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INDC International Nuclear Data Committee

International Nuclear Data Evaluation Network (INDEN) on the Evaluation of Light Elements (5)

Summary Report of the IAEA Consultants' Meeting

IAEA Headquarters, Vienna, Austria
29 August–1 September 2023

Prepared by

R.J. deBoer
University of Notre Dame
Notre Dame, IN, USA

Marco Pigni
Oak Ridge National Laboratory
Oak Ridge, TN, USA

P. Dimitriou
International Atomic Energy Agency
Vienna, Austria

March 2024

IAEA Nuclear Data Section

Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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Nuclear Data Section
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PO Box 100
1400 Vienna
Austria

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ABSTRACT

The INDEN for Light Elements network (INDEN-LE) held a Consultants' Meeting from 29 August to 1 September 2023, to review the status of the evaluations undertaken by the network as well as developments in R-matrix theory and new measurements. The summaries of the presentations and discussions can be found in this report.

March 2024

Contents

1. Introduction

The International Nuclear Data Evaluation Network on the evaluation of Light Elements (INDEN-LE) is continuing its efforts to evaluate charged-particle- and neutron-induced reactions in the resolved resonance region for light composite systems that are important in energy and non-energy applications. The work carried out by the INDEN-LE has been discussed and documented in the following reports:

Charged particle-induced reactions:
IAEA report INDC(NDS)-0703, 2016: (https://www-nds.iaea.org/publications/indc/indc-nds-0703/)
IAEA report INDC(NDS)-0726, 2017: (https://www-nds.iaea.org/publications/indc/indc-nds-0726/)
IAEA report INDC(NDS)-0737, 2017: (https://www-nds.iaea.org/publications/indc/indc-nds-0737/)
IAEA report INDC(NDS)-0767, 2018: (https://www-nds.iaea.org/publications/indc/indc-nds-0767/
IAEA report INDC(NDS)-0787, 2019: (https://www-nds.iaea.org/publications/indc/indc-nds-0787/
IAEA report INDC(NDS)-0827, 2021: (https://www-nds.iaea.org/publications/indc/indc-nds-0827/
Neutron-induced reactions:
IAEA report INDC(NDS)-0788, 2019: (https://www-nds.iaea.org/publications/indc/indc-nds-0788/
IAEA report INDC(NDS)-0827, 2021: (https://www-nds.iaea.org/publications/indc/indc-nds-0827/
Joint report:
IAEA report INDC(NDS)-0853, 2023: (https://www-nds.iaea.org/publications/indc/indc-nds-0853/

The 8th R-matrix codes and 5th INDEN-LE meetings were held back-to-back from 29 August to 1 September 2023, at the IAEA Headquarters, Vienna. The meetings were hybrid and were attended by: H. Leeb, T. Srdinko (Austria); Z. Chen, X. Cong, and H. Xu (China); P. Tamagno (France); G. Arbanas, C. Brune, R.J. deBoer, G. Hale, M. Paris , M. Pigni, I.J. Thompson (USA); S. Kopecky (EC-JRC); D. Foligno, A. Holcomb (OECD/NEA), with 15 participants from five members states (MS) and two international organizations, including IAEA staff P. Dimitriou (Scientific Secretary). A guest presentation was given by Y. Otake (RIKEN, Japan).

Arjan Koning, NDS Section Head, gave a welcome address and the scientific secretary of the meeting and project officer, Paraskevi (Vivian) Dimitriou, gave a short summary of the goals of the meeting and the status of the project. Helmut Leeb and R. James DeBoer were elected chair and rapporteur of the meeting, respectively. Status reports and presentations were given by the participants, followed by technical discussions and recommendations.

The summaries of the presentations are given in Section 2, while a summary of the technical discussions is provided in Section 3 and the conclusions in Section 4. The adopted Agenda and List of participants are given in Annexes 1 and 2, respectively. Links to participants' presentations can be found at: https://conferences.iaea.org/event/364/contributions/

2. Presentation Summaries

2.1. New measurements of $^{14}N(n,\alpha)$ and $^{16}O(n,\alpha)$ reactions, X. Cong (Peking Univ.)

New measurements of (n,α) reactions on ^{14}N and ^{16}O have been performed at Peking University (PKU). One of the motivations for studying these reactions is that Nitrogen fuel is widely used in Gen IV nuclear power systems. However, there are significant uncertainties in the existing data that reach 40% in the energy range from 4 to 12 MeV for the reaction channels $^{14}N(n,\alpha_0)$ and $^{14}N(n,\alpha_1)$. Similarly, the data for $^{16}O(n,\alpha_0)$ have large associated uncertainties at energies above 5 MeV. New measurements of the $^{14}N(n,\alpha_{0,1})$ reactions were performed at energies ranging from 4.53 to 5.51 MeV and from 7.09 to 11.48

MeV, and of the $^{16}O(n,\alpha_0)$ reaction at energies from 6.89 to 11.67 MeV at the PKU and CIAE facilities. The two accelerator facilities were selected because their accelerators cover different, complementary, energy ranges. The measurements were performed with a typical 50 keV energy resolution which was in certain cases increased to 100 keV. Preliminary results show that the new cross sections are higher than previous measurements. There is some significant uncertainty associated with the conversion from differential to angle-integrated cross sections that could contribute to this effect, along with contributions from low energy neutrons. In addition, the (n,α_0) and (n,α_1) partial cross sections were hard to separate. At higher energies, wall effects and background reactions on Kr are the most significant sources of uncertainty. Measurements of the $^{19}F(n,\alpha)^{16}N$, $^{20}Ne(n,\alpha)^{17}F$, and $^{16}O(n,\alpha1,2,3)$ reactions are planned for the future.

2.2. New evaluation of the ^{17}O and ^{15}N systems, Z. Chen (Tsinghua Univ.)

The classical reduced R-matrix theory, covariance statistics and the corresponding program RAC are used to complete these evaluations. A detailed description of the methodology has been reported in Ref. [1]. Here, we limit ourselves to introducing the improved evaluation of the ^{17}O system and the new evaluation of the ^{15}N system that were performed last year.

For the ^{17}O system, the new (n,α_0) experimental data of Peking University which was measured in the energy range from 6.5 to 13.5 MeV has been considered in the evaluation of (n,α_0) and (n,α) and has improved it significantly, especially in the 6 - 8 MeV energy region.

For the ^{15}N system, the fitting included the following 15 channels:

'N14(N,N0)N140', 'N14(N,4HE)11B0 ', 'N14(N,4HE1)11B1 ', 'N14(N,N1)N141', 'N14(N,P)C140 ',

'N14(N,D)C130 ', 'N14(N,T)C120', 'N14(N,4HE2)11B2', 14(N,4HE3)11B3', 'N14(N,N2)N142',

'N14(N,N3)N143', N14(N,N4)N144 ', 'N14(N,N5)N145', '14(N,N6)N146 ', 'B11(4HE,4HE)B11 '.

The relationship between the different channels of the ^{15}N system is described as follows:

$(n,tot) = (n,el) + (n,inl) + (n,\alpha) + (n,p) +(n,d) +(n,t) +(n,left)$, $(n,inl) = (n,n_{0,1,2,3,4,5,6}) + (n,inl_{else})$,

$(n,\alpha) = (n,\alpha_{0,1,2,3}) + (n,\alpha_{else})$, (n,all_else) = (n,inl_else) +(n,α_else) +(n,left) = (n,tot) - (n,allr)

Here, (n,tot) represents the contribution from all channels of the ^{15}N system. (n,allr) represents the contribution from retained channels, which includes the contribution from $(n, n_{0,1,2,3,4,5,6})$, $(n, \alpha_{0,1,2,3})$, (n,p), (n,d) and (n,t), for there is available experimental data. (n,inl_else) and (n,αelse) mean the reduced channel from (n,inl) and (n,α), respectively. (n,left) represents the contribution from all left (remaining) channels, mainly from the multi-body reactions.

In the RAC parameter file, each level has a 'reduced channel width' parameter, which can be adjusted to control the contribution of the reduced channel. RAC can calculate the integral cross section of each retained channel, but it cannot directly calculate the total contribution of the reduced channel. The total contribution of the reduced channel is obtained by subtracting the integral cross sections of all retained channels from the total cross sections. It is necessary to obtain a satisfactory fit for the total (n,α) cross section, a satisfactory fit for the total (n, inl) cross section and a satisfactory fit for the multi-body reaction value through appropriate allocation of the cross sections. These three components are represented by a combination of suitable multiple polynomials and resonance expressions whose coefficients are adjustable parameters.

Determining the contribution of the reduced channel is an iterative process. Firstly, by fitting the primary experimental data base, the calculated values of the total cross section and each retained channel can be obtained after a better fitting. According to the quality of the fit to the experimental data, the new reduced-channel values for (n,α) and (n, inl) are assigned. The respective contributions are represented by a new combination of multiple polynomial and resonance expressions whose coefficients can be taken as adjustable parameters. Then one proceeds to the next iteration of the fit.

We are continuously exploring ways of correctly estimating the contribution of the reduced reaction channel. Our goal is to build evaluated files of neutrons and charged particles for light nuclear systems, which however, is a long process. We are looking for the best way to provide our results in the ENDF-6 format.

References

[1] Z. Chen, Y. Sun, IAEA Report INDC(NDS)-0791, IAEA, Vienna, 2019, available at: https://www-nds.iaea.org/publications/indc/indc-nds-0791/

Discussion:

- The total cross section data of Cierjacks are not included in the fit.
- The ^{16}O(n,α) evaluated cross section is lower than ENDF/B-8 at neutron energies above about 8 MeV along with ^{16}O(n,inl) due, in part, to the new Peking University data presented above.
- The ^{17}O evaluation still includes the ^{13}C(α,n) data of Harissopulos et al. The evaluation extends up to 30 MeV.
- Unitarity is not conserved in the fitting.
- For the ^{15}N system, the total cross section data of Harvey and the ^{11}B(α,n) data from Wang et al. are not considered.
- What is the difference between the different “else” eliminated channels? The answer to this question was unclear.

2.3. New experimental results for n+^{14}N, R.J. deBoer (Notre Dame Univ.)

New measurements have been performed for reactions that populate the ^{15}N compound system at both the CASPAR underground facility and the ELBE facility at HZDR. At CASPAR, measurements of the ^{11}B(α,n)^{14}N reaction were made at low energies for nuclear astrophysics application. The new measurements span the center-of-mass energy range from 0.33 to 0.55 MeV, overlapping with previous published measurements of Wang et al. [1] and unpublished higher energy measurements at the University of Notre Dame. A new resonance was observed which corresponds to the known level at an excitation energy of 11.240 MeV, which corresponds to the very strong 433 keV resonance in the n+^{14}N total cross section and has been observed by Wang et al. (1991) in the ^{14}C(p,n)^{14}N reaction as a very weak resonance. These measurements were the thesis project of Tyler Borgwardt at the South Dakota School of Mines and Technology and have been published in Physical Review C [2].

New measurements of the n+^{14}N reaction have been made at the ELBE facility at HZDR in Dresden. These measurements cover the energy range from 0.1 to 12 MeV laboratory neutron energy. The measurements basically confirm those of Harvey et al. [3], but there are some significant differences. In particular, the resonance heights are all somewhat smaller than those of Harvey. The difference is most significant for the 433 keV resonance, where preliminary results give an on-resonance cross section of about 9.5 barn, while that of Harvey gives 11.5 barn. If the new result is correct, it means that the 7/2 spin assignment of Harvey is incorrect and that a 5/2 assignment is implied. While at this energy the resolution of the present measurements should be negligible, a smaller peak height is hard to understand. The experimental data analysis is still preliminary, so these conclusions could still change before publication.

References

[1] T.R. Wang, R.B. Vogelaar, R.W. Kavanagh, Phys. Rev. C **43** (1991) 883.
[2] T.C. Borgwardt, R.J. deBoer, A. Boeltzig, et al., Phys. Rev. C **108** (2023) 035809.
[3] J.A. Harvey, N.W. Hill, N.M. Larson, D.C. Larson, Proc. Int. Conf. on Nuclear Data for Science and Technology (S.M. Qaim, Ed.), Jülich (Germany), 13-17 May 1991, pp. 729-731 (1992).

2.4. Status of the LANL ^{15}N Analysis, G.M. Hale (LANL)

We reported on the status of the LANL R-matrix analysis of reactions in the ^{15}N system. This includes data for five reactions among the three channels p+^{14}C, n+^{14}N, and α+^{11}B, which are open below about 13 MeV excitation energy in ^{15}N. In all, there are more than 2100 data points that are fitted with a chi-squared per degree of freedom of 2.14. We showed reasonably good fits to ^{14}N(n,n)^{14}N and ^{14}C(p,n)^{14}N differential cross sections at lab energies up to about 2 MeV, as well as some ^{14}C(p,n)^{14}N analyzing-power measurements below 2.5 MeV. A few ^{11}B(α,p)^{14}C differential cross section measurements were also well described at E_{α} < 2.65 MeV.

The analysis resulted in good fits also to the integrated cross sections of the system. The best fit by far (c2 per point = 0.93) was to the n+^{14}N total cross section data of Harvey et al. [1] up to 2.5 MeV. However, differences with these data have been observed in a new measurement by deBoer et al., at the ELBE facility in Germany, especially over the 433-keV resonance, which require further investigation. Integrated cross sections for other reactions, including ^{14}N(n,p)^{14}C, ^{14}N(n,a)^{11}B, and ^{11}B(a,n)^{14}N, and ^{11}B(a,p)^{14}C, are well described by the analysis, with the notable exception of the low-energy ^{11}B(a,p)^{14}C data of Wang et al. [2]. The ^{11}B(a,n)^{14}N data set includes a newly-measured [3] low-energy extension of the cross section down to 334 keV at the underground CASPAR facility in South Dakota. We are very grateful to James deBoer for sharing these and other data with us prior to publication.

The results of this fit are encouraging, but they need to be extended to higher energies to be useful in an R-matrix evaluation of the cross sections for n+^{14}N. The Jπ assignments for some of the resonances differ from the accepted values. In addition to the narrow resonances, broad, underlying structure is important for most of the reactions. A higher-energy extension of this analysis could also be used to provide evaluated cross sections for incident p+^{14}C and α+^{11}B reactions.

References

[1] J.A. Harvey, N.W. Hill, N.M. Larson, D.C. Larson, Proc. Int. Conf. on Nuclear Data for Science and Technology (S.M. Qaim, Ed.), Jülich (Germany), 13-17 May 1991, pp. 729-731 (1992).
[2] T.R. Wang, R.B. Vogelaar, R.W. Kavanagh, Phys. Rev. C **43** (1991) 883.
[3] T.C. Borgwardt, R.J. deBoer et al., Phys. Rev. C **108** (2023) 035809.

Discussion:

- Are the angular distributions given an energy uncertainty? They are not but this is a good idea and should be implemented.
- The (α,p) data of Wang were obtained with a very thick target and the resolution effect has not been corrected for.
- The need for additional angular distribution measurements was stressed.
- Secondary gamma-ray angular distributions are highly desired.

2.5. A review of experimental capture data for the ^{7}Be evaluation, R.J. deBoer (Notre Dame Univ.)

The radiative capture reaction ^{3}He(α,γ)^{7}Be has a very well-known cross section due to several sets of consistent data taken after the year 2000. Prior to this, experiments suffered from inconsistencies between those obtained using the activation technique and those detecting prompt gamma-rays. However, after the Solar Fusion I evaluation (1998) where these deficiencies were highlighted, consistent results could be obtained with a new set of experimental measurements using both activation and prompt gamma-ray techniques in the same experimental campaign. This was then summarized in Solar Fusion II in 2011. Measurements performed afterwards have remained consistent, indicating that the systematics are well under control. Now new measurements have pushed to higher energy in order to better understand the ^{6}Li(p,γ) reaction and to try gain a better understanding of the mix of direct and internal reaction mechanisms that seem to make up the low energy cross section. One somewhat glaring open question for this reaction is that the angular distribution has not been studied and total cross section measurements rely completely on theory predictions. Also, first measurements have been made of the alpha particle ANC for the ground and first excited state of ^{7}Be, but they are inconsistent with those obtained from R-matrix and EFT analyses.

The situation is much worse, and more typical, for the ^{6}Li(p,γ) reaction. As a reaction that is not as important for nucleosynthesis, its low energy cross section has not undergone rigorous study. The reaction saw some renewed interest when He et al. [1] reported an unexpected downturn in the cross section at low energies, which they claim was the result of a new resonance. This was followed by some theory and indirect works that did not support this claim. In 2020 the LUNA collaboration published a new direct measurement where this downturn was not observed. However, the LUNA data have their own issues, including underestimated uncertainties and an upturn at low energy.

References

[1] J.J. He, S.Z. Chen, C.E. Rolfs, et al., Phys. Lett. B **725** (2013) 287.

2.6. Light element R-matrix analysis with SAMMY, M.T. Pigni (ORNL)

SAMMY has been modified to handle multiple entrance channels simultaneously. This is a significant improvement for evaluation work. The code uses the fit parameters (energies and reduced widths) in the lab frame, which requires additional calculations to convert from or to the CM frame. One special feature of SAMMY is the capability to perform simultaneous analyses of different isotopes, e.g., for neutrons on natural abundance targets. Benchmark tests have been performed using the ^{13}C(α,n)^{16}O and ^{16}O(n,α)^{13}C reactions. The code generates ENDF files to facilitate ENDF evaluations, i.e., it produces files 3 and 6. Some additional work is needed to create the covariance file.

The group should try to publish the results from Test 2 for ^{7}Be in a peer-reviewed journal, before completing the evaluation that would be the subject of a separate publication. The use of reduced R-matrix at higher energy is also proposed, using an approach like Reich-Moore. There is a lot of motivation to use the reduced R-matrix approach, but it must be used with extreme care.

2.7. Current status of LANL ^{7}Be evaluation, M. Paris (LANL)

We reported on the current status of the ^{7}Be system evaluation, which has been performed with the LANL R-matrix codes (EDA5, EDAf90). The configuration includes the following three partitions:

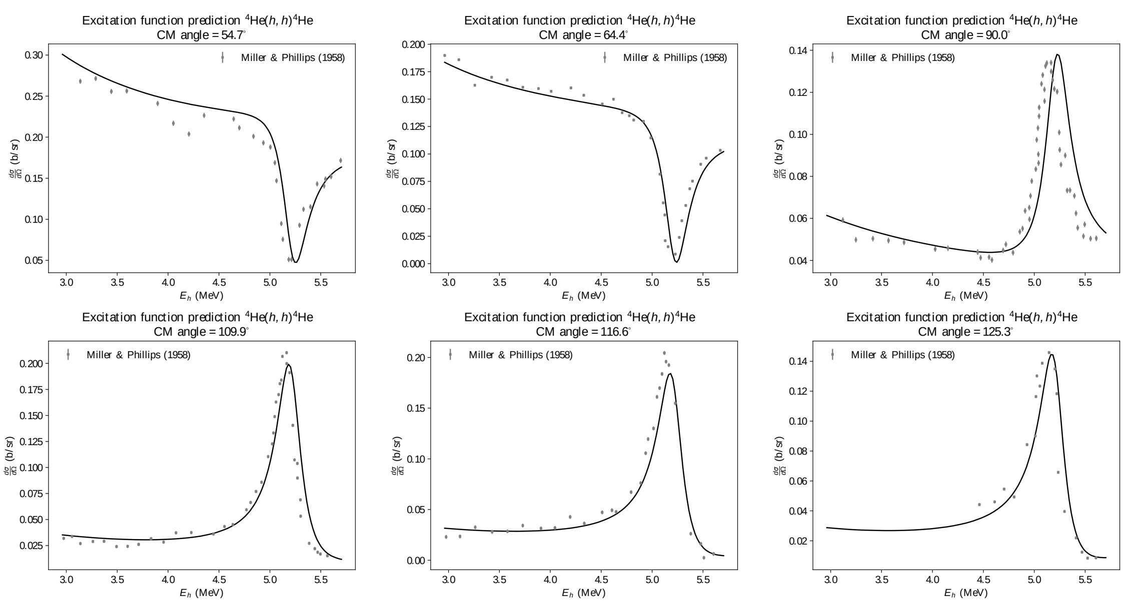
Here, we have shown the partitions/channels in the left-hand column (with target nuclei spin-parity shown), the channel radii (a_c), and the maximum orbital angular momentum (l_{max}) per partition.

Channel	a_c(fm)	$\ell_{\max}$
h+^{4}He (0^+)	4.43	4
p+^{6}Li(1^+)	3.13	1
γ+^{7}Be $(\frac{3}{2}^-)$	50.0	1

The current evaluation, which was recently updated for a recent LANL-internal project (the CP2020 Level II Milestone [1]), included a large amount of ^{3}He (h) induced elastic scattering for unpolarized σ(θ) and polarization A_y (θ) (polarization asymmetry) data, (h,p) unpolarized proton production angular distributions, (h,γ) angle-integrated cross sections and proton induced data on ^{6}Li including a large set of unpolarized, polarized, angle-integrated and angular distributions, as shown in the following table. This fit gives an overall $\chi^2/N_{dat} \approx 3.0$.

Process	Energy range (MeV)	N_{dat}	χ^2/N_{dat}	Observables
^{4}He(h, h)^{4}He	(1.2, 10.8)	1575	1.96	$\sigma(\theta), A_y(\theta)$
^{4}He(h, p)^{6}Li	(7.8, 10.8)	130	1.25	$\sigma(\theta)$
^{4}He(h, γ)^{7}Be	(0.287, 2.18)	40	1.32	σ
^{6}Li(p, h)^{4}He	(0.025, 2.97)	875	5.10	$\sigma, \sigma(\theta), A_y(\theta)$
^{6}Li(p, p)^{6}Li	(0.495, 2.6)	200	3.23	$\sigma(\theta)$
^{6}Li(p, γ)^{7}Be	(0.157, 1.17)	28	3.04	σ

The fit quality is fairly good across a wide range of energies and observables but there are inconsistent data sets, particularly in the angle-integrated σ(E) for (p,h) above a few hundred keV. We have made a comparison to the Miller and Phillips [2] excitation function data in the following figure.



This data was not included in the determination of the fit parameters and constitutes a prediction over the region of the included data. Ongoing studies will include data from ^{4}He(h,γ)^{7}Be, ^{6}Li(p,γ), ^{6}Li(p,p) from over 30 currently not included data sets.

References

[1] Charged Particle Transport Libraries (Final Report FY2020 Level-2 Milestone #7127), Report LA-UR-20-26607-Rev.01, https://www.osti.gov/biblio/1770083

[2] P.D. Miller and G.C. Phillips, Scattering of He^3 from He^4 and States in Be^7, Phys. Rev. **112** (1958) 2048.

2.8. Extending the ^{7}Be evaluation to include ^{6}Li exited states and capture to ^{7}Be excited state, I. Thompson (LLNL)

Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

In November 2022, I submitted as a candidate to ENDF/B-VIII.1 an evaluation for ^{3}He + ^{4}He reactions based on the evaluation work that our INDEN-LE group has produced over recent years. I now show R-matrix models which include the ^{6}Li first excited state (3^+ resonance) and which include capture channels (either by Reich-Moore, or as primary channels). I also consider further data up to 20 MeV. We might also consider using these models for a p+^{6}Li evaluation.

For the ^{6}Li 3^+ excited state, I include in the fit data of Gould, Harrison, Laurat and Merchez for proton-induced reactions, and 3 sets from Spiger for helion-induced reactions. Together these could be reasonably fit, although the Gould, Laurat and Spiger data was scaled down by about 30% (except for Laurat's A1508007 set). This reduced output from the R-matrix models suggests that either more poles are needed or larger R-matrix radii, or both. (a trial later with R_m=8 fm instead of 4 fm brings the Gould and Laurat rescaling closer to unity, but not for Spiger, with the overall χ^2/dof reduced from 2.52 to 2.32).

Capture channels can be modeled in 2 ways. First by the Reich-Moore approximation where the total capture probabilities are described by fitted damping widths of each pole, and second by including the primary gamma reactions as full two-body channels in the R-matrix set, with individual widths to be fitted (this last method requires extension of the ENDF6 format to include the primary gammas as, say, MT=900 and 901 for the ^{7}Be ground state and excited states respectively. I fitted the Notre Dame capture data set by both methods, using R_m=10 fm. Again, in both methods, the predicted R-matrix cross sections were typically deviating by –37% to +30% at the final fit (later trials with R_m=50 fm reduced these variations). Further model verifications are advisable.

Finally, I showed fits of further EXFOR data sets up to higher helion and proton energies than used in the 2022 submission. I think that, when the above R_m dependencies are resolved, there will be enough improvement in the fits to submit both ^{3}He+^{4}He and p+^{6}Li evaluations to ENDF/B-VIII.1 as improvements over existing models.

Discussion:

- Is there a way to calculate direct reaction mechanisms from coupled channels and combine this with the R-matrix approach to dividing the radiative capture into internal and external capture? Unknown.

2.9. Nuclear data (p+^{9}Be) for compact neutron sources, Y. Otake (RIKEN)

The RANS systems have been developed at RIKEN. These are three compact neutron sources based on small linacs. RANS-III will operate in a truck! These systems are designed for medical applications and nondestructive assays. Neutron source development is driven by societal needs. For example, new needs include salt damage to concrete, bridge collapse, to investigate inside the structure of large structures. These facilities can produce 10^{12} to 10^{11} neutrons/s using the ^{9}Be(p,n) and ^{7}Li(p,n) reactions. The system includes a bunched beam system. Without moderator, a fast neutron peak and a thermal neutron peak are obtained.

The components needed to calculate the neutron energy spectrum are:

1) Total neutron cross section
2) Angular distribution
3) Neutron energy based on kinematics.

The total cross sections are fitted with Breit-Wigner functions and Gaussians. Angular distributions are fitted with polynomials. The method has been benchmarked by separate studies using the ^{115}In(n,n') reaction, however, the experiment was quite complex. The yields can be overestimated by 30 to 50%. However, for the ^{7}Li(p,n) reaction, there is only a 5% deviation between the new calculations and the ENDF/B and JENDL evaluations. Several experimental issues still exist, but it is unclear how significantly they affect the data.

2.10. ^{19}F(α,n) progress report, P. Dimitriou (IAEA)

Preliminary R-matrix fits have been made using the AZURE2 code. Resonance information was taken from ENSDF based on the (α,p) angular distribution measurements of Kuperus et al. [1] and Schier et al. [2], (α,p) and α–elastic scattering data of Cseh et al. [3]. For the Wrean et al. (α,n) data [4], the fit doesn't look bad, but there are a couple of features that are not reproduced. The fits to the (α,α) data look good, but large normalizations need to be applied. The reproduction of the (α,p) angular distributions is still a struggle. The plan is to extend the R-matrix analysis up to 5 MeV and include the (α,n) data of Balakrishnan et al. [5]. New (α,n) cross-section measurements are expected from NPL (UK), but angular distribution data would be very useful too.

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[3] J. Cseh, E. Koltay, Z. Máté, E. Somorjai, et al., Nuc. Phys. A **413** (1984) 311.

[4] P.R. Wrean, R.W. Kavanagh, Phys. Rev. C **62** (2000) 055805.

[5] M. Balakrishnan, S. Kailas, M.K. Mehta, Pramana **10** (1978) 329.

2.11. Experimental results for the ^{13}C(α,n)^{16}O reaction, R.J. deBoer (Notre Dame Univ.)

As detailed in previous INDEN-LE reports, new measurements of the ^{13}C(α,n)^{16}O reaction have been made over a wide energy range. The results seem to be in good agreement with the, still unpublished, OU total reaction cross section in the region where only the ground state is accessible. However, the OU data have quite large uncertainties. The absolute cross section is about 20% smaller than that of the recent measurements of Prusachenko et al. [1]. The low energy part of this data set, center of mass energy below 2 MeV, has been fit with R-matrix, based on the initial parameters of Gerry Hale, which closely reproduced the data. Only one resonance was found to need a spin adjustment, that of a 7/2+ level, which was changed to 7/2-, although the fit to the total neutron cross section data was then somewhat worse, indicating that perhaps something more complicated is going on, like a doublet here. The focus has been an extrapolation into the very low energy range of astrophysical interest, down to a few 100 keV. This has been largely successful but some inconsistencies have cropped up such as inconsistent energy calibration between the (α,n) and (n,total) data. However, the absolute value of the cross section is much more consistent, and a Bayesian uncertainty analysis preformed using an MCMC routine resulted in an uncertainty of 5% or even smaller at low energies.

References

[1] P.S. Prusachenko, T.L. Bobrovsky, I.P. Bondarenko, M.V. Bokhovko, A.F. Gurbich, and V.V. Ketlerov, Phys. Rev. C **105** (2022) 024612.

2.12. Status of R-matrix Based Evaluation, H. Leeb (TUW)

Light nuclear systems have low level density and statistical considerations are not applicable. There are several codes that are used for R-matrix fit purposes.

R-matrix analysis strengths:

- Provides excellent description of the resonance cross sections;
- Satisfies conservation rules.

R-matrix analysis limitations:

- It is not a microscopic model, so it doesn't have predictive power;
- In general, not all the channels are included in the analysis, so unitarity is not strictly conserved; the method is also limited to binary channels;
- The analysis is practically limited in energy range.

The R-matrix method can describe a wide range of reaction data, but it cannot handle multiparticle breakup reactions. Some attempts have been made to treat the multiparticle breakup channels as two bound particles. Lane and Thomas [1] introduced the "Reduced" R-matrix, which is like the Reich-Moore approach.

The reduced R-matrix adds an additional term to the denominator of the R-matrix itself. We have developed a helpful approximation, which works if the two poles are not too close together in energy. This reduced R-matrix approximation has now been tested. The "defect" from unitarity can be calculated to get the cross section of the excluded channels. Cross sections are quite well reproduced up to 10 MeV for nearly all the ^{9}Be+n reactions. In particular, the ^{9}Be(n,α2n)^{4}He reaction is reproduced quite well from the unitarity defect. Differential cross sections for (n,n) and (n,n_2) are also reproduced quite well.

Can we now do an evaluation? The R-matrix fit is the first part of the procedure, but then one needs to perform a Bayesian analysis to complete the evaluation. In the past, typically, a generalized least squares method was used. It should be noted that Linearized Bayesian assumes normal distributions for the parameters, and so does the generalized least squares method.

Discussion:

- What priors can we use in the Bayesian approach to R-matrix analysis?
- Can we do a Bayesian evaluation of n+^{9}Be using GLS? Correlations could then be calculated.
- Cross correlations between different channels are not limited to -1 to 1 range.
- Model defects could also be included in the Bayesian statistical analysis.
- What are the model defects? Some examples are given:
    - Matching radii;
    - Finite number of pole terms;
    - Violation of unitarity by missing channels;
    - Use of approximations;
    - Unrealistic channel radii and/or background contributions.

References

[1] A.M. Lane, R.G. Thomas, Rev. Mod. Phys. **30** (1958) 257.

3. Technical discussion

Discussions evolved around the status of Tests 2 and 3 (described in detail in Refs [1–3]).

Participants agreed that the two separate projects should be concluded and published separately:

1. Focus on Test 2, i.e., statistical methods applied to the R-matrix analysis of ^{7}Be.

   Action on deBoer, Hale, Leeb, Paris, Pigni, Tamagno, and Thompson: finalize Test 2 and publish the results of the comparison of minimization methods, uncertainties and covariances produced by each code.

2. Focus on Test 3, i.e., an evaluation of the ^{7}Be compound system.

   Action on deBoer, Hale, Paris: to check whether Thompson's evaluation of the ^{7}Be system qualifies for inclusion in ENDF/B.

Capote suggested that the comparisons in Action #1 should be made separately between the correlation matrix and uncertainties.

For the needs of Action #1, Pigni and Thompson agreed to use primary gamma-rays instead of the Reich-Moore approach. ENDF-6 files 5 and 6 would be used for charged-particles. For the type of cross sections involved, one could use a uniform grid because the resonances are narrow, but it would have to be a fine enough grid for the linear interpolation to give a good reproduction of the cross sections.

For charged particle elastic scattering there will be no MF3 file. The Ferdinand code has the capability of reconstructing angular distributions from Legendre coefficients.

Appendix D of the ENDF-6 manual should be revised to include charged-particle information. Thompson will take care of this.

Rflow code is now available on GitHub.

The second topic of discussion was a comparison between the Brune basis and Park's parameterization [4] used in R-matrix theory:

It was stated that the Brune basis had the disadvantage that one must invert a matrix of a size equal to the number of levels, which would not be advisable for any analysis of high-mass nuclei where there are hundreds of levels. However, for most charged particle analyses there is no such problem. Park's parameterization on the other hand does not require such inversion.

Both Paris and Brune argued that Park's and Brune's parameterizations were the same, however, Arbanas and Leeb claimed that while they may be equivalent, Park's parameterization was more stable computationally. deBoer clarified that Brune's parameterization involves physical widths, and one does not have to convert to the B=-L parameterization. Arbanas compared Eq. 34 of Park's article to Eq. 16 of Brune's preprint https://arxiv.org/pdf/nucl-th/0207048.pdf, adding that Park fits observed partial widths directly without reference to "formal" widths, whether they are from Brune's or Wigner-Eisenbud's parameterization. While it is true that Brune's parameterization does not require a conversion back to B=-L, both B=-L and Brune widths are formal and not the observed widths. Park's widths on the other hand, are both observed and formal widths within Park's R-matrix formalism which is different from the Wigner's or Brune's R-matrix formalism (the latter two being equivalent). Paris commented that since Park introduces a separate boundary condition for each Wigner-Eisenbud level energy, it was not clear that the inverse transformation back to Wigner-Eisenbud parameters existed. At least, it had not been proven.

Participants also discussed the importance of performing R-matrix analysis of gamma-producing reactions, as these are important in a range of applications. In this context, Arbanas asked whether different EM multipolarities were treated as different channels in the implementation of such reactions in the R-matrix formalism. Hale clarified that in the implementation of the R-matrix formalism, photons that were emitted from excited states of the residual nucleus with different energies were considered as separate channels, something like separate "particle arrangements" and that the multipoles within an arrangement were considered as terms of the partial-wave expansion.

Finally, while comparisons with integral benchmark experiments can offer insight on the performance of the different evaluated libraries, it was acknowledged that criticality tests depend on too many parameters to be used to constrain the $^{16}O(n,\alpha)$ reaction. "Broomstick" measurements are very sensitive to the total cross section, but the uncertainties are also rather large.

References

[1] IAEA Report INDC(NDS)-853, 2023, see: https://www-nds.iaea.org/publications/indc/indc-nds-0853/

[2] IAEA Report INDC(NDS)-827, 2021, see: https://www-nds.iaea.org/publications/indc/indc-nds-0827/

[3] IAEA Report INDC(NDS)-787, 2019, see: https://www-nds.iaea.org/publications/indc/indc-nds-0787/

[4] T.-S. Park, Phys. Rev. C **104** (2021) 064612.

4. Conclusions

Participants presented the status of their evaluations of compound systems produced in both charged-particle and neutron-induced reactions relevant to a host of applications. Discussions evolved around various technical issues related to R-matrix theory and its' implementation in the various codes.

Agreement was reached to finalize Tests 2 and 3 and produce separate publications as the work that has been done so far is significant and merits to be published and shared with the user community.

The dates of the next meeting will be set after online discussions and depending on the progress of the two new, agreed actions.

IAEA Consultancy Meeting of the International Nuclear Data Evaluation Network – Light Elements

29 August – 1 September 2023
IAEA, Vienna
MOE7 (virtual component)

ADOPTED AGENDA

Tuesday, 29 August (14:00 – 18:00, open 13:45 Vienna time)

14:00	**Opening of the meeting,** A. Koning / NDS Section Head	
	Welcome and Introduction, P. Dimitriou / Scientific Secretary	
	Election of Chair and Rapporteur(s), Adoption of Agenda	
	Participants' Presentations *(60' each w/ discussion)*	*Breaks as needed*
	X. Cong	New measurements of ^{14}N(n,alpha) and ^{16}O(n,alpha)
	H. Xu /Z. Chen	Improved evaluation of n+^{14}N and n+^{16}O using new data
	R.J. deBoer	New experimental results on n+^{14}N
	G. Hale	Status of LANL R-matrix analysis of reactions in the ^{15}N system
	Discussion	

Wednesday, 30 August (14:00 – 18:00, open 13:45 Vienna time)

14:00	**Participants' Presentations** cont' *(60' each w/ discussion)*	*Breaks as needed*
	R.J. deBoer	Review of experimental capture data for ^{7}Be evaluation
	M. Pigni	Results on ^{7}Be evaluation using new SAMMY module
	M. Paris	Current status of LANL ^{7}Be evaluation
	I.J. Thompson	Extending the ^{7}Be evaluation to include ^{6}Li exited states and capture to ^{7}Be excited states
	Discussion	

Dinner at a restaurant (separate information)

Thursday, 31 August (14:00 – 18:00, open 13:45 Vienna time)

14:00	**Participants' Presentations** cont' *(60' each w/ discussion)*	*Breaks as needed*
	Y. Otake	Nuclear data (p+^{9}Be) for compact neutron sources
	P. Dimitriou	Progress report on ^{19}F(alpha,n)
	R.J. deBoer	Experimental results for ^{13}C(alpha,n) and future (alpha,n) studies at Univ. Notre Dame
	H. Leeb	Status of R-matrix based evaluation of n-induced reactions on ^{9}Be
	Discussion	

Friday, 1 September (14:00 – 18:00, open 13:45 Vienna time)

<table>
<tr><td>14:00</td><td>Round Table Discussion Breaks as needed</td></tr>
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Treating primary gammas as two-body channels in R-matrix codes (e.g. as in the ENDF proposal to use MT=900-999 for these)
Deriving MT=102 data from MT=900-999 for legacy code continuity
Methods for point-wise cross-section reconstructions from R-matrix parameters for charged-particles in all R-matrix formats
Recommendations for using Brune basis in data libraries
Any needed improvements to Appendix D in the ENDF-6 format manual?
R-matrix search code Rflow using tensorflow on cpu or gpu (will be) on github
Inclusion of covariance information in ENDF files for charged-particle induced evaluations
Timeline for following evaluations:

^{7}Be evaluation
^{15}N evaluation (n+^{14}N)
^{17}O evaluation

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<tr><td></td><td>Drafting of the meeting summary report</td></tr>
<tr><td></td><td>Closing of the meeting</td></tr>
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PARTICIPANTS

Country		Name	Surname	Affiliation	Email
AUSTRIA		Helmut	LEEB	Technical University Vienna	helmut.leeb@tuwien.ac.at
		Thomas	SRDINKO	Technical University Vienna	thomas.srdinko@tuwien.ac.at
CHINA	🎧	Zhenpeng	CHEN	Tsinghua University	zhpchen@mail.tsinghua.edu.cn
FRANCE	🎧	Pierre	TAMAGNO	Commissariat à l'énergie atomique et aux énergies alternatives	pierre.tamagno@cea.fr
USA	🎧	Ian	THOMPSON	Lawrence Livermore National Laboratory	thompson97@llnl.gov
	🎧	Gerald	HALE	Los Alamos National Laboratory	ghale@lanl.gov
	🎧	Mark	PARIS	Los Alamos National Laboratory	mparis@lanl.gov
	🎧	Goran	ARBANAS	Oakridge National Laboratory	arbanasg@ornl.gov
		Marco	PIGNI	Oakridge National Laboratory	pignimt@ornl.gov
		Richard	deBOER	University of Notre Dame	richard.j.deboer.12@nd.edu
	🎧	Carl	BRUNE	Ohio Universtiy	brune@ohio.edu
INT. ORGANIZATION	🎧	Stefan	KOPECKY	EC / Joint Research Centre	stefan.kopecky@ec.europa.eu
	🎧	Daniela	FOLIGNO	OECD Nuclear Energy Agency	daniela.foligno@oecd-nea.org
	🎧	Andrew	HOLCOMB	OECD Nuclear Energy Agency	andrew.holcomb@oecd-nea.org
		Paraskevi (Vivian)	DIMITRIOU	International Atomic Energy Agency	p.dimitriou@iaea.org

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: https://nds.iaea.org