

INDC International Nuclear Data Committee

International Nuclear Data Evaluation Network (INDEN) on the Evaluation of Light Elements (4)

Summary Report of the IAEA Consultants' Meetings

IAEA Headquarters, Vienna, Austria
20-23 June 2022

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

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

Paraskevi Dimitriou
International Atomic Energy Agency
Vienna, Austria

February 2023

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or to:

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Printed by the IAEA in Austria

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ABSTRACT

The INDEN for Light Elements network (INDEN-LE) held a Consultants' Meeting from 20 to 23 June 2022, 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.

February 2023

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1. Introduction

The IAEA Nuclear Data Section is coordinating an international effort to (i) compare and verify existing R-matrix codes on charged-particle reactions in the resolved resonance region, (ii) produce evaluations of charged-particle cross sections for applications and, finally, (iii) disseminate the evaluated data through general and special purpose nuclear data libraries.

Six IAEA consultants' meetings have been held since the start of this project, to address the capabilities of existing R-matrix codes and the translatability of the corresponding R-matrix calculations. So far, three exercises have been performed, the first one on an inter-comparison of R-matrix algorithms implemented in the codes, published in Ref. [1], the second on the inter-comparison of minimization techniques and fitting procedures applied by the evaluators, and the third and final one on the evaluation of the ${}^7\text{Be}$ system. The exercises involved the two incident channels ${}^3\text{He}+{}^4\text{He}$ and $p+{}^6\text{Li}$ forming the ${}^7\text{Be}$ compound system at sufficiently low excitation energies to exclude other reaction channels. Details of the exercises, the results as well as additional comparisons that were performed, can be found in the summary reports of the six meetings:

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/>)

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. The network activities are split into three groups focusing on nuclear data for actinides (and heavy elements), structural materials and light elements, respectively (see also: [TM IAECIELO](#)). 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 ([TM IAECIELO](#)): neutrons on ${}^9\text{Be}$, ${}^{14,15}\text{N}$, ${}^{23}\text{Na}$. These four light systems as well as (α,n) reactions on F and O isotopes, which are of particular interest in the field of spent fuel management, and the re-investigation of neutrons on ${}^{16}\text{O}$ following the conclusions of the CIELO project, were discussed at the first meeting on the Evaluation of Light Elements (INDEN-LE) which was held from 30 to 31 August 2018, and a work plan was agreed among participants ([INDC\(NDS\)-0768](#)). The subsequent two INDEN-LE meetings were held in 2019, and 2021, and the corresponding summary reports were published as:

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/>)

The seventh R-matrix codes and fourth INDEN-LE meetings were held back-to-back from 20 to 23 March 2022, at the IAEA Headquarters, Vienna. The meetings were hybrid with a virtual component, and were attended by: H. Leeb, B. Raab, T. Srdinko (Austria); Z. Chen, Jie Liu (China); P. Tamagno (France); S. Kunieda (Japan); G. Arbanas, C. Brune, R.J. deBoer, G. Hale, M. Paris, M. Pigni,

I.J. Thompson (USA); S. Kopecky (EC), making a total of 17 participants from five member states (MS) and one international organization, including IAEA staff P. Dimitriou (Scientific Secretary) and R. Capote (NDS Deputy Section Head).

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. Ian Thompson and Helmut Leeb were elected chairs of the meeting and R. James DeBoer and Marco Pigni the rapporteurs. The meeting continued with status reports and presentations by the participants, followed by technical discussions.

The summaries of the presentations are given in Section 2, while the summaries of the technical discussions are provided in Sections 3 and 4. The adopted Agenda and List of Participants are given in Annexes 1 and 2, respectively. Links to participants' presentations are given in Annex 3.

References:

- [1] I.J. Thompson, R.J. deBoer, P. Dimitriou, et al., Verification of R-matrix calculations for charged-particle reactions in the resolved resonance region for the ^7Be system, *Eur. Phys. J. A* **55** (2019) 92.

2. Presentation Summaries

2.1. Progress in the new reduced R-matrix theory, H. Leeb (TU Vienna)

Efforts are continued to develop a reduced R-matrix analysis to span the range between the RRR and URR region by members of the group (Thomas Srdinko and Tanja Stary). One of the main challenges is the presence of non-binary channels at low energies that dominating in some reaction systems. The method being used is that proposed by Lane and Thomas [1] where unitarity is broken and a reduced R-matrix is defined. The R-matrix is then divided into sub-matrices of a group of channels that can be fit, and a group of channels that cannot. The only approximation that is similar to this approach and has so far been used in nuclear data evaluation, is the Reich-Moore approximation; therefore, it is the first time, that a simplified reduced R-matrix parametrisation has been developed. The current test case is that of $^9\text{Be}+n$, which has a dominant four-body breakup at $E_n \sim 1.66$ MeV and several non-binary channels beyond $E_n = 10$ MeV.

What are the problems with extending the theory to multi-channel breakup channels? The internal wave function is of many-body structure and cannot be determined quantitatively. Because there are more than two particles in the exit channel a finite channel region, essential for R-matrix theory, cannot be defined. Frequently, breakup reactions are approximated as two-step processes, assuming that the intermediate state has a long decay time. This works well as long as it is not a dominant channel. Long-range interactions become problematic. Breakup reactions have been approximated and calculated as two-step processes of two-particle channels by Mark Paris and Gerry Hale. Secondary gamma rays are determined using the same approach.

What is the reduced R-matrix? Because only part of the open channels are explicitly considered in the reduced R-matrix analysis, the corresponding S-matrix is of reduced dimension and not unitary. Consequently, the reduced R-matrix is complex-valued. The imaginary part of the reduced R-matrix describes the flux loss into not included channels similarly to the imaginary part of an optical potential.

Can we calculate the cross sections for ignored states? We divide the standard R-matrix into a solvable part, and a part we cannot solve. If the solvable part does not contain all open channels, the corresponding S-matrix is not unitary. We end up with a reduced R-matrix that has an additional logarithmic derivative (L) in the denominator.

What is L? The logarithmic derivative L is a complex entity and consists of the shift factor (real part) and the penetration factor (imaginary part). The logarithmic derivative L becomes real below the threshold of the considered channel. The form of the reduced R-matrix has been derived for a case with one pole and an arbitrary number of channels. The two-pole solution has also been worked out. We assume that the one-pole approximation works well for separated resonances (no interference). We have suggested this form for the reduced R-matrix, but for an arbitrary number of poles its applicability has not been proven mathematically.

We have applied this to the four-body break up of $n+{}^9\text{Be} \rightarrow \alpha + \alpha + n + n$, assuming we have ${}^9\text{Be}(n,n)$, ${}^9\text{Be}(n,\alpha)$, and ${}^9\text{Be}(n,n')$ channels. The break-up channel is ignored but we can calculate the cross section of the ignored channel. We defined a unitarity defect parameter to determine the cross section of this break-up channel.

Comment: The L&T approach is a "sequential decay" model, in which each step is treated as a two-body process. Our (LANL) approach in SPECT is a three-body resonance model, in which three-body kinematics are used, and recently are being made relativistic.

From the comparisons with existing experimental data, we see that the elastic differential cross sections are reasonable, but still need some work. The $n+{}^9\text{Be}$ system is roughly described, but a lot of work is still needed.

We have also applied the reduced R-matrix method to the ${}^6\text{Li}+n$ system, which is an easier system. The breakup channel is at $E_n=1.47$ MeV. For the eliminated channel, the shape is reasonably reproduced, but there is room for improvement. The goal is to reach the level of agreement required for data evaluation. The current fit probably needs more levels than those reported in the ENSDF tables.

Q&A:

- For these reactions, what is the expected relative contribution of direct processes with respect to resonant processes? The motivation for asking is to suggest a parameterization of direct processes within the R-matrix formalism.

Answer 1: Depending on the compound system, both can be important. Broad resonances, which in the R-matrix formalism mock up the effect of direct reactions, modify the phase-space contributions that underlie the narrow resonance structure in the spectra.

Answer 2: So far, we (LANL) have been able to describe the spectra pretty well for the cases we have considered, with combinations of known narrow and broad resonances in the two-body sub-systems of the three-body final states. However, the experimental data in these cases are not known well enough to say anything definite about reaction mechanisms, and we certainly have not considered all cases, even for light nuclei.

References:

- [1] A.M. Lane, R.G. Thomas, R-Matrix Theory of Nuclear Reactions, Rev. Mod. Phys. **30** (1958) 257.

2.2. A novel R-matrix formalism for Three-Body Channels, B. Raab (TU Vienna)

In light nuclear systems, three-body breakup processes may occur even at low energies and contribute significantly to the reaction cross section. Up to now, these channels have been treated approximatively e.g., using the sequential approach, where the total three-body process is considered as two successive two-body processes. However, if the breakup channel dominates the reaction cross section, the use of the approximative method is questionable.

This was the motivation to develop a novel R-matrix formalism which provides a full quantum mechanical treatment of the three-body process based on the Faddeev equations. A first proposal for such a method was presented by W. Glöckle in 1974 [1]. Originally developed for three identical particles, we could generalize the formalism to three arbitrary masses and interactions. Several essential modifications were necessary to apply the three-body R-matrix theory to real nuclear systems. After probing the stability of the algorithm, it was applied on the neutron+deuteron system. We calculated the angle-integrated elastic cross section and the breakup cross section. The results were very promising and described the experimental data very well. However, the calculated experimental cross section data were systematically too low in the energy range above 8 MeV. To solve that problem, we changed the matching radius in R-direction (coordinate of the free spectator particle in the Faddeev-components), to restore continuity in the first derivative of the three-body wave function at the matching radius, which is not originally included in the formalism. This led to matching radii, depending on the incident energy yielding cross sections, in very good agreement with experimental data.

Next, we studied the neutron+⁹Be system which is important e.g., for fusion devices where it serves as a neutron multiplier. The calculated breakup cross section is in good accordance with experimental data up to 4 MeV. Above that energy higher partial waves begin to contribute significantly. However, since our formalism is restricted to s-waves, our results are no longer reliable in this energy range. The elastic cross section exhibited some problems due to the opening of the ⁹Be(n,α)⁶He channel at 0.597 MeV which was not included in our three-body structure.

To our knowledge this is the first available three-body R-matrix formalism which was successfully applied to nuclear systems.

Q&A:

- Do you expect that with this method you will be able to perform a full R-matrix analysis similar to the analysis performed by the standard R-matrix analysis codes?

Answer: This approach is well suited for a calculable R-matrix method.

- Lane and Robson [2] show that there is a delta function in the block operator that allows to pick the boundary conditions arbitrarily.

Answer: If you take the boundary condition with a vanishing derivative, you get a zero derivative at the boundary.

Rebuttal: No, this is not the case if you use integration by parts.

Comment: It is true that the boundary condition does not need to be zero to maintain the orthogonality. The important point is that the boundary condition cannot be energy dependent. In the case of the three-body break up, you need to impose an energy dependent boundary condition.

- Why isn't the low-energy structure reproduced? You have the entrance channel pole.
 Answer: The three-body theory does not have such a pole at low energies. There is no resonance related to the $\alpha+{}^6\text{He}$ system since the ${}^8\text{Be}$ has no structure in our theory.
 Comment: From the point of view of evaluating the experimental data, the resonance observed at low energies needs to be reproduced.
- How do you know that the value of the regulator has converged?
 Answer: We look at the trend of the value and once it reaches a plateau, we assume it has converged.
- What's the physical significance of the regulator?
 Answer: This is a case of an ill-posed problem where you get many solutions (states), but only the first few are physical. The others lead to numerical problems and are not significant. You need to introduce a criterion to cut off the number of states. For example, if you go too far and remove too many states, you may lose physical states which will affect the solution. There is a similar situation in optical models.
 Comment: The R-matrix poles are not all resonances. The R-matrix can describe any process, even a direct process by introducing distant poles. If you could include an infinite number of poles, then you could mockup any type of reaction.
- Is there a better way to parameterize direct reactions in the R-matrix theory?
 Answer: Some attempts were made in the past. Lane and Thomas describe such a procedure extensively in Lane and Thomas mentioned in the previous section 2.1.

References:

- [1] W. Glöckle, R-matrix approach to the 3-body problem, *Z. Phys.* **271** (1974) 31.
- [2] A.M. Lane, D. Robson, *Comprehensive Formalism for Nuclear Reaction Problems. I. Derivation of Existing Reaction Theories*, *Phys. Rev.* **151** (1966) 774.

2.3. Linking optical potentials to resonances at lower energies, I. Thompson (LLNL)

The $n+{}^{14}\text{N}$ system has been used as a test case. Similar work has been done in the past mostly for higher mass. The problem is that one wants to know what gamma rays are produced from neutron-induced reactions. This information is easy to extract from the Hauser-Feshbach (HF) theory at higher energies with overlapping resonances. But it is also possible to derive HF from the R-matrix theory. For HF, we ignore all off-diagonal terms (which is identical to the single-level Breit-Wigner approximation). We use average widths with correction. An optical potential can be used to produce widths if you know the average spacing "D". HF (n, n') cross sections vary smoothly with energy. Users also need to know the cross sections for gamma production, i.e. ($n, n\gamma$). Transfer reactions also produce gamma rays that can be measured for applications. It is quite a demand to make an R-matrix fit up to 14 MeV. An R-matrix with widths sampled over a Porter-Thomas distribution matches fairly well with the HF calculation, but there is a deviation at higher energies. Width fluctuation corrections with HF are needed. A full Porter-Thomas statistics for the reduced width amplitudes used in the R-matrix is needed. Partial waves were used up to rather high values.

Q&A:

- These calculations involve a large number of channels, how practicable are they?
 Answer: I envision a hybrid approach. Comparing theory to data where it is available, and then using some approximation when it is not.

- Is there a way to define some statistical parameters that are more directly related to R-matrix parameters?

Answer: People have been trying to do this for many years, with limited success. HF is the approximation we have now, we want to do something better.

Comment: The HF formulas were created in a time when calculations were limited by calculation power. These constraints do not longer apply, so there may be other ways of doing this.

- Toshihiko Kawano uses the K-matrix instead of the R-matrix [1]. Would this be a better approach?

Answer: The K-matrix theory is formulated in a way that conveniently links to the HF theory.

- Would it make sense to perform the calculations in channel space since the number of channels is very large?

Answer: Maybe.

- Is there any sensitivity to the radius parameter?

Answer: Yes, there could be.

Comment: I found it convenient to use a larger channel radius for the alpha particle (8 to 10 fm) so that the Brune transformation could be successful.

References:

[1] T. Kawano, P. Talou, H.A. Weidenmueller, Phys. Rev. C **92** (2015) 044617.

2.4. Improved evaluation of the ^{17}O system, Z. Chen (Tsinghua University)

Four improvements over the 2021 evaluation were presented:

- KFK white source measurements are considered;
- Parameters in the high energy region (8-30 MeV) are expressed as polynomial + peaks;
- Total widths were calculated;
- ENDF file was produced with 1000 neutron energy points. Problems were encountered with the large covariance matrix.

A reduced total width 8—30 MeV is implemented for

1. $^{16}\text{O}(n,nx)$, $x \geq 5$
2. $^{16}\text{O}(n,ax)$, $x \geq 3$.

KFK white source measurements 0.5—6.2 MeV were included in the fit. A binomial smoothing of the measured data was required so as to use the additional $^{12}\text{C}(n,n)$ differential cross sections. The advantage of the binomial smoothing is that it preserves the peak information in the original form and the width is not changed much. In the valley, the Savitzky-Golay filtering method is used: the weights for the average are larger as the energy is closer to the center point (peak). The extraction of angular distributions from excitation functions is a good constraint for the fit (see appendix).

Present results: the fit from 0 up to 32 MeV considers 186 energy levels and gives good agreement with the measured data. In the fitting process (n,tot) plays a dominant role. Up to 20 MeV the agreement with ENDF/B-VIII.0 is very good. Above 20 MeV, there are some differences.

For elastic scattering, angular distributions play an important role. The agreement with ENDF/B-VIII.0 is similar to the (n,tot) channel.

For the (n,a) channel, the agreement with ENDF/B-VIII.0 is good up to 7 MeV. Between 7—12 MeV there are large differences, but the RAC fit is closer to the measured data. These differences may be explained by the fact that the RAC fitting procedure included all the available experimental data.

For inelastic scattering the agreement with ENDF/B-VIII.0 is reasonably good up to 12 MeV. In the range 12—16 MeV there are large differences. This channel is influenced strongly by data of Boromiza [1]. Above 16 MeV the agreement with ENDF/B-VIII.0 is good.

The (n,p) and (n,n α) evaluated channels are close to ENDF/B-VIII.0.

The evaluation method has been introduced in detail in [2] and is not repeated here. The main feature of RAC is to adopt the χ^2 expression of 'General Least-Squares'(GLS), instead of 'Approximate Least-Squares' (ALS) which is widely used to date. When GLS was used to fit experimental data, the χ^2 was relatively large in the beginning and PPP occurred as a result of the excessively large systematic error. In the process of the RAC evaluation, the χ^2 of GLS and the χ^2 of ALS are displayed at the same time. By carefully adjusting the normalization coefficient and reducing the systematic error as much as possible, the χ^2 (GLS) and χ^2 (ALS) get closer and closer, until they converge. In other words, adopting GLS will force the evaluator to carefully normalize the experimental data, so that the experimental data set can achieve a high degree of internal consistency, and hence obtain the most reliable evaluation value and corresponding covariance matrix.

References:

- [1] M. Boromiza, et al., Phys. Rev. C **101** (2020) 024604
- [2] Zhenpeng Chen, Yeying Sun, A Global Fitting Method with the R-Matrix Code RAC, IAEA report INDC(NDS)-0791, Dec 2019, <https://www-nds.iaea.org/publications/indc/indc-nds-0791/>

2.5. Cross sections of the $^{12}\text{C}(n,\alpha_0)^9\text{Be}$ and $^{12}\text{C}(n,n+3\alpha)$ reactions in the 10-MeV region, J. Liu (Peking University)

Carbon is one of the most widespread elements in nature and organism. The neutron-induced charged-particle emission reactions on carbon in the MeV region are of interest for both nuclear technology applications and nuclear physics theories. Cross sections of the $^{12}\text{C}(n,\alpha_0)^9\text{Be}$ and $^{12}\text{C}(n,n+3\alpha)$ reactions were measured with high accuracy in the neutron energy region of 9.50 – 14.67 MeV using a single crystal chemical vapor deposited (sCVD) diamond detector as an active target. Quasi monoenergetic neutrons were produced through the $^2\text{H}(d,n)^3\text{He}$ reaction based on the HI-13 tandem accelerator and the $^3\text{H}(d,n)^4\text{He}$ reaction based on the Cockcroft-Walton generator at the China Institute of Atomic Energy. The measured pulse height spectra of the diamond detector were compared with those from Monte Carlo simulations to determine the events of the $^{12}\text{C}(n,\alpha_0)^9\text{Be}$ and $^{12}\text{C}(n,n+3\alpha)$ reactions. The cross sections of the two reactions are measured simultaneously, and they can be checked against each other. The *R*-matrix analysis for the $n+^{12}\text{C}$ system was carried out using the RAC code. The calculation results for the (n,tot), (n,el), (n,inl), (n,p), (n,d), (n,g) reactions using the RAC code are consistent with the measurements and evaluations. For the (n, α_0) reaction, as shown in FIG. 1 (a), the calculation results using the RAC code are fitting better with the measurements than the evaluations. The present measurements are in good agreement with the calculation results using the RAC code, which proves the validity of this measurement. For the (n,n+3 α) reaction, as shown in FIG. 1 (b), the calculation results using the RAC code are in good agreement with the present measurements.

Our results are useful in constraining the $^{12}\text{C}(n,\alpha_0)^9\text{Be}$ and $^{12}\text{C}(n,n+3\alpha)$ excitation functions near ten-MeV neutron energy region where large differences exist between the data of previous measurements and evaluations.

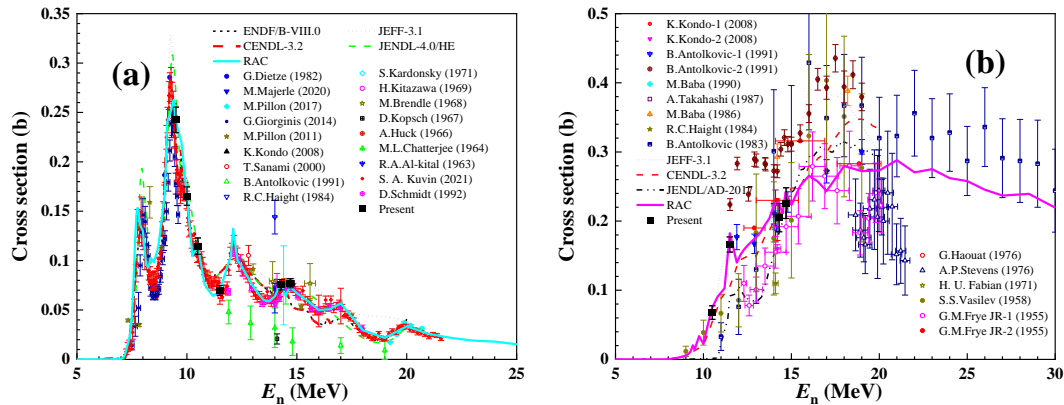


FIG. 1. The cross sections of the $^{12}\text{C}(n,\alpha_0)^9\text{Be}$ (a) and $^{12}\text{C}(n,n+3\alpha)$ (b) reactions.

Q&A:

- The $^{12}\text{C}(n,n+3\alpha)$ reaction can decay in many different ways, including sometimes emitting a triton plus an alpha particle. Sometimes you can think about it as neutron inelastic scattering to an excited state of ^{12}C , so to what extent with your experimental technique are you able to resolve anything about these different final states reaction channels with 3 alpha particles?

Answer: Based on our experimental technique using a diamond detector, the different branch channels of the $^{12}\text{C}(n, n+3\alpha)$ reaction cannot be separated. In our work, only the total $^{12}\text{C}(n, n+3\alpha)$ cross sections were measured.

Comment: there is a recent publication by Jack Bishop et al. [1] on measurements with the time projection chamber at slightly lower energies from 8 to 10 MeV, where they track and sort out all the produced charged particles. It is a very nice technique because it can separate the different reactions and, in particular, one can measure the direct branching ratio of the decay of the ^{12}C second excited state which is very interesting for studying the triple alpha process. This technique should be considered in the future.

- Are these data available?

Answer: Data are not yet included in EXFOR. And we will submit our manuscript to a journal in future.

References:

[1] J. Bishop, et al., Phys. Rev. C **100** (2019) 034320.

2.6. Evaluation of $^{16}\text{O}+n$ and $^{37}\text{Cl}+n$ systems, M. Pigni (ORNL)

A preliminary fit to the total $^{16}\text{O}+n$ cross section up to 10 MeV has been performed. Background poles (BGPs), specifically $\frac{1}{2}+$, can have a strong impact on the fit over the entire energy range.

- It is suggested that a $\frac{1}{2}+$ BGP should not be used, because the subthreshold $\frac{1}{2}+$ level creates a strong correlation between different $\frac{1}{2}+$ levels throughout the region of the entire fit.
- It is suggested that the Cierjacks data could have a systematic uncertainty as small as 1%.

For $^{37}\text{Cl}+n$, only total neutron cross-section data for $^{\text{nat}}\text{Cl}$ is available. Unfortunately, ^{35}Cl abundance is not negligible. The available (n,p) data are scarce and there are energy regions that have not been well measured. For example, the Harvey natural Cl abundance data have been corrected to just ^{37}Cl abundance. This seems to work on average. Discrepancies are observed between directly measured (n,p₀) data and (n,p) measured via activation.

2.7. New $^{13}\text{C}(\alpha,n)^{16}\text{O}$ measurements and the beginning of a new evaluation for the ^{17}O system, R.J. deBoer (Notre Dame University)

The motivation for nuclear astrophysics are as follows:

- The reaction rate of $^{13}\text{C}(\alpha,n)$ in the energy range between 0.2—0.3 GK is needed for s-process neutron production; 0.2—0.3 Giga Kelvin relates to 0.2 to 0.5 MeV energy (in center of mass).
- $^{13}\text{C}(\alpha,n)^{16}\text{O}$: there is a 20-40% inconsistency among S-factor measured data (as of 2 years ago). This is evident in the normalization issues across the full energy range for $^{13}\text{C}(\alpha,n)$ differential data.

The $^{13}\text{C}(\alpha,n)$ S-factor today includes LUNA, JUNA, and ND measurements leading to two conclusions: Kellogg and Harrisopoulos data are systematically too low and, at the lowest energies, the Drotleff and Heil data are systematically high.

Why are there such large differences in the cross-section magnitude? The reason is the detection efficiency. The calibration of a neutron detector efficiency is more difficult than the calibration in other detectors. The resonance strength for the 1.05 MeV resonance given in the Nuclear Data Project (TUNL) database is low. This is a big problem because it would otherwise be a natural and convenient method of obtaining the target thickness.

New measurements at University of Notre Dame facility:

Measurements were performed with deuterated liquid scintillators with intrinsic efficiency whose curve is flat or slowly varying above 1 MeV. Detailed simulations indicate that corrections for neutron scattering is very significant, especially from the target holder and, resulting in larger uncertainties. Improvements should be made in the future to reduce these effects. The setup that was utilized was designed more for γ -ray experiments.

Large differential datasets (14000 datapoints) in energy (0—7 MeV and angles (0—160 degree) were measured fulfilling the idea of full data range datasets.

Comparison with this data, OU (α,n) (unpublished), and Febbraro (α,n_0) [1] measured data between 2.5-5.5 MeV shows that OU data agrees in shape but not in magnitude (Note: This seems to have been resolved in the few months after the meeting. Again, a result of detector efficiency.). A scaling factor of 1.3 is needed to match ND and Febbraro data when comparable, for instance when there is only the (α,n_0) channel open.

After summing the partial ND cross-section data to get the total, we find a good agreement with scaled OU data although there are a couple of points that are low overall. However, the comparison with Febbraro's data [1] shows some differences in the shape in some points above 5.2 MeV.

Comparison with ENDF/B-VIII.0 for $^{13}\text{C}(\alpha,n_0)$ at zero degree shows good agreement with data below 2.5 MeV and not too good above it.

There is quite a lot of discrepancy among world measured data at 0 degree for $^{13}\text{C}(\alpha, n_0)^{16}\text{O}$. For the total (α, n) cross section comparison, the situation is not too bad for the resonances, but there are a lot of discrepancies in the valleys between the resonances, where the cross section is very small, and in the energy dependencies.

The focus of the fit is on the Febbraro 2020 [1] data for (α, n_0) above 5 MeV incident alpha particle.

Progress has been made in fitting with AZURE2 starting from EDA parameters (in B=-1 and relativistic kinematics) transformed to the Brune basis. The following energy adjustments are reported: -7 keV energy shift is needed for the Cierjacks [2] total neutron data: this is a large correction, but a possible reason may be the $^{27}\text{Al}(n, \alpha)$ calibration. Bair and Hass [3] required more complicated linear corrections. For Harissopulos [4], the uncertainties were inflated to 10% and no energy shift was needed up to 2.6 MeV energy in the CM.

Angular distribution effects related to angular attenuation coefficients lead to energy dependent normalization differences at higher energies.

R-matrix fit to higher energies: there is a good comparison with (n, tot) and (n, α) data and the S-factor of Bair Hass (1973) [3].

There is an Improvement in the uncertainty analysis using Markov-chain Monte Carlo (MCMC). The use of a Monte Carlo sampling has the advantage that one can get the final probability distributions for all the parameters, so it is easy to see if there is a problem related to a background level or something that is statistically insignificant.

Normalization of the data is reported. Some of the resulting chi2 are very small. Cierjacks [2] seems to have a large normalization factor (about 5%). Gerry Hale mentioned Lubitz's comment that the normalization factor should not be larger than 3.5% while Hale got 3.8%. Hale agrees with the energy shift found in this work.

Q&A:

General comment: the new Notre-Dame data are very useful to pin down the ^{16}O cross sections better than before.

Comment on the angular attenuation effects: the expansion of the measured angular distribution in Legendre polynomials should be done in the laboratory system, not in the center of mass system. For gamma rays the difference may be small, but in this case, it may be large.

References:

- [1] M. Febbraro, R.J. deBoer, et al., Phys. Rev. Lett. **125** (2020) 062501.
- [2] S. Cierjacks, et al., Nucl. Instr. Meth. **169** (1980) 185.
- [3] J. K. Bair and F. X. Hass, Phys. Rev. C **7** (1973) 1356.
- [4] S. Harissopulos, H.W. Becker, J.W. Hammer, A. Lagoyannis, C. Rolfs and F. Strieder, Phys. Rev. C **72** (2005) 062801(R).

[2.8. Update of R-matrix evaluations with EDAf90, M. Paris \(LANL\)](#)

A new implementation of the code EDAf90 was presented. A new activity on data evaluation is now underway for the $(n, n\gamma)$ reaction in cooperation with LLNL. Work is underway to add relativistic level parameters to ENDF.

The $\frac{1}{2}+$ levels create the “window” in the $^{16}\text{O}+n$ cross section. This results from strong interference between pole terms.

The level parameters from the LANL fit of $^{16}\text{O}+n$ are mostly in agreement with the TUNL nuclear data library, but there are some differences in the spin-parities.

ENDF/B-VII.1: Assumed Harissopoulos [1] data was correct, and Bair and Haas data was wrong. This caused a 32% reduction in the $^{16}\text{O}(n,\alpha)$ evaluation from ENDF/B-VI.

New channels have been added to the evaluation as it is extended to higher energies: (α,n_1) and (α,n_2) . The Nelson (n,n_2) data [2] have been added for example. Normalizations between different data sets are typically within 10%. The lowest energy LUNA and JUNA data are below the current fit. A complete evaluation up to 7 MeV neutron energy is underway.

The full set of parameters that are required to reproduce the fit will be provided.

Q&A:

Comments:

- There is a place to put boundary conditions in ENDF.
- The Shouky (n,n) data [3] are not included currently, because they were previously found not to be consistent.
- There are a lot of other angular distributions besides Shouky that seem to be in better agreement.
- The LANL group is working to put all of their data base in EXFOR, but they also need to include information on the systematic uncertainties and other experimental details.
- There is already a correction system in EXFOR. It accepts energy shifts and renormalizations.
- If the metadata information from the EDA fit is not stored somewhere, it will be lost.
- Could the neutron ANC of the bound state help constrain the $\frac{1}{2}+$ non-resonant contribution?
Answer: ANC information is not yet included in the EDA analysis, but perhaps could be thought about.

References:

- [1] S. Harissopoulos, H.W. Becker, J.W. Hammer, A. Lagoyannis, C. Rolfs and F. Strieder, Phys. Rev. C **72** (2005) 062801(R).
- [2] R.O. Nelson, et al., Nucl. Sci. Eng. **138** (2001) 105.
- [3] I. Schouky, Kernforschungszentrum Karlsruhe Report, KFK-2503, 1977.

2.9. Evaluation of light nuclei for JENDL-5 from R-matrix analysis with AMUR, S. Kunieda (JAEA)

JENDL-5 was released at the end of 2021. The new JENDL logo was made by Satoshi Kunieda himself. No major developments have been made in the AMUR code in the last 3 years due to the unavailability of the developer. An important technical improvement is that an energy resolution for angular distributions has been implemented and found to be impactful yet computationally intensive.

Due to the fact that molten salt reactors could contain LiF compounds, there is interest in the $n+^{19}\text{F}$ system. In the previous evaluation, there were issues fitting the Elwyn angular distribution data. However, the experimental energy resolution was not taken into account although it is rather large, i.e. 100 keV FWHM. Using the new energy resolution routine in AMUR, the fit has been greatly improved. The

JENDL-5 evaluation has been improved with respect to JENDL-4 by moving from a Breit-Wigner calculation to an R-matrix analysis. In the actual JENDL-5 file only the angular distribution part (DA) was replaced with the new R-matrix analysis. This had a significant and systematic impact on neutronics calculations (criticality simulation) of k_{eff} .

For Nitride fuel sources, both ^{14}N and ^{15}N isotopes are needed, even though ^{15}N is only 0.37% abundant. The AMUR fit looks very good, but there are only 3 data sets available. The differential data require a 16% normalization factor.

In the case of the $^{13}\text{C}(n,\gamma)$ reaction, the fit to the angular distribution data required contribution from a distant pole, which could be mimicking direct capture. The different “blocks” in the covariance matrices correspond to the different energy ranges of evaluated data from R-matrix analysis and of experimental data, respectively. R-matrix resonance parameters are not included in JENDL-5, but they can be provided to the group upon request.

2.10. Evaluation of $^{19}\text{F}(\alpha,n)$: first steps, P. Dimitriou (IAEA)

This reaction is important for non-destructive assay analysis using (α,n) reactions with up to 6.5 MeV alpha energy. It is also needed to model backgrounds for rare event experiments at energies up to 9 MeV. Only a few data sets exist for alpha-induced reactions and there are discrepancies between the different (α,n) data. A first attempt to fit the Wrean (α,n) data [1] gives reasonable results; however, the issue is that the structure of the compound nucleus ^{23}Na is unknown at those excitation energies. As a result, some of the spin-parity assignments were deduced from the fit to the cross-section data. Statistical model calculations using the Talys code reproduce the average cross section, doing a bit better than JENDL. An estimate of the model uncertainties resulting from the different models available in Talys was given. The (α,α) data cannot be reproduced by existing alpha optical potentials. Overall, the experimental data for this system are scarce and in poor agreement. Additional measurements are highly recommended.

References:

[1] P.R. Wrean, et al., Phys. Rev. C **62** (2000) 055805.

2.11. Overview of ^{16}O , R. Capote (IAEA)

A dramatic increase in neutron absorption is observed, mainly in the (n,α) reaction channel, when going from ENDF/B-VII.1 to ENDF/B-VIII.0. The increased absorption impacts selected criticality benchmarks and dosimetric response in shielding (deep penetration benchmark). Two sets of oxygen evaluations are used in the validation exercise. One is based on the JENDL-AN or JENDL-HE release that can be tracked down as one of the earliest ENDF/B-VI releases. The other one is ENDF/B-VII.1.

Regarding scaling factors for measured data, a comparison of the total cross shows that the RPI measurements scale with the ENDF/B-VII.1 results within a factor of 0.996 which agrees with the scaling factor of more than -3% obtained from Cierjacks 1980 data [1].

A comparison of the results for the (α,n) channel above 5–6 MeV shows that the main difference among ENDF/B-VII.1, ENDF/B-VIII.0 and the INDEN oxygen evaluation (composed by JENDL as described above) is in the energy region above the first excited state and up to 9 MeV.

The normalization of measured data below 5 MeV is based on the results of Urllass et al. [2]. A comparison with the (n,α_0) data of Prusachenko et al. [3] shows that while these data are generally consistent with ENDF/B-VIII.0.

Results from benchmark calculations of the thermal solution of ^{235}U testing the two oxygen evaluations, INDEN 24a (^{16}O ENDF/B-VIII.0) and 24b (^{16}O INDEN), were presented. The largest differences are found above 0.45 ATLF (above thermal leakage fraction), i.e. for larger solutions rather than the other solutions related to smaller ATLF. INDEN 24b seems to have a larger deviation than INDEN 24a. The same trend is found for ^{239}Pu thermal solutions, i.e. larger impact on solution with large ATLF.

In the reactor core simulations: according to the reactor core scheme, neutrons interact first with Al, then measurements (of number of neutrons per fission per second per cm²) are performed in the two water sections and in the PV simulator.

Results for PCA shielding benchmarks were presented showing $^{27}\text{Al}(n,\alpha)$ as function of the penetration depth. The impact of the two evaluations 24a and 24b is clearly seen, with the INDEN (24b) evaluation showing better agreement except for one benchmark for which 24a performs better. These benchmarks are particularly sensitive to neutron energies above 6 MeV (at which $^{27}\text{Al}(n,\alpha)$ is a dosimetry reaction). For $^{238}\text{U}(n,f)$ the results also seem to favor the INDEN evaluation despite the underestimation of the calculated reactions.

Then main conclusion is that a new ^{16}O evaluation is needed above 5 MeV.

References:

- [1] S. Cierjacks, et al., Nucl. Instr. Meth. **169** (1980) 185.
- [2] S. Urllass, et al., EPJ Web of Conferences **239** (2020) 01030.
- [3] P.S. Prusachenko, T.L. Bobrovsky, I.P. Bondarenko, et al., Measurement of the cross section for the $^{13}\text{C}(\alpha,n)^{16}\text{O}$ reaction and determination of the cross section for the $^{16}\text{O}(n,\alpha)^{13}\text{C}$ reaction, Phys. Rev. C **105** (2022) 024612.

3. The ^7Be system

The discussion focused on the full evaluation of the ^7Be system up to 20 MeV. The following issues were raised:

- ENDF-6 format:

Relativistic kinematics is now defined in ENDF-6 format.

The reference channel is the first in the list of channels and the list goes from lowest mass to highest mass. In current practice, the first channel is often the Reich-Moore channel. LRF=7 is R-matrix unlimited. Partition pairs (PPI) can be in any order for KRM = 4, while for KRM=3, the first channel is always gamma.

Currently, relativistic kinematics cannot be used in conjunction with the Reich-Moore approach in ENDF-6. Therefore, there is still an option to use non-relativistic kinematics for the evaluation.

Action on M. Paris: Create an example showing the effect of relativistic kinematics.

- Metadata is an important part of the output of an evaluation.

The metadata describing the evaluation, the parameters, and the data that were used, should be provided in the same folder or file. Provision of metadata enables the exchange of data and parameters allowing the evaluation to be tested and validated.

– ⁷Be evaluation:

The goal should be to submit an evaluation of ⁷Be that is of better quality than what is available. Gamma rays should be included.

The covariance matrix calculation and comparison should be deferred to the end of the exercise when a full evaluation is available.

In a follow-up meeting that was held on 1 September 2022 at the IAEA Headquarters, the conditions of the evaluation of ⁷Be were revised as follows:

Test 3 – Full evaluation of ⁷Be compound system

[Summary of discussions of the follow-up meeting held on 01-09-2022.
Present: P. Dimitriou, H. Leeb, M. Pigni, I. Thompson]

The conditions for performing a full evaluation of ⁷Be have been laid out at previous meetings and are mentioned in the corresponding meeting reports (INDC(NDS)-0787; INDC(NDS)-0827).

Herein we repeat the specifications of the exercise and list the requirements for submitting a final evaluation for discussion at the next INDEN-LE meeting and consideration for ENDF/B-8.1.

Three incident channels will be considered according to the experimental data available in EXFOR:

$p+^6\text{Li}$, $E_x = 11.5$ MeV at least ($E_p \approx 7$ MeV (lab));

$^3\text{He}+^4\text{He}$, $E_x = 11.5$ MeV at least ($E_{^3\text{He}} \approx 23$ MeV (lab));

$^4\text{He}+^3\text{He}$, $E_x = 11.5$ MeV at least ($E_{^4\text{He}} \approx 17$ MeV (lab)).

All outgoing channels including gamma channels should be considered if possible.

a. Experimental data

All EXFOR data files (and others) compiled by I. Thompson and available on GitHub and on Shared OneDrive will be used. A csv file with metadata is also available (dataprop.csv).

Additionally, data files provided by James deBoer and Zhenpeng Chen (also available on GitHub and Shared OneDrive), should also be consulted and used.

Note: deBoer data files do not contain any metadata (units, type of data, etc.)

b. Input resonance energies, widths, spins and parities

This information will be taken from TUNL website, and if additional data are needed in the higher excitation energies, theoretical values will be used. Ian Thompson will provide shell-model calculations.

c. Output data (to be provided by evaluators)

- Chi²/dof
- Resonance parameter (RP) files

- Reconstructed cross-section files
 - Use Legendre expansions for elastic scattering charged-particle angular distributions - if possible
 - Covariances of RP and/or reconstructed cross sections (ENDF6 specifications)
 - List of data normalizations
 - Experimental data - metadata (whatever modifications have been implemented)
- d. Requirement for participation in INDEN evaluation**
- To provide all output listed in (c) by agreed deadlines
- e. Actions and Deadlines**
- January 2023 **online** meeting: present evaluations; obtain feedback.
[Sec. note: an online poll resulted in the following dates for the online meeting: 13-16 February 2023]
 - Provide all output data listed in (c) – evaluators could use this information to improve their own evaluation (at or immediately after February meeting)
 - INDEN-LE **hybrid** meeting (Spring 2023: dates tbd): agree on final INDEN evaluation.
 - Submit to CSEWG

4. Technical discussions

The following groups are interested in performing or have performed a new evaluation of the $n+^{16}\text{O}$ system: LANL, Tsinghua, ORNL, TUW, ND (limited energy), JAEA.

Though the different evaluators take different approaches, they all have to produce resonance parameter files and cross-section files that can be submitted to CSEWG for consideration for ENDF/B-VIII.1.

The first step in the evaluation is to resolve the discrepancies observed between the different data sets using energy-independent normalization factors, preferably.

Action on James deBoer: examine the renormalization of all new data sets (Prusachenko, Lenz, OU, new ND).

LANL has used the χ^2 distribution to eliminate spurious parameters in a χ^2 fit. Issues with very small uncertainties have been somewhat relieved by this correction. This approximately corresponds to scaling up the $\Delta\chi^2$ value by the square root of the number of fit parameters, e.g. for 100 parameters $\Delta\chi^2$ would get increased by 10.

ORNL aims at providing resonance parameters for ENDF/B-VIII.1 using the $B=-l$ boundary condition. They will produce test files that will be used by the various processing codes to check and resolve any arising processing issues and finally, arrive at a fully processable resonance parameter file that can be validated. This of course, presupposes that Fudge, NJOY, NPEX, etc. are updated to treat the $B=-l$ basis.

Other remarks:

- A full evaluation of the ^{10}Be system was completed at Tsinghua University. The question is how to produce ENDF-6 files and furthermore, how to reproduce the double differential cross section data which are important for applications.
- Thermal capture data for the $n+^{23}\text{Na}$ system seem to converge.
- New measurements of $n+^{\text{nat}}\text{N}$ have been made in Dresden that seem to agree with the previous ORNL data.
- There is a new project on measurements and evaluations of $(n,n'\gamma)$ data involving LANL and LLNL among other institutions. Another topic of the project is bridging the RRR and URR. The project also involves machine learning.
 - Both primary and secondary gammas are important for many applications. Primary gammas are of interest because they are often higher energy, therefore above the natural background, see for example the SBEND collaboration.
 - The list of materials of interest includes carbon, oxygen, and nitrogen. The goals overlap considerably with the goals of INDEN-LE, with emphasis on inelastic scattering whereas capture gamma rays are of secondary focus.

Given that many different evaluation efforts are currently underway due to the planned release of ENDF/B-VIII.1 and JEFF0-4 in 2024, it was decided to organize a virtual meeting in early 2023 to discuss the status of the evaluations of ^{10}Be and ^{17}O evaluation. There was a proposal to include the ATOMKI group for 1 day in this virtual meeting to discuss their high-energy $^3\text{He}(\alpha,\gamma)$ measurements.

ND2022 paper:

An invited talk (P. Dimitriou) will be given at ND2022 covering the work on R-matrix codes for charged-particle reactions and INDEN-LE. Participants were asked to provide 1 or 2 slides on their activities to include in the presentation. Separate talks will be given by Ian Thompson on the Ferdinand translation code, Helmut Leeb on the reduced R-matrix approach, James deBoer on $^{13}\text{C}(\alpha,n)$ data, I. Thompson on RRR to URR, M. Paris and G. Hale on the ongoing evaluations and development of SPEC, S. Kunieda on the evaluation of $^{15}\text{N}+n$ and $^3\text{He}+\alpha$, and Zhenpeng Chen on his evaluations.

ANNEX 1

ADOPTED AGENDA

Monday, 20 June (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) <i>Breaks as needed</i>	
	H. Leeb	Progress in new reduced R-matrix theory
	B. Raab	R-matrix formalism for 3-body channels
	I. Thompson	Linking optical potentials to resonances at lower energies
	Discussion	

Tuesday, 21 June (14:00 – 18:00, open 13:45 Vienna time)

14:00	Participants' Presentations cont' (60' each w/ discussion) <i>Breaks as needed</i>	
	Z. Chen	Improved evaluation of ^{17}O system
	J. Liu	Cross section measurements of the $^{12}\text{C}(n, \alpha_0)^9\text{Be}$ and $^{12}\text{C}(n, n+3\alpha)$ reactions in the MeV region
	M. Pigni	Progress on $n+^{16}\text{O}$ R-matrix evaluation and analysis on the $^{35}\text{Cl}(n, p)$ reaction channel
	R. deBoer	New $^{13}\text{C}(a, n)^{16}\text{O}$ measurements and the beginnings of a new evaluation of the ^{17}O system
	Discussion	

Wednesday, 22 June (14:00 – 18:00, open 13:45 Vienna time)

14:00	Participants' Presentations cont' (60' each w/ discussion) <i>Breaks as needed</i>	
	S. Kunieda	Evaluation on light-nuclei for JENDL-5 - from R-matrix works with AMUR
	P. Dimitriou	Progress report
	M. Paris	Update of R-matrix evaluations with EDAf90
	Discussion	

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

Thursday, 23 June (14:00 – 18:00, open 13:45 Vienna time)

14:00	Round Table Discussion <i>Breaks as needed</i>	
	<ul style="list-style-type: none"> • ^7Be evaluation • ^{17}O evaluation • Treatment of uncertainties • Depletion benchmarks in $n+^{16}\text{O}$ evaluation • $^{35}\text{Cl}(n, p)$ experimental data • ND2022 paper 	
	Drafting of the meeting summary report	
	Closing of the meeting	











ANNEX 2

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

20 – 23 June 2022

IAEA, Vienna

PARTICIPANTS

Country	Name	Surname	Affiliation	Email	
AUSTRIA		Helmut	LEEB	Technical University Vienna	helmut.leebe@tuwien.ac.at
		Benedikt	RAAB	Technical University Vienna	benedikt.raab@tuwien.ac.at
		Thomas	SRDINKO	Technical University Vienna	thomas.srdinko@tuwien.ac.at
CHINA		Zhenpeng	CHEN	Tsinghua University	zhpchen@tsinghua.edu.cn
		Jie	LIU	Peking University	1901110257@pku.edu.cn
JAPAN		Satoshi	KUNIEDA	Japan Atomic Energy Agency	kunieda.satoshi@jaea.go.jp
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	m paris@lanl.gov
		Goran	ARBANAS	Oakridge National Laboratory	arbanasg@ornl.gov
		Marco	PIGNI	Oakridge National Laboratory	pignimt@ornl.gov
		Richard J.	DEBOER	University of Notre Dame	rdeboer1@nd.edu
		Carl	BRUNE	Ohio University	brune@ohio.edu
INT. ORGANIZATION		Stefan	KOPECKY	EC / Joint Research Centre	stefan.kopecky@ec.europa.eu
		Paraskevi (Vivian)	DIMITRIOU	International Atomic Energy Agency	p.dimitriou@iaea.org
		Roberto	CAPOTE	International Atomic Energy Agency	r.capotenoy@iaea.org

ANNEX 3

Presentation Links

#	Author	Title	Link
1	LEEB, Helmut	Progress in new reduced R-matrix theory	INDEN-LE2022_Leeb.pptx
2	RAAB, Benedikt	A novel R-matrix formalism for 3-body channels	INDEN-LE2022_Raab.pptx
3	THOMPSON, Ian	Linking optical potentials to resonances at lower energies	INDEN-LE2022_Thompson.pptx
4	CHEN, Zhenpeng	An improved evaluation of ^{17}O system	INDEN-LE2022_Chen.pdf
5	LIU, Jie	Cross section measurements of the $^{12}\text{C}(n,\alpha_0)^9\text{Be}$ and $^{12}\text{C}(n,n+3\alpha)$ reactions in the ten-MeV region	INDEN-LE2022_Liu.pdf
7	DEBOER, Richard J.	New $^{13}\text{C}(\alpha,n)^{16}\text{O}$ measurements and the beginnings of a new evaluation of the ^{17}O system	INDEN-LE2022_deBoer.pdf
8	CAPOTE, Roberto	Impact of ^{16}O on integral performance	INDEN-LE2022_Capote.pptx
9	HALE, Gerry PARIS, Mark	Update of R-matrix evaluations with EDAf90	INDEN-LE2022_Paris.pdf
10	KUNIEDA, Satoshi	Evaluation on light-nuclei for JENDL-5 - from R-matrix works with AMUR	INDEN-LE2022_Kunieda.pdf
11	DIMITRIOU, Paraskevi	Preliminary work on $^{19}\text{F}(\alpha,n)$	INDEN-LE2022_Dimitriou.pdf

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: <http://www-nds.iaea.org>
