

INDC(NDS)-0768 Distr. G,IBA,IN,J,NM

INDC International Nuclear Data Committee

International Nuclear Data Evaluation Network (INDEN) Meeting on the Evaluation of Light Elements

Summary Report of the IAEA Consultants' Meeting

IAEA Headquarters, Vienna, Austria 30-31 August 2018

> Richard J. deBoer University of Notre Dame Notre Dame IN, USA

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November 2018

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Printed by the IAEA in Austria November 2018

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ABSTRACT

A Consultants' meeting on the Evaluation of Light Elements within the International Nuclear Data Evaluation Network (INDEN) was held at the IAEA headquarters in Vienna from 30 to 31 August 2018. The goal of the meeting was to review the existing evaluations for light elements ⁹Be, ^{14,15}N, ¹⁶O and ²³Na, to identify areas for improvements in the evaluations, and to define the timeline to provide improved evaluations.

November 2018

Contents

1.	Intro	oduction	7
2.	Pres	entation summaries	7
	2.1.	LANL R-matrix work on n+ ⁹ Be and n+ ¹⁴ N, G. Hale	7
	2.2.	Sodium evaluation, P. Archier	10
	2.3.	Status of n-induced cross sections for O-16, S. Kopecky	11
	2.4.	A ⁹ Be(p,n) ⁹ B model of Geant4 and aspects of effective field theories for light nuclei, TS. Park	12
	2.5.	User Assessment of light elements two-body, neutron & gamma-production cross-sections, I. Thompson	13
	2.6.	Global fitting of ⁷ Be system, Z. Chen	14
	2.7.	¹⁵ N compound system at low energies, J. deBoer	17
	2.8.	Evaluation of n+ ¹⁵ N, S. Kunieda	20
	2.9.	n+ ^{28,29,30} Si, n+ ¹⁶ O, a+ ^{17,18} O and future work, Marco Pigni, Oak Ridge National Laboratory	21
	2.10.	Evaluation of Light Nuclei with GECCCOS, H. Leeb	23
3.	Tecł	nnical discussions	25
	3.1.	Current status of listed light systems	25
	3.2.	From Resolved Resonances to Unresolved Resonances	27
	3.3.	Data processing	27
	3.4.	Other items	27
	3.5.	Work to be done	28
4.	Sum	mary	29
5.	List	of Actions/Tasks	30

Annex 1 – Adopted Agenda	32
Annex 2 – Participants' List	34
Annex 3 – Presentation Links	37

1. Introduction

The International Nuclear Data Evaluation Network (INDEN) is an initiative of the IAEA which aims at continuing the success of the NEA CIELO project in expediting advances in nuclear data evaluation through international collaboration among experts (<u>https://www-nds.iaea.org/index-meeting-crp/TM_IAEACIELO/</u>).

The INDEN main goal is not only to produce improved (in terms of physics and/or performance in selected applications) evaluated data files, but in the process, to gain better understanding of the physics, to improve the models and approaches, the statistical analysis and treatment of uncertainties and hence to develop an evaluation methodology that is broadly accepted and adopted by the nuclear data community.

The INDEN activities are split into three groups that focus on nuclear data for actinides (and heavy elements), structural materials and light elements, respectively.

The INDEN meeting on the Evaluation of Light Elements was held from 30 to 31 August 2018, with the purpose of bringing together the experts in the field to discuss the outstanding issues in the evaluation of light elements in the energy range from a few keV to 20 MeV. Such issues include lack of experimental data or discrepancies in experimental data, implementation of R-matrix algorithms at higher energies where many channels are open and/or three-body decays can occur, connecting the resolved-resonance region with unresolved resonance region and the statistical model regime, treating uncertainties and producing covariance matrices, and data processing codes.

Four light systems were identified as priorities for nuclear criticality and nuclear safety applications at the CIELO follow-up meeting that was held in December 2017 (<u>https://www-nds.iaea.org/index-meeting-crp/TM_IAEACIELO/</u>): neutrons on ⁹Be, ^{14,15}N, ²³Na. These four light systems were the focus of this INDEN meeting, however, other cases with equally challenging issues, such as the (α ,n) reactions on F and O isotopes which are of particular interest in the field of spent fuel management, were also discussed, in particular ¹⁶O which was among the CIELO project priorities.

The meeting opened with a welcome address and brief introduction to the INDEN network by IAEA staff Andrej Trkov. Nine experts from China, France, Japan, Korea, USA and the European Commission including IAEA staff Paraskevi Dimitriou (Scientific Secretary) and Andrej Trkov attended. Gerry Hale (LANL) was elected chairman and James deBoer (Univ. Notre Dame) rapporteur of the meeting. The meeting continued with presentations by the participants which were then followed by discussions on technical issues.

Summaries of the presentations are given in Section 2 of this report, while the summary of the technical discussions is presented in Section 3. The meeting agenda and list of participants are provided in Annexes 1 and 2. Links to the presentations are given in Annex 3.

2. Presentation Summaries

2.1. LANL R-matrix work on n+⁹Be and n+¹⁴N, G. Hale

The results of R-matrix work that has been done at Los Alamos for reactions in the ¹⁰Be and ¹⁵N systems was presented. The n+⁹Be work illustrated that approximating the low-lying (2n,2 alpha) breakup channel as a two-body nn+⁸Be channel did not work at all well to describe the experimental (n,2n) cross section data. However, the total cross section and the (n, α) cross section were described fairly well in the analysis,

and they were used in the ENDF/B evaluation. It was suggested that perhaps a description of the breakup channel in a hyper spherical basis would improve its representation.

The ¹⁵N analysis includes data for the channels and reactions shown in the table below:

TABLE 1. SUMMARY OF THE ¹⁵N R-MATRIX ANALYSIS.

The top part of the table gives the channel configuration, the lower part gives the data included for each reaction.

channel	a _c (fm)	I _{max}
n+ ¹⁴ N	2.5	2
p+14C	4.3	3
α+ ¹¹ Β	5.1	2

Reaction	Energies (MeV)	# data points	Types of data	χ²
¹⁴ N(n,n) ¹⁴ N	$E_n = 0 - 2.5$	932	σ _τ , σ(θ)	935
¹⁴ N(n,p) ¹⁴ C	$E_n = 0 - 3.0$	350	σ _{int}	621
¹⁴ N(n,α) ¹¹ B	E _n =1.33 – 2.32	104	σ _{int}	233
¹⁴ C(p,n) ¹⁴ N	$E_p = 1.17 - 3.1$	335	σ(θ)	858
¹¹ Β(α,p) ¹⁴ C	E _α =1.45 - 2.94	110	σ(θ)	112
	Total	1831	$\sigma(\theta), \sigma_{int}$	2759

Overall, the fit has a chi-squared per degree of freedom of 1.61. The fits to the integrated cross sections for most of the reactions are reasonably good. The ORELA total cross section data measured by Jack Harvey [1] in the early 1990s have exceptionally small statistical scatter and high resolution, as shown in the figure below. The fit to these data resulted in changes of the resonance parameters for some of the resonances [2].



FIG. 2.1. The total cross section for neutrons on ¹⁴N at energies below 2.5 MeV. The data points are from the measurement of Harvey et al. [1], and solid red line is the calculation from the ¹⁵N R-matrix analysis. Resonance assignments are indicated on the figure, and those in red are new from this analysis [2].

References

- J.A. Harvey, N.W. Hill, N.M. Larson, and D.C. Larson, "Measurement of the Nitrogen Total Cross Section from 0.5 eV to 50 MeV. And Analysis of the 433 keV Resonance", Proc. Int. Conf. on Nuclear Data for Science and Technology, Julich, Germany, 13-17 May 1991, S.M. Qaim, ed., pp. 729-731, Springer-Verlag, Berlin (1992).
- [2] G.M. Hale, P.G. Young, and M.B. Chadwick, "Cross Sections for n+14N from an R-matrix Analysis of the 15N System", Proc. Int. Conf. on Nuclear Data for Science and Technology, Gatlinburg, TN, USA, 9-13 May 1994, J.K. Dickens, ed., pp. 607-609, Am. Nucl. Soc., IL, USA (1994).

Discussion:

The n+⁹Be system has a low energy 4 body break up threshold (2n, 2α) which is why the available data cannot be reproduced with standard R-matrix. Hyper spherical coordinates for the penetrability of multi-particle breakup seem to match the energy dependence of data.

For n+¹⁴N, a small channel radius of 2.5 fm was used: the hard sphere scattering was very sensitive to the channel radius and drove it down to a very low value. At a smaller radius you reduce the density of

background states. So in the phenomenological model where you have a very limited number of states, this naturally drives the fit to a smaller radius.

How do we go to higher energies? Above break up, we have to extend the usual R-matrix calculations as high as possible and see when it breaks down. However, it may be necessary to use the Reduced R-matrix at higher energies but we need to find a way to preserve unitarity at lower energies where there are only two-body channels.

2.2. Sodium evaluation, P. Archier

An overview of ²³Na evaluations performed at CEA Cadarache over the last ten years was presented.

First, a brief history of sodium evaluation in JEFF-3.1.1 was given. In particular, large discrepancies with experimental data and no covariance information being available are the main drawbacks with this evaluation. Since CEA Cadarache is involved in the French Sodium cooled Fast Reactor (SFR) project named ASTRID, it was important to revisit neutron-induced sodium nuclear data.

²³Na evaluation was produced for JEFF-3.2 (=JEFF-3.3) using the CONRAD code. The Resolved Resonance Range was analyzed using Larson total (1976) and Rouki first inelastic (2012) experimental data. Hence, this energy domain has been extended from 350 keV to 2 MeV and the first inelastic level has been taken into account to reproduce resonant structures for this reaction. For the continuum (En>2 MeV), multiple experimental data sets (total, six inelastic levels, (n,p), (n, α) and (n,2n) reactions) were simultaneously analyzed with CONRAD, coupled with the ECIS/TALYS codes.

Covariance matrices covering the whole energy range have been produced using Monte Carlo marginalization techniques, which enable to propagate all systematic experimental uncertainties to model parameters in a consistent way.

In order to improve this ²³Na evaluation in JEFF-3.3, a new resonance analysis is planned using also existing differential data on elastic angular distributions available on EXFOR. Furthermore, an extension of the current resonance range beyond 2 MeV is forecast.

Discussion:

It was noted that the original evaluation of ²³Na+n for JEFF-3.1.1 was adjusted to the integral measurements for the MASURCA core. That is why there were large differences with respect to differential data from EXFOR.

The radius parameter used in the R-matrix fit was energy dependent so that they could fit up to higher energies.

Covariances are calculated by propagating model and experimental uncertainties using a Monte Carlo procedure. R-matrix parameters and optical model parameters are treated at the same time so that correlations can be seen.

The fit to the angular distribution data is very poor, but the fit for just the angle integrated cross section is very good.

It turns out that the angular distributions are very important in resolving the integral measurements because in edge regions of applications backscattering differential cross sections must be accurate. Better to just interpolate data in any region where you may be missing resonances or cannot fit the differential data. One can use benchmarks to test the description of differential data in off resonance regions.

2.3. Status of n-induced cross sections for O-16, S. Kopecky

An overview of the available experimental data for neutron induced reactions on ¹⁶O was given. The goal is to identify the most reliable experimental data sets, data sets that should be included in all evaluations. A selection of data for the total cross section and the discrepant measurements for the coherent scattering length were discussed.

The main focus is on the status of the ${}^{16}O(n,\alpha){}^{12}C$ cross section. For this reaction rather large discrepancies between the experimental data sets exist and so far no satisfying reason for the differences was found. Most of the data sets have been using the inverse reaction ${}^{13}C(\alpha,n){}^{16}O$. In the presentation it was recommended to normalize all data sets to the thick target neutron production yield of the same reaction. For the thick target yields three different experimental data sets exist, performed at three different laboratories, using three different detection methods, and all these three data sets agree within their experimental uncertainties. The data for the energy loss of the alpha particle in carbon is well characterized as all. Therefore a reliable normalization and a correct estimate of the uncertainty can be derived, and all the corrected ${}^{13}C(\alpha,n){}^{16}O$ sets are then consistent up to the threshold of the (n, α_1) reaction.

Discussion:

A huge amount of data exists in EXFOR, what data should be used?

Scattering length: the two measurements are very discrepant. However, these data can nail down the thermal cross section. Both experiments seem solid, hard to resolve the inconsistency.

(n,total): the very low energy data are measured with water samples that have a (n,p) background that has to be subtracted. First resonance, a lot of experimental distortions to the shape. A lot of this is from uncorrected background contributions.

Even the best measurement still has a transmission of less than 0.2, which is questionable.

The higher energy total neutron cross sections: From the transmission point of view, the Johnson (1974) data [private communication] are again the best.

Subthreshold state dip: Again, Johnson (1979) [private communication] data look best from transmission point of view but all are in good agreement here (Fowler et al, Phys. Rev. C 8, 545 (1973)) is a bit off in energy). Cierjacks (Nucl. Instrum. Methods 169,185 (1980)) has highest resolution but doesn't know his target thickness (3 to 7 MeV)

Somehow the target thickness measurement uncertainties are underestimated.

2.4. A ⁹Be(p,n)⁹B model of Geant4 and aspects of effective field theories for light nuclei, T.-S. Park

Three topics were presented, development of a ROOT-based nuclear data library project, a chargeexchange model of Geant4 dedicated to ⁹Be(p,n)⁹B reaction and discussions on effective field theories for light nuclei.

Development of a ROOT-based nuclear data library.

We developed a nuclear data library for ENDF data based on ROOT, which is named as TNudy. Developing as a library of ROOT, TNudy can enjoy all of the powerful set of mathematical and graphical routines and tools. In particular, the C++ interpreter of ROOT, cint, makes it possible to use TNudy interactively. TNudy is developed in C++ language, the inheritance technique of which makes the development and the management of the library highly efficient. Each structure of ENDF is implemented as a C++ class with suitable member functions relevant to the structure, which enables us to access systematically not only total and differential cross sections but also every subset of ENDF. With a few examples, we demonstrated its graphical visualization of data, interactive usage and composition of macro files. Currently, MF=1 to MF=6 are implemented rather thoroughly, including the ability to construct cross sections with the resonance parameters. Partial implementation is done up to MF=28, but covariance data are yet to be implemented.

New charge exchange model of GEANT4 for ⁹Be(p,n)⁹B reaction.

We developed a charge-exchange model of GEANT4 dedicated for ${}^{9}Be(p,n){}^{9}B$ reaction. The popular hadronic models of Geant4 such as G4Bertini and G4BinaryCascade model are found to be quite inaccurate in describing the ${}^{9}Be(p,n){}^{9}B$ reaction, which is the dominant reaction for the production of neutrons by bombarding a proton bean on a beryllium target. Even the dedicated charge-exchange hadronic model of GEANT4, G4ChargeExchance, fails to meet the data, because it takes into account only n0 neutrons, while there are substantial contributions from ni, $i \ge 1$. We developed a hadronic model of GEANT4 dedicated for the charge-exchange reaction by taking the total and differential cross section data of ENDF VII.1 as input. The developed model is found to be in good agreement with the experimental data.

Aspects of EFTs for light nuclei.

The potentials and limitations of effective field theories for light nuclei are discussed. Heavy-baryon chiral perturbation theory (HBChPT) is based on the most important feature of low-energy QCD, spontaneous symmetry breaking of a chiral symmetry, and takes nucleons and pions as pertinent degrees of freedom. It enables us to have the first principle description of nuclear forces and electroweak current operators. Its success also includes getting accurate and robust theoretical predictions on important astro-nuclear reactions such as p+p and 3He + p reactions. Issues of HBChPT are discussed, which include the increasing number of low-energy constants when one extends the theory to higher orders, the renormalization procedure for the short-range physics and the non-perturbative nature of Schrodinger equation. Emerging of pionless EFTs by lowering the cutoff below the pion mass is discussed. Finally, we discussed halo or cluster EFT, pointing out the one-to-on correspondence between the parameters of halo EFT and those of the R-matrix theory. The correspondence of the propagator of a cluster in halo-EFT and the energy-level matrix was also discussed. New nuclear data library: ^TNudy

Discussion:

At the moment, with the TNudy application one cannot write an ENDF file nor can you reconstruct complex quantities like total neutron emissions at an angle without additional programming in root.

⁹Be(p,n)⁹B: with EFT one can increase the accuracy of the calculation order by order, however, the emerging low-energy constants spoil the predictive power of the theory.

Break up channels can be included but limited to 3 or 4 particles.

It is always possible to do R-matrix or EFT at low energy since the light systems studied behave like clusters.

t It would be interesting to see how EFT applies to a weakly bound or unbound system?

2.5. User Assessment of light elements two-body, neutron & gamma-production cross-sections, I. Thompson

We here compare ENDF/B-VIII.0 evaluations with EXFOR experimental data, to see where there might be gaps or deficiencies from the users' point of view. My method will use code in Fudge python to access EXFOR data with the x4i api of Dave Brown and compare with cross sections extracted from evaluations in the GNDS format (as implemented at LLNL). I focus on cross-sections $\sigma_c(E_n)$ and angular distributions $\sigma_c(\theta, E_n)$ for two-body channels *c* with neutron incident energies E_n . Then I look at gamma-production energy, angle or energy-angle distributions: $\sigma_\gamma(E_n)$, $\sigma_\gamma(\theta_\gamma, E_n)$, $\sigma_\gamma(\theta_\gamma, E_\gamma, E_n)$. For INDEN I will develop code for looking at neutron-production distributions in the same ways. I examine neutron reactions on targets of ⁹Be, ¹⁴N, ¹⁵N, ²³Na.

For n+⁹Be reactions, elastic-scattering angular distributions have been extensively measured, and are fit well by ENDF/B-VIII.0 evaluations, which are LANL R-matrix models most recently improved in 2009 and 2018. The total neutron cross section datasets are also extensive, but not so consistent with each other, so the evaluations are close to those experimental results evaluated as reliable. An important two-body channel is the reaction ⁹Be(n,t)⁷Li to the ground state and excited states of ⁷Li. The 478 keV from the ⁷Li^{*} decay is accurately reproduced by the evaluation. Since the $\alpha + \alpha + n$ breakup threshold in ⁹Be is only at 1.57 MeV, the breakup channel soon becomes dominant from the users' perspective, so it is extremely important that neutron breakup distributions are modeled correctly. Though I have not yet validated these channels myself, Trkov suggested using the EXFOR plotting routines at IAEA that use the code ENDVER.

For n+¹⁴N reactions, elastic-scattering angular distributions are generally good, though with some room for improvement at low energies. This region below 2.5 MeV was last modeled in 1990 by Hale with R-matrix methods. Cross-section measurements in the exit channels for p, t and α were well described, but there was little data to confirm the angular distributions in these channels. The gamma production distributions of [1] are well described, but the other data sets of [2] and of [3] not so well. There are extensive measurements of neutron production by [4], but I have not checked yet agreements with the evaluation.

For n+¹⁵N reactions, the extensive elastic-scattering angular distributions of [5] are plausibly modeled, but the previous R-matrix fit up to 5.4 MeV from ENDF/B-V could still be improved. There is very limited experimental data for the p, d and t exit channels, and even less for gamma production.

For n+²³Na reactions, there are strong fluctuations in the elastic-scattering angular distributions up to 2 MeV that are as yet difficult to describe in R-matrix theory because of overlapping resonances ($\Gamma/D \sim 1$

or higher). The gamma production seems to follow experimental data up to that 2 MeV, but above that energy the evaluation is quite inadequate. There are again extensive measurements of neutron production by [4] that I have not checked.

In conclusion, the R-matrix evaluations for all targets seem to be a good beginning, but only up to the few MeV limit of that fitting. Above the resolved resonance region, further work is needed in regions of strong (but not isolated resonance) fluctuations. In the statistical regions, then direct-reaction or pre-equilibrium models will be needed to predict neutron production cross sections. For neutrons on ⁹Be targets, some three-body breakup model should be investigated, even if it requires the two alpha particles to be treated as a ⁸Be cluster in specific states (0⁺, 2⁺ at 3 MeV, and 4⁺ at 11 MeV). In all cases, R-matrix methods should be extended beyond the first breakup thresholds, by, for example, fitting imaginary damping widths at those energies and then running limited-space Hauser-Feshbach models to find the decay products from the flux that had been absorbed.

References

- [1] V.C. Rogers *et al.*, report DNA-3495F (1974), EXFOR 10490004.
- [2] J.K. Dickens *et al.*, Nucl. Sci. Eng. **40**, 346 (1970), EXFOR 10095002.
- [3] H.E. Hall and T.W. Bonner, Nucl. Phys. 14, 295 (1959/60), EXFOR 1282004.
- [4] A. Takahashi et al., Osaka University Report OKTAV-A-87-01 (1987), EXFOR 22076026.
- [5] C.P. Sikkema *et al.*, Nucl. Phys. **32**, 470 (1962), EXFOR 20206002.

Discussion:

For ²³Na+n, there are lots of $(n,n'\gamma)$ data that needs improved evaluation. Users want to see this kind of gamma ray emission data (especially in IBA applications).

2.6. Global fitting of ⁷Be system, Z. Chen

Seven schemes of a global fitting about ⁷Be system have been done, with the same level structure and the same experimental data base, but with different χ^2 formulae and a different method to deal with the system error.

The formulae of χ^2 as follow:

$$\chi^{2} = (\vec{\eta} - \vec{y})^{+} V_{0}^{-1} (\vec{\eta} - \vec{y}) + ((N-1)/S)^{2} \Rightarrow \text{minuimum} (ALS) F1.$$

$$\chi^{2} = (\vec{\eta} - \vec{y})^{+} V_{0}^{-1} (\vec{\eta} - \vec{y}) \Rightarrow \text{minuimum} (CLS) F2.$$

$$\chi^{2} = (\vec{\theta} - \vec{\theta_{a}})^{+} V_{a}^{-1} (\vec{\theta} - \vec{\theta_{a}}) + (\vec{\eta} - \vec{y})^{+} V_{M}^{-1} (\vec{\eta} - \vec{y}) \Rightarrow \text{minuimum} (GLS) F3.$$

Name	Da	V		Sta	System	((NO		NO		EA		F		χ^2_{me}	Comme
of	ta	of	ti-		atic	N-1)	R-		R-		E/		0.		an		nt
Seven	Us	$\vec{\eta}$		stic	-Error	/S		Rel		Abs		EE		0		(fre	
Sche	ed			Err	(%))2	a.		о.		E		f		ed.		
mes	ή		or					dat		dat			Х	2		452	
							e.		e.						7)		
1-0-	Ori	V		OR	No(0.0	Y		Yes		No		EE		F		3.60	χ^2 too
N-ALS	gi	0	Ι		to 0.0)	es					E		1		2		larger
2-0-	Ori	V		OR	No(0.0	Y		Yes		Part		EE		F		2.61	As a
P-ALS	gi	0	Ι		to 0.0)	es					E		1		6		Reference
3-0-	Ori	V		OR	No(0.0	Y		Yes		Part		EE		F		2.11	Accepta
M-ALS	gi	0	Ι		to 0.0)	es					E		1		6		ble
4-0-	Mo	V		OR	ORI(1.	N		Yes		All		EE		F		0.96	As a
P-CLS	di	0	Ι		5 to 10)	0					E		2		1		Reference
5-S-	Mo	V		OR	STD(0.	N		Yes		Part		EA		F		1.46	Very
M-CLS	di	М	Ι		2 to 2.5)	0					E		2		2		good
6-S-	Mo	V		OR	STD(0.	N		Yes		Part		EA		F		1.54	The
M-GLS	di	М	Ι		2 to 2.5)	0					E		3		2		best one
7-S-	Mo	V		OR	STD(0.	N		Yes		All		EA		F		1.40	As a
A-GLS	di	М	Ι		2 to 2.5)	0					Е		3		4		Reference

Characteristics of the seven schemes

Most of the absolute data were normalized within some limits, but those data which are not in direct competition with other data-sets were not normalized. It is surprising that all the evaluated results are very close for the most of data points; the obvious differences only exist in χ^2 and the covariance matrix of evaluated values. The best results are obtained using 'General Least Square' (GLS) and 'Reduced R-matrix Theory' (χ^2 =1.542), which was based on the work of CLS (χ^2 =1.462). Generally speaking, the first step is to do CLS fitting, the second step is to do GLS fitting on the base of CLS fitting which has got a very good Evaluation Value already.

From this work the following conclusions can be drawn that need further in-depth discussion:

- The most important advantage of 'global fitting' is that, by systematic comparisons, the existing errors can be found in the original database and be deleted; the discrepancy existing between different datasets can be found and minimized; the systematic error of each dataset can be found and be decreased. So the improved database used in the fitting will be much closer to the real and objective world, and consequently the final unique evaluation result will be much closer to the real and objective world, which is no other than the expectation value in statistics.
- 2. A complete and accurate Covariance matrix of the Evaluated value (CE) should include both the contribution of Data and Model at the same time and should match the Evaluated value in the ENDF file. A method which only evaluates data using mathematics, or only makes calculations with the MC method, or misses the interference of statistical and systematic error, and so on, will not be good enough.
- 3. In a 'global fitting', the Covariance matrix of data(C) should be used, with diagonal element C_{ii}= Si²+Y_i², non-diagonal element C_{ij}= S_i*Y_j, in which Si is statistic error, Y_i is systematic error, C_{ij} represents the interference of statistical error and systematic error.
- 4. In the fitting procedure, using an 'Iterative process' has much advantage, as the normalization factor changes little by little, and the value of the normalized experimental data approaches the 'real value' little by little. At the same time, the relative statistical error is fixed always, but the relative systematic error of the data should be reduced little by little. In this way the CLS fitting can converge to the GLS fitting reasonably.
- 5. Duo to the R-matrix fitting being a kind of phenomenological fitting, there is no reason to limit the number of levels used; but every level used must be very sensitive to the total χ^2 , in other words the

level-set used finally should be **'not one more and not one less'**. There is no reason to limit the number of R-matrix parameters of the sub-channels considered, but they should be very sensitive to the mean χ^2 /degree of freedom (dof); the parameter-set used finally should be **'not one more and not one less'**.

- 6. Never think that the 'non-physical parameter' used has no meaning, in fact it may represent the contribution of the non-physical part in the actual data-base; or maybe the contribution of the non-compound nuclei; or maybe it is a real level which has not be recognized in the past. If the same new levels have been used in more than one independent fits with different codes, maybe the new levels should be recognized as real levels.
- 7. With regards to the energy calculation, for the Capture reaction or γ transition, the ' γ and residual nucleus' can be taken as a 'general particle pair' that is dealt with approximately. Our practices show that in this way the fit to the calculated integrated cross section and differential cross section looks very good.
- The γ is a kind of standing wave, the spin of γ is S=1, S₃=-1, +1, no S₃=0, so the special formulae for calculation of γ angular distribution will be used. The calculation looks rather complex, but the result is accurate.
- 9. With the Reduced R-Matrix theory in Lane and Thomas, Rev. Mod. Phys. **30**, 257–353. (1958), there is a possibility to do evaluation from 1.0E-07 MeV to 20 MeV for a nuclear system, if only there exists a very good experimental database.
- 10. Due to the fact that R-Matrix fitting is a kind of phenomenological fitting, the formulae in Lane and Thomas, Rev. Mod. Phys. **30**, 257–353. (1958) can be used for γ calculation approximately, the calculation looks rather simple, but the result is very good, too.
- 11. $\Gamma_{\lambda c} = 2P_c \gamma_{\lambda c}^2$ and $\Delta_{\lambda c} = -\gamma_{\lambda c}^2 S_c$ are approximate formulas for one-level R-matrix analysis; For multi-level and multi-channel R-matrix analysis the correct below formulas should be used (see in above reference for Lane and Thomas (1958) p. 273):

$$\begin{split} &\Gamma_{\lambda} = \sum_{c} \Gamma_{\lambda c}, \ \Gamma_{\lambda c} = 2P_{c}\gamma_{\lambda c}^{2}/d_{c}, \\ &\Delta_{\lambda} = \sum_{c} \Delta_{\lambda c}, \\ &\Delta_{\lambda c} = \frac{P_{c}(R_{cc}^{0}P_{c}) - S_{c}^{0}(1 - R_{cc}^{0}S_{c}^{0})}{d_{c}}\gamma_{\lambda c}^{2}, \end{split}$$

$$d_c = (1 - R_{cc}^0 S_c^0)^2 + (R_{cc}^0 P_c)^2,$$

 R_{cc}^0 , S_c^0 refer to the parameters of background.

- 12. Due to the R-matrix fitting being a kind of phenomenological fitting, the best fit should have the minimum χ^2 , the acceptable value is mean χ^2 /dof <3.0
- 13. Due to the use of different methods for dealing with errors, when checking an R-matrix analysis it is important to perform a visual comparison of data and calculations.
- 14. The basic criteria for a good fit is that the calculated value is close to the experimental data value, and that most of the calculations for a given data set are within the error bars.

Discussion:

What part of the data should we be able to vary? Systematic or statistical?

The formulas used in the calculations of Chen need to be checked so that one can try to reproduce his fit results.

2.7. ¹⁵N compound system at low energies, J. deBoer

Nucleosynthesis in the first generation of massive stars offers a unique setting to explore the creation of the first heavier nuclei in an environment that lacks any heavier nuclei impurities from earlier stellar generations. In later generations of massive stars, hydrogen burning occurs predominantly through the CNO cycles, but without the carbon, nitrogen, and oxygen that allow this catalytic reaction sequence, these stars would have to rely on the inefficient pp-chains for their energy production. However, there may be other reaction chain sequences that utilize only light elements and act as alternative pathways А = 5 and А = 8. One such chain could around masses reaction be 2 H(α , γ) 6 Li(α , γ) 10 B(p, α) 7 Be(β ν) 7 Li(α , γ) 11 C(β ν)) 11 B(α ,n) 14 N, which would also provide a neutron source to this early stellar environment. New measurements are reported for the ${}^{11}B(\alpha,n){}^{14}N$ reaction using a ${}^{3}He$ counter. An R-matrix analysis is performed in order to facilitate a comparison of the different reaction data.

Measurements

The ¹¹B(α ,n)¹⁴N reaction (Q = 0.15789(1) MeV) was studied over alpha-particle beam energies E_{α} ranging from 520 to 2000 keV and with beam intensities on target between 0.03 and 18 μ A. A ¹¹B enriched (>99%) target with a thickness of 8.4(4) μ g/cm2 was created by electron sputtering enriched ¹¹B powder onto a clean tantalum backing 2 mm in thickness. The detection system consisted of a ³He proportional counter, which is made up of 20 ³He tubes encased in a polyethylene moderator. The detector is described in [1,2]. The target was placed at the center of the moderator to measure the angle integrated cross section.

The energy dependence of the efficiency was modeled using MCNP and the absolute efficiency was obtained using the activation method and the ⁵¹V(p,n)⁵¹Cr reaction at 3.7 MeV. [3,4]. The resulting efficiency was found to be consistent with that found by [1] to within 1% using a nearly identical setup. The small Q-value of the ¹¹B(α ,n)¹⁴N and the range of alpha-beam energies that were investigated results in neutrons that cover the range from 0.4 < E_n < 2.0 MeV, taking into account the angular kinematic spread as well. The neutron detection efficiency of the ³He counter varies from about 30 to 45% over this neutron energy range. The overall uncertainty in the neutron efficiency is estimated to be ~5%. In addition, only the ground state in the ¹⁴N final nucleus is energetically accessible. The resulting cross section is shown in Fig. 2.2 compare compared to that of [5].



FIG. 2.2 Comparison of the angle integrated cross section of the present measurements (red points) with those of [5] (grey points).

R-matrix analysis

The ¹¹B(α ,n)¹⁴N reaction populates states in the ¹⁵N compound at an excitation energy range (for these measurements 11.2 < E_x < 12.6 MeV) where the proton decay (S_p = 10.20742(1) MeV) is also possible in addition to decay via alpha-particle (S_a = 10.99118(1) MeV) and neutron (S_n = 10.833.30(1) MeV) [6,7].

For the ¹⁵N system, a global R-matrix analysis is under construction that utilized data from the ¹¹B(α ,n)¹⁴N [5] reaction as well as the ¹⁴C(p,p)¹⁴C [8,9], ¹⁴C(p,n)¹⁴N [10], ¹⁴N(n, total) [11,12], ¹⁴N(n,p)¹⁴C [13,14,15], and ¹⁴N(n, α)¹⁰B [13,14,15,16] reactions. A preliminary fit is shown in Fig. 2.3. Target effects, experimental energy calibrations, and differing level spin assignments are under investigation to improve the level of agreement.



FIG. 2.3 Preliminary results for a global R-matrix fit of different reactions that populate the ¹⁵N compound system between $E_x = 11$ and 13 MeV. A general agreement is obtained but there are still several regions where some the R-matrix cross section does not describe the data well.

References

- [1] A. Best, M. Beard, J. Gorres, et al., Phys. Rev. C 87, 045805 (2013).
- [2] A. Best, S. Falahat, J. Gorres, et al., Phys. Rev. C 87, 045806 (2013
- [3] K.K. Harris et al., Nucl. Instrum. Meth. 33, 257 (1965).
- [4] G. Deconninck and J. Royen, Nucl. Instrum. Meth. **75**, 266 (1969).
- [5] T.R. Wang, R.B. Vogelaar, and R.W. Kavanagh, Phys. Rev. C 43,883 (1991).
- [6] W.J. Huang, G. Audi, et al. The AME2016 atomic mass evaluation (I). Evaluation of input data; and adjustment procedures. Chin. Phys. C 41(3), 030002 (2017).
- [7] M. Wang, G. Audi, et al. The AME2016 atomic mass evaluation (II). Chin. Phys. C 41(3), 030003 (2017).

- [8] W.R. Harris and J.C. Armstrong, Phys. Rev. 171, 1230 (1968).
- [9] J.D. Henderson, E.L. Hudspeth, and W.R. Smith, Phys. Rev. 172, 1058 (1968).
- [10] R.M. Sanders, Phys. Rev. **104**,1434 (1956).
- [11] J. J. Hinchey, P. H. Stelson, and W. M. Preston, Phys. Rev. 86, 483 (1952).
- [12] C. H. Johnson, B. Petree, and R. K. Adair, Phys. Rev. 84, 775 (1951).
- [13] F. Gabbard, H. Bichsel, and T.W. Bonner, Nucl. Physics 14, 277 (1959).
- [14] G.L. Morgan, Nucl. Sci. Eng. 70, 163 (1979).
- [15] C.H. Johnson and H.H. Barschall, Phys. Rev. 80, 818 (1950).
- [16] V.A. Khryachkov et al., EPJ Web of Conferences, 21:03005, 2012.

2.8. Evaluation of n+¹⁵N, S. Kunieda

The preliminary results of the $n+^{15}N$ cross-sections evaluation in a resolved resonance energy region were presented. Although natural abundance of ^{15}N is very small (0.366%), this isotope is drawing attention as a structural material. That is because the production of ^{14}C is strongly minimized as the energy threshold of the $^{15}N(n,p)$ reaction is around 10 MeV.

The R-matrix code AMUR [1] was used for the preliminary analysis of the ¹⁶N compound system. The energy eigenvalues, spin and parity (J π) of each level are basically taken from ENSDF. However, values of J π for some levels needed to be changed in order to reproduce the shape of experimental total cross-sections. The values of the energy eigenvalues and reduced width-amplitudes are searched for while the boundary condition parameters are fixed as R_c = 5 fm and B_c = -L. In a preliminary analysis, only measured total cross-section of Zeitnitz et al. [2] up to 5.5 MeV and recommendation value of Mughabghab at 0.025 eV [3] were fitted. Reasonable results had been obtained, however, the fitting itself has not yet perfect as he still need to fix the assignments of J π . The experimental differential cross-sections also need to be analyzed in order to constrain the parameter values. Besides, the experimental condition should be considered as much as possible in the later stage.

The preliminary correlation matrix obtained by the Kalman filtering method [4] is shown for the total cross-sections (Fig. 2.4). High correlations are seen in the lower and higher energy region due to the effect of tails from the negative levels and distant poles. A trace of the (near) unitarity limits is seen at resonance energies, which should give a strong constraint on the behavior of resonance parameters.



FIG. 2.4. Correlation matrix for neutron total cross-section on ¹⁵N.

References

- [1] S. Kunieda et al., Nucl. Data Sheets **123**, 159 (2015).
- [2] B. Zeitnitz et al., Kernforschungszentrum Karlsruhe Reports, No.1443 (1971).
- [3] S. Mughabghab et al., Atlas of Neutron Resonances, (2006), Netherlands.
- [4] T. Kawano et al., J. Nucl. Sci. Technol. (Tokyo) **37**, 327 (2000).

Discussion:

¹⁵N(n,total) evaluation is very similar in JENDL and ENDF/B-VIII.0.

Uncertainties in evaluations are completely based on the experimental uncertainty. Very good reproduction of the total cross section up to nearly 6 MeV, however the uncertainties seem to be quite small.

High correlation caused by S-wave dominance at low energy and from background states at high energy. Will go up to higher energy, above 6 MeV but only for (n,total) data. Can add differential data in the low energy.

2.9. n+^{28,29,30}Si, n+¹⁶O, a+^{17,18}O and future work, Marco Pigni, Oak Ridge National Laboratory

A set of resonance parameters for ¹⁶O in the neutron energy range of thermal up to about 6 MeV has been generated using the R-matrix code SAMMY. The evaluation work builds on a comprehensive analysis of experimental data sets performed by [1] who derived a set of Reich-Moore parameters describing ¹⁶O neutron cross sections in the resolved resonance region up to about 6 MeV. The resonance analysis was initiated in FY16¹ and was updated through FY17².

The aim of the present work is to provide a set of improved resonance parameters able to describe n+¹⁶O cross sections to provide an alternative to the extant point-wise evaluation of oxygen in the ENDF/B-VII.1 nuclear data library.

There are two major features of the present resonance parameter evaluation. The first one is the use of the $B_c = -L$ boundary condition commonly used in the formal R-matrix theory. This boundary condition is used here to correct the effect of an approximation introduced into previous evaluations of resonance parameters that employ the $B_c = S_c(E)$ energy-dependent boundary condition, where $S_c(E)$ is the shift function defined as the real part of the logarithmic derivative of the wave function at the channel radius for the channel c. The $B_c = S_c(E)$ has been routinely used because it yields resonance energies that correspond to peaks in measured cross sections, thus providing an intuitive way of verifying fitted resonance energies. The effect of this approximation is removed in SAMMY by using the $B_c = -L$ boundary condition of the formal R-matrix theory that retains energy dependence of the shift functions for L > 0 partial waves. Because deviations introduced by the $B_c = S_c(E)$ approximation are expected to be larger for light nuclei like ¹⁶O than for heavy nuclides, the magnitude of deviations found here for ¹⁶O may be considered as an upper bound for deviations on heavier nuclides.

The second main feature of the present work is to report R-matrix calculations without the Reich-Moore approximation (by treating capture channels as particle channels whose penetrability factors are set to 1 in the SAMMY input file) that is used to quantify accuracy of Reich-Moore approximation. For light nuclei,

¹ Notes on the consistency of $16O(n, \alpha)$ cross sections

² ORNL contribution to ENDF/B-VIII.0 and progress on light nuclei evaluations

direct capture cross section is a significant contributor to the total capture and it is conventionally added to resonant capture cross section computed by the Reich-Moore approximation. The scarcity of capture data and the smallness of the capture cross sections on ¹⁶O makes it difficult to analyze differences between the full R-matrix (explicitly accounting for all capture channels) and its Reich-Moore approximation. An extension of the ENDF format [3] is suggested to accommodate multiple gamma-ray channels reported in this work, as ENDF is presently limited to just one exit channel in the capture particle-pair definitions.

Particular emphasis was devoted to the fit of the experimental data for total and (n,α) cross sections as well as for elastic angular distributions. Based on the two features described above and introduced in the evaluation methodology, the evaluation work on the $n+^{16}O$ cross sections, their covariance matrices, and comparison to experimental data from the thermal up to the resolved resonance region will be reported.

^{28,29,30}Si

Since 1997 Hetrick evaluation [4] till the recent release of the ENDF/B-VIII.0 library (2018), the silicon cross section evaluations were not updated in the releases of the ENDF library although a new set of silicon evaluations [5,6] in the RRR was performed at ORNL in 2002 and submitted for inclusion into the ENDF/B-VII.0 library. One of the reasons may have been the difficulty, at that time, to include in the processing procedure of the ENDF files the neutron direct component of the capture cross sections.

After the recent release of the ENDF/B-VIII.0 library and testing a group of benchmarks designed to validate the predictions of reactivity for criticality safety in systems containing silicon, it was found that the prediction for these benchmarks remarkably improved and the remaining outliers had a pronounced thermal spectrum suggesting the possibility that the silicon thermal capture was underestimated.

In the present work, two sets of silicon evaluations were generated ORNL(2018¹) and ORNL(2018²). ORNL(2018¹) accounted for an updated value of the $28Si(n_{th},\gamma)$ cross section and a direct capture contribution decreased by 20% from the ORNL(2002) evaluation in order to match the thermal capture cross section suggested by a study performed at IAEA [7]. For ORNL(2018¹), the ^{29,30}Si evaluations were kept unchanged.

The ORNL(2018²) set of evaluations accounted for updating the direct capture contributions for all three isotopes and the ²⁸Si(n_{th} , γ) value as done for ORNL(2018¹). This was motivated by the unfavorable behavior of the component of the direct capture cross sections reported in ORNL(2018¹). The newly calculated direct capture cross sections were performed with the CUPIDO code [8,9].

Due to both changes in the thermal cross section value and the direct capture cross section, an improved agreement with benchmarks in the thermal spectrum was achieved for ORNL(2018¹). ORNL(2018²) is still under testing.

^{17,18}O

The R-matrix SAMMY analysis -in the Reich-Moore approximation- of the $^{17,18}O(\alpha,n)$ reaction, needed for modeling the neutron emission processes essential for nuclear material verification [10], has been improved, albeit in a preliminary fashion, by an updated set of resonance parameters and related covariance information in the energy range up to 5 MeV. The partial cross section of the (α,n) to each excited states were computed by the R-matrix formalism and were fitted to presently available experimental cumulative data sets and, partially, to Hauser-Feshbach (HF) calculations. Therefore, we recommend that the measurements of exclusive partial cross sections data be performed to better define the resonance widths. Since in our analysis we used branching ratios obtained from HF calculations for the excited states, the impact of the newly evaluated partial cross sections to the excited states on the emerging neutron spectra should be tested.

This work was motivated by (1) the need to provide evaluated data to improve the state of the art in modeling neutron emission processes essential for nuclear material verification and (2) to estimate uncertainty in the neutron generation rates.

Future work will finalize and formalize the evaluation work on $^{17,18}O(\alpha,n)$ cross sections by including the evaluated set of resonance parameters and related covariance information in the charged-particle ENDF/B-VIII sub-library.

References

- [1] R.O.Sayer et al., ``R-Matrix Evaluation of 16O Neutron Cross Sections up to 6.3 MeV,'' ORNL/TM-2000/212, August 2000.
- [2] Collaborative International Evaluated Library Organisation Pilot Project, WPEC Subgroup 40 (SG40) - CIELO Pilot Project, https://www.oecd-nea.org/science/wpec/sg40-cielo/. Where is this reference cited in the text?
- [3] A.Trkov et al., ENDF-6 Formats Manual, Report BNL-0365-2009 Rev.2, Brookhaven National Laboratory Upton, NY 11973-5000, October 2012.
- [4] D.M.Hetrick, ``Evaluation of 28,29,30Si neutron induced cross section for ENDF/B-VI," ORNL/TM-11825 (1997).
- [5] K. H. Guber et al., ``Neutron Cross Section Measurements for Light Elements at ORELA and Their Application in Nuclear Criticality,'' Nuclear Data for Science and Technology, Tsukuda (Japan), p. 346 (August 2002).
- [6] H.Derrien et al., ``Evaluation of silicon neutron resonance parameters in the energy range thermal to 1800keV,'' ORNL/TM-2001/271 (2002).
- [7] R.B.Firestone, ``Thermal neutron capture cross-sections and neutron separation energies," International Atomic Energy Agency STI-PUB-1263 (2007).
- [8] G.Arbanas et al., ``Direct-Semidirect Thermal Neutron Capture Calculations," UCRL-PROC-217859 report (2005).
- [9] W.E.Parker et al., Phys. Rev. C 52, 252 (1995).
- [10] M.T.Pigni et al., "Uncertainty Quantification in (α,n) Neutron Source Calculations for an Oxide Matrix," Progress in Nucl. Energy 91, 147 (2016).

Discussion:

ENDVER package which has lots of plotting and data exporting capabilities using ENDF-6 files can be easily downloaded from IAEA main web page.

2.10. Evaluation of Light Nuclei with GECCCOS, H. Leeb

A good knowledge of nuclear reaction data of light nuclear systems is needed in several fields of research (e.g. nuclear astrophysics) and nuclear technology (e.g. nuclear fusion, decision on structure materials). At present the evaluation of nuclear reaction data of light nuclear systems represents still a challenge and available evaluated nuclear data files are not fully satisfactory. Light nuclear systems are characterized by an extended energy range (system dependent up to 10 MeV and higher) for which resonant behaviour of the reaction cross sections occurs. One major problem is the fact that at present no quantitative semi-microscopic method is known which provides a quantitative description of this resonance regime. In addition, the applicability of statistical model calculations is questionable even for high energies, especially for the lightest nuclear systems. Under these circumstances unitary R-matrix models are used

for the description of reaction data in light nuclear systems. Albeit phenomenological this approach may lead to a consistent description of reactions due to the constraints of unitarity if sufficient experimental information is available.

A successful nuclear data evaluation consists essentially of three steps: (1) The retrieval of all available experimental data sets and a careful assessment of the uncertainties of the experiments. (2) A proper set of models with reasonable parameters which provides a fair description of reaction data. (3) An evaluation procedure which starts from the best description and consistently combines the model with the experimental data in order to find our best knowledge of reaction cross sections and associated covariance matrices. In this contribution we presented our considerations to (2) and (3) which are summarized below.

The first part of the presentation was dedicated to the hybrid R-matrix model, a unitary approach developed by our group recently [1]. Key point is the use of a physically reasonable matching radius and the enforcement of a continuous transition between resonance regime and statistical model calculations. The latter is argued that beyond a sufficiently high energy (dependent on the considered nuclear systems) the level density of the compound nucleus becomes almost continuous and a statistical model description can be applied. Matching at the transition energy reaction cross sections and if compound-elastic scattering is negligible also the S-matrix of the elastic channel ensure a smooth transition. Furthermore, the background poles are determined via the calculable R-matrix from the real part of the optical potential used in the statistical model calculation. Some additional pole terms are added and fitted together with the background poles in the energy regime considered by the R-matrix representation to the set of available experimental data. With increasing matching radius this fit can become rather intriguing. Therefore, we presented a method which allows a transformation of the R-matrix at different matching radii which leads to the S-matrix and thus equivalent observables. As an example, we presented a unitary description of the ¹⁷O compound nucleus including all binary reaction channels up to 13 MeV incident neutron energy within the hybrid R-matrix approach.

In the second part of the contribution we discussed the concepts of Bayesian evaluation techniques and presented a Modified Generalized Least Square method suitable for large scale evaluations [2]. The latter point is of particular importance for evaluations which extend over energy regions which are described by different nuclear models, e.g. the hybrid R-matrix approach presented previously. In general, the parameters of different nuclear models are mutually not related and do not present a proper basis for the evaluation. Therefore, extending over the regime of different models it is preferable to work with a surrogate model based on the observables. In the resonance regime this ansatz automatically implies the necessity of a great number L of data points of observables in order to provide a fair description of the reaction data. Thus, the Bayesian evaluation becomes a large-scale problem for the handling of covariance matrices even for the linearized form of a Generalized Least Square technique. The Modified Generalized Least Square method [2] makes use of the fact that the original models depend on a relatively small number of parameters. Thus, a much smaller number $N \ll L$ of Monte Carlo sweeps suffice for a proper determination of the *a-priori* covariance matrix A_0 . Thus, neither an explicit calculation of A_0 nor of the updated covariance matrix A_1 is required. Instead one has to store only the N Monte Carlo sweeps, a vector of N weights and an auxiliary N x N matrix W thus reducing the storage requirements, e.g. for N =2000 Monte Carlos sweeps and $L = 10^6$ the method reduces the required storage from 7.6 TByte to 15.3 MByte. From this information the covariance matrices for all observables as well as cross nuclide and cross reaction channels can easily be reconstructed.

In summary we presented the Hybrid R-Matrix method, a tool for the description of reactions in light nuclear systems, which combines the resonance range with statistical model calculations. For the Bayesian evaluation step, we presented the Modified General Least Square method which significantly reduces the storage requirements and accelerates the update process. At the same time, it offers a very effective way of storage organisation, which still contains the full information and allows the

reconstruction of all required covariance matrices as well as a complete update of the evaluation with new experimental data. Thus, it offers a promising new and efficient way for the storage of nuclear data libraries.

References

- [1] Th. Srdinko, H. Leeb, R-matrix approach at the intersection with the statistical model regime, EPJ Web of Conferences **146** (2017) 12030
- [2] G. Schnabel, H. Leeb, A modified Generalized Least Square method for large scale nuclear data evaluation, Nucl. Instr. Meth. A **841** (2017) 87.

Discussion:

For the moment the code provides total cross sections. It will be developed to provide partial cross sections.

The model deficiencies are reflected in the uncertainty analysis. All the sources of uncertainty including correlations have to be calculated.

Plan to demonstrate the method in the evaluation of ¹⁶O+n first and then ⁹Be+n next.

3. Technical discussions

The discussion opened with a survey of who is working on which reaction from the INDEN list of reactions of interest for light systems. In addition to which reaction would be taken on by whom, there was also the issue of how high in energy the analysis should go. It has been proposed that the high energy of interest is 20 MeV, at minimum, to be acceptable for an evaluation.

These projects being long-term, the question was raised how many years INDEN would go on. It was stated that this evaluation group did not have any end date. Also, participants are free to move to a different reaction once they finish work on another.

3.1. Current status of listed light systems

⁹Be+n:

Hale (LANL), Thompson (LLNL), Leeb (TUW), Chen (Tsinghua) and Pigni (ORNL) are all working on ⁹Be+n. They are all concentrating on the break up aspect of the reaction, as it occurs very low in energy and is essential for this reaction. Hale is limiting his calculations to the resolved resonance region. Thompson is going to use a multi-step breakup model and analyze above the RRR up to 20 MeV. Leeb will also go into the high energy region up to 20 MeV. Archier (CEA Cadarache) will also collaborate but it is not clear whether the group will actually produce an evaluation. Chen will also try to perform this evaluation and has requested that Hale send him the data. Related to this, Hale has emphasized that the first step will be to collect a common data set. If any data is not in EXFOR he will provide it to EXFOR. It was also mentioned that new data from RPI are available [3.1].

Action on G. Hale: to provide all data on $n+{}^{9}Be$ that is not already in EXFOR to IAEA (N. Otuka) for compilation.

¹⁴N+n:

Hale (LANL), deBoer (U. Notre-Dame), and Kunieda (JAEA) are working on $n+^{14}N$. Hale and deBoer will examine the RRR up to a few MeV, but do not plan to go into the unresolved resonance region. Kunieda, on the other hand, will look at the higher energy region only.

¹⁵N+n:

Kunieda (JAEA) is the only person investigating ¹⁵N+n. From his presentation, he seems to already have a good start on the resolved resonance region. Next year, he will work on using statistical methods to go up to 20 MeV, and maybe even higher.

¹⁶O+n:

While not listed in the INDEN list of reactions, it has become clear that ¹⁶O+n has issues remaining that were left unresolved from the CIELO working group. Pigni (ORNL), Hale (LANL), and Kopecky (JRC-EC) will all work on this. Pigni will publish his parameters when he gets the Brune transformation working in SAMMY. Hale will also publish his results in Physical Review soon. Kopecky is continuing with the analysis of the thick target yield normalization technique that he has used. The results look very promising. Again, there is still a need to form a common data set for the analysis.

There was considerable discussion on this topic on several issues. It was recommended that the results of Kopecky's analysis of normalization based on measured Thick Target Yields (TTY) should be uploaded on the EXFOR Correction System. Each evaluator can in fact upload the corrections introduced to the data as a result of the assessment of all the experimental data sets in a separate EXFOR correction file. Details about how to upload onto the correction system are provided at https://www-nds.iaea.org/exfor/x4guide/x4renorm2/index.htm. There will be a need to re-evaluate the Bair & Haas [3.2] data as well as all the other data after Kopecky gives his re-normalizations to thick target yields. It was emphasized that there is a strong correlation between the normalizations of the different data sets, in particular unitarity causes an anticorrelation between the reaction cross section and the total cross section. So if you push the Bair & Haas [3.2] data down, it will push the total data up. There was also mention that the *shape* of Harissopulos et al. data [3.3] may be incompatible with that of the other data sets as bove the threshold for excitations to excited states.

From recent publications this past year by Peter Mohr [3.4] and Bill Peters [3.5], it has been pointed out that the long counter measurement of Harissopulos et al. is not correct at energies above the threshold for de-excitations to excited states in ¹⁶O because they did not know the branchings to these states and did not have a flat efficiency function for their neutron detector. In addition, Giorginis' [3.6] reanalysis of the target thickness of Harissopulos' data [3.3] does not seem to be correct. The thick target method seems more promising at the moment.

It was also mentioned that using other reaction cross sections for normalization/calibration of a relative measurement needs to be done with care to avoid circular normalizations. There have been cases, for example, where the n+H cross sections were used to calibrate measurements of $n+^{16}O$, and then for measurements of n+H the $n+^{16}O$ was used for calibration, which had been originally calibrated to n+H.

For ¹⁶O there should also be an assessment of all of the $(n,n\gamma)$ data, as there is interest in this data, in particular in the 6.13 MeV transition, and the present evaluation is quite preliminary. It is clear that more work needs to be done on oxygen.

²³N+n:

Archier's group (CEA Cadarache) is the only group working on ²³Na+n, but Pigni (ORNL) and Kunieda (JAEA) would also like to look at it if they can find some time. There was also the question of whether this analysis should be moved to the INDEN group on structural materials as it is rather high in mass and the RRR only goes up to about 2 MeV before it evolves into the Unresolved Resonance Region (URR) which is quite common in medium mass nuclides.

3.2. From Resolved Resonances to Unresolved Resonances

The next point of discussion was the connection of the RRR with the URRR. There has not been a good connection between the resolved and unresolved region because, while it appears still resolved, you begin to accidently start missing a lot of resonances in the analysis. For applications you always use Monte Carlo probability tables to do this intermediate range instead. However, at this point there is no general recipe for how this should be done. For example, Kopecky and Pigni use the average resonance characteristics in the GNASH code, but this depends on what application you are using this for. Another real problem is even trying to apply a statistical model to a light nuclear system. Often the data are just used directly when no model can reproduce them well, but there is definitely not enough data to do this in many cases.

3.3. Data processing

Processing for neutron data was the next point of discussion. However, this instead mostly focused on processing issues for charged particles. The main issues are that PREPRO [3.7] and NJOY [3.8] are not able to handle charged particle data. The processing issue is for the B = -L basis. For charged particles the problem is both B = -L and to get cross sections from a resonance file. Or it can, but its output is not cross section, but is the cross-section ratio to Rutherford. This last part was not confirmed. It was emphasized that the final goal here is to have an ENDF parameter file and the processing codes so that cross sections. It has all of the proper updates that have been made to SAMMY as a result of the IAEA meetings on R-matrix Codes. (refer to: <u>https://www-nds.iaea.org/index-meeting-crp/CM_R-matrix2018/</u>) A new version of AMPX has just been released. These codes also need to be able to handle parameters in the Brune basis.

3.4. Other items

Secondary gamma rays: At this point several other minor issues were discussed. It was first discussed how Carl Brune had worked up some nice notes on how to implement angular distributions for secondary gamma-rays. AZURE2 and Fresco have been updated with this capability. SAMMY is also being updated but there needs to be a better emphasis for why it is needed for its user community. Carl's notes were distributed to the group by deBoer (with C. Brune's permission).

Higher energies: The next question was if the Reduced R-matrix could be used to fit in these higher energy regions above the breakup thresholds. Chen is using this approach, but the issue is that it has yet to be determined exactly how it is implemented in RAC. In addition, the technique needs to be refined so that unitarity can still be maintained below the 3 body thresholds. There is also the issue that a method like Reich-Moore cannot be used to calculate angular distributions. The question is how does a multibody penetrability act? This could also be used when there are many channels. But it was heavily emphasized that this needs to be done with great care. For the present, it is only an issue with the ⁹Be+n system.

There was also the question of whether the charged particle and neutron groups should merge, but since the charged particle group is still working out comparison issues (Chen, deBoer, Hale, Kunieda, Thompson, Pigni) they will remain separate for now.

3.5. Work to be done

Progress made by participants by the time of the next meeting is estimated as follows:

⁰Be+n

Hale will try to push all of the reactions up to higher energies than he had in previous analyses. There is total cross section data, but some of the other channels do not have data. The breakup channel is also a problem.

Thompson will show preliminary calculations for breakup at higher energies. He will extract angular distributions from CDCC calculations.

Leeb will try to have the 3 body R-matrix theory implemented. This will be a more general thing. He will use a reduced R-matrix.

Pigni will also investigate alternative approaches and see where he is in a year.

Chen will also evaluate this system.

¹⁴N+n

deBoer will aim at getting a good fit of the low energy region by the next meeting.

Hale will also aim for a good fit of the low energy region and also push the calculations up to high energy. Kunieda will present results on the higher energy region.

¹⁵N+n

Kunieda will complete his R-matrix analysis and then he will try to go to higher energies.

²³Na+n

Archier will include differential cross sections and will produce an ENDF6 file to share with everyone.

Kunieda will look at the high energy data.

Thompson will look at the effect of deformation.

Pigni will make a fit in the B=-L basis. This needs to be done because the previous fit doesn't conserve unitarity due to the use of energy dependent boundary conditions.

¹⁶0+n

Kopecky will give a normalization for the data with his thick target calculations, maybe even a paper.

Hale and Thompson will define what the relativistic corrections mean, these are more like the Klein-Gordon equation.

Chen will revisit the previous evaluation he performed in 2005.

Action on all: For each reaction the subgroups will create an experimental data base. They will distribute to one another (possibly the entire group).

References

- [3.1] M.J. Rapp et al., Nuclear Science and Engineering, Vol.**172**, 268 (2012); Y. Danon et al., Conf. on Nucl. Data for Sci. and Technology, Nice 2007, Vol.1, p. 401 (2007), France.
- [3.2] J.K. Bair and F.X. Haas, Phys. Rev. C 7, 1356 (1973).
- [3.3] S. Harissopulos et al., Phys. Rev. C 72, 062801 (2005).
- [3.4] P. Mohr, Phys. Rev. C 97, 064613 (2018).
- [3.5] W.A. Peters, Phys. Rev. C 96, 029801 (2017).
- [3.6] G. Giorginis, private communication.
- [3.7] PREPRO, ENDF/B Pre-processing codes, <u>IAEA-NDS-39 REV. 16</u>
- [3.8] R.E. MacFarlane, et al., The NJOY Nuclear Data Processing System, Version 2012, LA-UR-1227079, August 2013.
- [3.9] AMPX, A modular code system for processing ENDF/B, ORNL/TM-2016/43, 2016.

4. Summary

The current status of the evaluations of the light systems identified as being of top priority for nuclear reactor criticality and safety studies was reviewed at the meeting. Participants presented their current and future plans for evaluations. A list was produced of the groups working on the five light targets, ⁹Be, ^{14,15}N, ¹⁶O and ²³Na, including their objectives/goals as well as the results expected to be delivered by the next meeting. All the evaluations delivered to the INDEN network will be made available to the user community from a dedicated website.

The next meeting will be held in Autumn 2019.

5. List of Actions/Tasks

Action/task	Responsible	Deadline
Provide all data on n+ ⁹ Be that is	G. Hale	Next INDEN meeting
not already in EXFOR to IAEA (N.		
		Continuous
subgroups will create an	All	Continuous
experimental data base and		
distribute it among each other		
and the whole group		
⁹ Be+n		
Push all of the reactions up to	G. Hale	Next INDEN meeting
higher energies than in previous		
breakup at higher energies	1. Thompson	Next INDEN meeting
Extract angular distributions from		
CDCC calculations.		
Implement 3-body R-matrix	H. Leeb	Next INDEN meeting
theory. Use reduced R-matrix.		
Consider alternative approaches	M. Pigni	Next INDEN meeting
to break-up		
Perform evaluation	Z. Chen	Next INDEN meeting
¹⁴ N+n	D. de De est	
Get a good fit of the low energy region	R. deBoer	Next INDEN meeting
Get a good fit at low energy and	G. Hale	Next INDEN meeting
extend to higher energies as		
Fit higher energy region	S. Kunieda	Next INDEN meeting
Complete B-matrix analysis at low	S Kunieda	Next INDEN meeting
energies and then extend to	5. Runeud	Next molen meeting
higher energies		
¹⁶ O+n		
Provide normalization based on	S. Kopecky	Next INDEN meeting
analysis of thick target data		
Define relativistic corrections	G. Hale, I. Thompson	Next INDEN meeting
Update evaluation of 2005	Z. Chen	Next INDEN meeting
²³ Na+n	D. Austrian	
Include differential cross sections	P. Archier	Next INDEN meeting
share with everyone		
High energy data	S. Kunieda	Next INDEN meeting
Effect of deformation	I. Thompson	Next INDEN meeting
Re-fit using B = -I	M. Pigni	Next INDEN meeting
	·····	



International Nuclear Data Evaluation Network (INDEN) Meeting on the Evaluation of Light Elements

IAEA, Vienna, Austria 30 to 31 August 2018 Meeting Room VIC MOE15

ADOPTED AGENDA

Thursday, 30 August

- 08:30 09:00 Registration (IAEA Registration Desk, Gate 1)
- 09:00 09:30 Opening Session

Welcoming address (Arjan Koning, NDS Section Head)

Election of Chairman and Rapporteur

Adoption of the Agenda

09:30 – 17:30 Presentations by participants (~ 40 min each)

- 1) P. Dimitriou, A. Trkov: Introduction to INDEN II
- 2) LANL R-matrix work on $n + {}^{9}Be$ and $n + {}^{14}N$, G. Hale (LANL)
- 3) CEA contribution to Sodium nuclear data evaluation, P. Archier (CEN Cadarache)
- 4) Status of experimental data for n-induced reactions on ¹⁶O, S. Kopecky (EC-JRC)
- 5) A new ⁹Be(p,n) model of Geant4 and aspects of effective field theories for light nuclei, T.-S. Park (Sungkyunkwan Univ.)
- 6) Assessment of two-body and gamma-production cross-sections with EXFOR, I. Thompson (LLNL)
- 7) Global fitting of ⁷Be using GLS, Z. Chen (Tsinghua Univ.)
- 8) Preliminary results of $n + {}^{15}N$ analysis, S. Kunieda (JAEA)
- 9) R-matrix analyses and evaluation work on light nuclei: $n + {}^{28,29,30}Si$, $n + {}^{16}O$, $\alpha + {}^{17,18}O$, M. Pigni (ORNL)
- Progress towards a global R-matrix fit of the ¹⁵N system at low energy, R. deBoer (Univ. Notre-Dame)
- 11) T. Srdinko (TUV)

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

19:00 Dinner at a restaurant downtown (see separate information in folder)

Friday, 31 August

09:00 – 17:00 Round Table Discussion – Drafting of report

Topics for discussion on systems:

- Neutrons on ⁹Be; ^{14,15}N, ²³Na at energies up to 20 MeV

What needs to be done? When were the last evaluations done? What new experimental data have become available? Are new evaluations needed?

- Issues with R-matrix fitting and evaluation:
 - How is the resolved-resonance region (RRR) and unresolved-resonance region connected (URR)?
 - $\circ~$ How are RRR, URR and statistical model regime connected? How are fluctuations treated?
- Data processing? Codes and methods (charged particles)
- Other items from CM on Charged-particle induced reactions:
 - Plans for new fits of nuclear reaction: Data assessments, data error checking, use of previous fits, etc.
 - Going above dissociation thresholds: Is there a general method?
 - Can we extend R-matrix theory to higher energies by any simple and welldefined method (to deal with large number of open channels)? – related to point above.
 - Analysis of the 3 He(α , γ) 7 Be data with AZURE2
 - ²⁷Al+p work done with AZURE2

How ${}^{12}C(p,p)$ and ${}^{12}C(a,a)$ scattering would be extremely useful as charged particle standard reactions, similar to the way ${}^{12}C(n,n)$ is a neutron standard.

INDEN II project organization:

- How is the work going to be organized? Priorities, evaluators, timeline.
- Next meeting

Drafting of the summary report

Coffee break(s) as needed

12:30 – 14:00 Lunch break

International Nuclear Data Evaluation Network (INDEN) Meeting on the Evaluation of Light Elements

30 to 31 August 2018 IAEA, Vienna

List of Participants

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ANNEX 2

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ANNEX 3

Presentations

#	Author	Title	Link
1	G. Hale	LANL R-Matrix Work on $n+^{9}Be$ and $n+^{14}N$	PDF
2	S. Kopecky	The European Commission science and knowledge service	PDF
3	P. Archier	CEA Cadarache Contribution to Sodium Nuclear Data Evaluation	PDF
4	T-S. Park	A ⁹ Be(p,n) ⁹ B Model of Geant4 and Aspects of EFTs for Light Nuclei	PDF
5	I.J. Thompson	User Assessment for light elements: two-body, n- & gamma- production cross-sections	PDF
6	Z. Chen	The Global Fitting Resulta of ⁷ Be System - GLS	PDF
7	R.J. deBoer	¹⁵ N Compound System at Low Energies	PDF
8	S. Kunieda		PDF
9	M.T. Pigni		PDF
10	T. Srdinko		PDF
11	P. Dimitriou		PDF

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