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R-Matrix Codes for Charged-particle Reactions in the Resolved Resonance Region (5)

Summary Report of the Consultants' Meeting
IAEA Headquarters, Vienna, Austria
13-14 May 2019

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September 2019

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ABSTRACT

A Consultants' Meeting was held at the IAEA Headquarters from 13 to 14 May 2019, to discuss the results of a coordinated effort to verify the minimization techniques implemented in the R-matrix codes through a well-defined exercise. Five R-matrix codes were included in this second exercise: AZURE2, CONRAD, EDA, SFRESCOX, and SAMMY. Furthermore, the final exercise which is the evaluation of the ^{7}Be system was agreed upon at this meeting. This report summarizes the presentations and technical discussions of the meeting, as well as any additional actions that were proposed.

September 2019

Contents

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.

The kick-off meeting of this coordinated project was held on 7-9 December 2015 at the IAEA in Vienna. The focus of the first meeting was the identification of specific capabilities of existing R-matrix codes and the translatability of R-matrix calculations produced by the various codes. A summary report of the meeting is published as INDC(NDS)-0703 (https://www-nds.iaea.org/publications/indc/indc-nds-0703/).

In the two subsequent meetings held on 5-7 December 2016 and 28 to 30 June 2017 at the IAEA in Vienna, the working group met to discuss the details and results of a common exercise that was carried out in two parts: the first part aimed at comparing the R-matrix algorithms implemented in the codes (Test 1a), while the second part compared the minimization techniques and fitting procedures applied by the evaluators (Test 1b). The exercises involved fitting the two channels ^{3}He+^{4}He and p+^{6}Li forming the ^{7}Be compound system at sufficiently low excitation energies to exclude other reaction channels. The details of the exercise and results, as well as additional systematic comparisons that resulted from the technical discussions can be found in the summary reports of the meetings, INDC(NDS)-0726 (https://www-nds.iaea.org/publications/indc/indc-nds-0726/) and INDC(NDS)-0737 (https://www-nds.iaea.org/publications/indc/indc-nds-0737/), respectively.

The fourth meeting was held from 27 to 29 August 2018 with the purpose of reviewing the final conclusions of part one (Test 1) and preparing the relevant publication, and finalizing the second exercise (Test 2). The results of Test 1 were published in the article "Verification of R-matrix calculations for charged-particle reactions in the resolved-resonance region for the ^{7}Be system", I.J. Thompson et al., Eur. Phys. J. A (2019) 55: 92; DOI 10.1140/epja/i2019-12753-y.

The fifth meeting was held from 13 to 14 May 2019, to assess the results of Test 2 and to agree on the details of the final exercise (Test 3) which is the evaluation of the compound system ^{7}Be. While only five codes participated in Test 2, namely, AZURE2, CONRAD, EDA, SFRESCO and SAMMY, seven will be involved in the evaluation of ^{7}Be: AZURE2, CONRAD, EDA, GECCCOS, RAC, SFRESCO, SAMMY.

Seven participants from four countries attended the meeting: Z. Chen (People's Rep. of China), R.J. deBoer (USA), H. Leeb (Austria), M. Pigni (USA), T. Srdinko (Austria), I.J. Thompson (USA), G. Hale (USA), P. Tamagno (France) and S. Kopecky (EC), including IAEA staff P. Dimitriou (Scientific Secretary) and R. Capote.

The participants were welcomed to the IAEA by the Nuclear Data Section Head, Arjan Koning. P. Dimitriou briefly introduced the objective and scope of the meeting. I. Thompson was appointed Chairman and H. Leeb rapporteur. After the Agenda was adopted, the meeting continued with participants' presentations according to the Agenda. The meeting agenda and participants' coordinates can be found in Annexes 1 and 2, respectively, while the links to the presentations are given in Annex 3.

2. Test 2

The main aim of Test 2 was to compare the minimization techniques implemented in the different codes, i.e. how the codes reach the local minimum from a given starting point. To test how the different codes perform this basic function, the same compound system ^{7}Be that was used in the previous Test 1 was adopted, and a consistent set of experimental data was selected among the whole set of data retrieved from the EXFOR database for Test 1. One data set was included for each channel ((α,α), (p,p), (α,p) and (p,α)). In addition, using the same input parameters that were adopted in Test 1, the starting input values were defined carefully so that convergence to a fully concave-upward minimum was possible. The minima as well as the covariance matrices would have to be compared. The covariance matrix should also contain the normalisations.

The bound channels were fixed following Hale's prescription, i.e. using boundary condition for bound state B = S(E_{bound}) and for all others B = -L. The matching radii were the same as in Test 1.

Hale and deBoer were responsible for selecting the experimental database and determining the starting parameters of the fit.

The results of Test 2 are summarized in the following.

2.1. AZURE2, Richard J. deBoer, Univ. Notre Dame

Results were presented for Test 2 to compare the fitting procedure used by different codes. AZURE2 uses a χ^2-function to gauge the goodness of the fit. It has contributions from both the fit through the individual data points and a contribution from an overall normalization, where the systematic uncertainty is given from the experiment. To minimize the χ^2-function, AZURE2 uses the MINUIT2 library using the function MnMIGRAD. It is unclear what method is actually used by this function other than that it is a variable metric method. The criterion used by MnMIGRAD is the Estimated Distance to Minimum. For some cases it was found that the default value was too conservative and resulted in the code "grinding" on some parameters for many iterations with very little improvement in χ^2. When the tolerance value was increased from 1 to 100, this resulted in a significant reduction in the number of iterations to achieve a similar value of χ^2. From experience with the current example and others, it has been found that MINUIT2 needs very good starting parameters or it gets stuck in local minima.

Results for AZURE2 for Test 2:

- Did the fit converge? Yes
- Iterations (calls) needed to reach convergence: 4000
- Final χ^2: 3654.67 (points) + 37.68 (systematic)
- Total number of data points: 1874
- Number of free R-matrix parameters: 16

The breakdown of the number of iterations and χ^2 per data set is given below:

filename	reaction	data type	syst. unc. (%)	point χ^2	N	norm	norm χ^2	total χ^2/N
Barnard.dat	^{4}He(^{3}He,^{3}He)^{4}He	dσ/dΩ	5	762.212	810	0.999668	4.40755×10^{-5}	0.94100
Ivanovic.dat	^{4}He(^{3}He,^{3}He)^{4}He	dσ/dΩ	5	194.725	90	1.05072	1.029	2.17529
Spiger_3He3He.dat	^{4}He(^{3}He,^{3}He)^{4}He	dσ/dΩ	1.5	1378.95	488	0.923847	25.7743	2.87853
Spiger_3Hep.dat	^{4}He(^{3}He,p)^{6}Li	dσ/dΩ	1.5	171.869	120	1.02392	2.54213	1.45343
Fiedler.dat	^{6}Li(p,^{3}He)^{4}He	σ	-	11.4024	6	1.47521	-	1.90040
Elwyn.dat	^{6}Li(p,^{3}He)^{4}He	σ	9	7.61053	30	1.09472	1.10758	0.29060
Tumino.dat	^{6}Li(p,^{3}He)^{4}He	σ	-	17.7375	29	1.11946	-	0.61164
Elwyn_dXS.dat	^{6}Li(p,^{3}He)^{4}He	dσ/dΩ	9	490.774	110	1.08493	-	4.47144
Fasoli.dat	^{6}Li(p,p)^{6}Li	dσ/dΩ	-	94.6888	33	0.988927	-	2.86936
McCray.dat	^{6}Li(p,p)^{6}Li	dσ/dΩ	5	434.209	132	1.13445	7.23046	3.34423
Harrison.dat	^{6}Li(p,p)^{6}Li	dσ/dΩ	-	52.8134	26	1.20971	-	2.03128

The final values obtained for the 16 fitted R-matrix parameters are shown in the following table (the bold values are the fitted values while the other parameters were kept fixed):

$J^\pi = 1.5^-$				
E	He3+He4	H1+Li6	H1+Li6	H1+Li6
(MeV)	LS: 1, 1/2	LS: 1, 1/2	LS: 1, 3/2	LS: 3, 3/2
−3.8579830	**−0.85175861**	−0.01150	−1.38640	1.06791
$J^\pi = 0.5^-$				
E	He3+He4	H1+Li6	H1+Li6	
(MeV)	LS: 1, 1/2	LS: 1, 1/2	LS: 1, 3/2	
−14.826003	**−1.2397242**	3.16021	0.71913	
$J^\pi = 3.5^-$				
E	He3+He4	H1+Li6	H1+Li6	H1+Li6
(MeV)	LS: 3, 1/2	LS: 3, 1/2	LS: 3, 3/2	LS: 5, 3/2
−10.912503	**3.4097015**	−1.04027	−9.53490	3.45889
$J^\pi = 2.5^-$				
E	He3+He4	H1+Li6	H1+Li6	H1+Li6
(MeV)	LS: 3, 1/2	LS: 1, 3/2	LS: 3, 1/2	LS: 3, 3/2
7.9057480	**0.41851923**	**1.0493521**	**1.6204186**	**1.1505310**
8.2967806	**−0.63950896**	**0.80826284**	**1.3598557**	**0.0376158**

2.2. CONRAD, Pierre Tamagno, CEA Cadarache

The CONRAD code has joined the group for about a year with the objective of catching up with the group efforts to perform Test1. The CONRAD code was originally developed to deal with neutron-induced reactions mainly on actinides therefore significant changes had to be made in the code in order to cope with charged particles as entrance and exit channels. The neutron/actinides constraining programming choices that were preventing the use of CONRAD for charged-particles-induced reactions have been listed during the meeting. The main changes that had to be introduced were:

- The inclusion of the Coulomb scattering amplitude and the related interference term in the angular-differential cross section.
- The use of user-defined boundary conditions B_c that were neglected so far. The original code choice was to set $B_c = S_c$ which is valid only for neutron channels with l = 0 ($S_c = 0$). This choice for other channels leads to non-orthogonal expansion wave functions in the internal region of the R-matrix theory. The code can now deal with arbitrary boundary conditions, namely $B_c = -L$ that is used in the present group tests.
- The computation of S_c that was neglected in the code so far was thus upgraded in order to treat charged particles and closed channels as these latter were also neglected when treating actinides.

- Some dovetailing modifications in terms of kinematics were also necessary in order to treat non-elastic angular distributions (threshold energy and exit particle masses).
- To prevent having non-unitarity of the collision matrix, the R-matrix and collision matrix sizes are non-longer adjusted to the number of open channels as was done in the past.

The above modifications have removed all the limitations and the CONRAD code can now be used further in the charged-particle reaction evaluation process. To facilitate the treatment of experimental data used by the present group the code was also upgraded to treat data provided in various forms: energies, angles or cross sections provided in the CM or Lab frame. Finally - as the group is focusing on evaluating data related to ^{7}Be compound nucleus and not on separated target and projectile pairs - the code was also updated to treat resonance parameters in the CM (amplitudes and energies scaled) and in the CN frame (energies shifted).

When transforming the input resonance parameters to the CN frame special attention must be paid to the number of significant digits used in the input files in order to have results comparable with results in the Lab frame. As working in the CN frame [will be hazardous] is not recommended when dealing with actinides both possibilities are maintained in the code.

The results for Test2 have been presented in the present meeting. Some differences (up to 17%) have been found in the initial χ^2 quoted in the Test2 instructions paper, yet the final χ^2-value obtained after minimization is close to results obtained by the other group members.

2.3. EDA, Gerry Hale, Los Alamos National Laboratory

Starting from the previously agreed-upon initial parameters and experimental data for Test-2, EDA obtained a solution in 127 iterations (~2160 function evaluations) having an overall χ^2 of 3521 (including normalizations) for 1874 data points (χ^2 per datum=1.879). The breakdown of how this χ^2 is distributed among the data sets is given in the table below:

Data set	Reaction	χ^2_{rel}	Norm	χ^2_{norm}
Barnard $\sigma_{el}(\theta)$	^{4}He(^{3}He,^{3}He)^{4}He	787.6	1.0011	0.00049
Ivanovich $\sigma_{el}(\theta)$	^{4}He(^{3}He,^{3}He)^{4}He	180.2	1.0515	0.95831
Spiger $\sigma_{el}(\theta)$	^{4}He(^{3}He,^{3}He)^{4}He	1308.0	0.92435	29.767
Spiger $\sigma_{r}(\theta)$	^{4}He(^{3}He,p)^{6}Li	169.9	1.0233	2.3028
Fiedler σ_{int}	^{6}Li(p,^{3}He)^{4}He	11.40	1.4770	-
Elwyn σ_{int}	^{6}Li(p,^{3}He)^{4}He	7.49	1.0951	0.93151
Tumino σ_{int}	^{6}Li(p,^{3}He)^{4}He	17.62	1.1190	-
Elwyn $\sigma_{r}(\theta)$	^{6}Li(p,^{3}He)^{4}He	491.03	1.0884	0.81437
Fasoli $\sigma_{el}(\theta)$	^{6}Li(p,p)^{6}Li	109.85	0.98245	-
McCray $\sigma_{el}(\theta)$	^{6}Li(p,p)^{6}Li	322.76	1.1298	5.2812
Harrison $\sigma_{el}(\theta)$	^{6}Li(p,p)^{6}Li	75.31	1.1876	-
	Total	3481.1		40.06

These results are somewhat better than those reported in other searches, and the reason may be that the EDA minimization algorithm terminates only when the modulus of the gradient vector of χ^2 with respect to parameters becomes small enough to ensure that a good solution has been reached. The eigenvalues of the parameter covariance matrix (H-matrix) are all positive, and its condition number, ~3.5 x 10^{-7}, shows that the matrix is not singular,

which are indications of a stable solution. However, the solution covariance matrix gives high correlation coefficients, ρ > 0.9, for some of the parameters, including the eigen-energies of the negative-energy levels with the alpha-particle reduced-width amplitudes of those levels, and several of the parameters of the two closely-spaced $J^{\pi}=5/2^{-}$ levels. These high levels of correlation were even more prevalent when the proton widths in the negative-energy levels were allowed to go free in the search, and they led to unstable solutions with unphysically large parameter values, so we decided to fix them for the remainder of the exercise.

2.4. SFRESCO, Ian J. Thompson, Lawrence Livermore National Laboratory

As originally specified by an email sent to the group on April 25 2019, this Test2 problem had 1874 data points to be fitted by varying 24 of 74 R-matrix parameters, 4 free data scale factors, and 8 scale factors targeted to 1.0 with specified uncertainties. This give 1846 degrees of freedom for the χ^2 fit, in my case performed with Minuit (Version 1) with strategy 2 that attempts to 'Make Sure Minimum True, Errors Correct'.

Although this specification was supposedly chosen to make fitting straightforward, I had problems in finding a converged χ^2-minimum. I found solutions at χ^2/dof = 1.910 , but not a clear minimum, as 4 parameters become large with the energy of the bound $3/2^{-}$ pole tending to –3 GeV! Fixing the parameter at the beginning gave a solution with 1.92, but some proton widths of the bound states still becoming large, and still 4 negative eigenvalues of the covariance matrix. It appears that those widths tend to have canceling effects, so can become large together, as if 'narrow canyons' lead away from apparent χ^2-minima.

The specification sent by email on 6 May 2019 tried to simplify the problem by fixing all the proton widths of the $1/2^{-}$, $3/2^{-}$, and $7/2^{-}$ states, so only 16 R-matrix parameters were to be varied. The simplified specification allowed the fitting algorithm to find a solution with χ^2/dof = 1.94. In the presentation, the R-matrix parameters obtained for B = –L , as well as in the Brune parametrization were shown. Some of the transformations still took many iterations (277 for $1/2^{-}$, and 524 for the $7/2^{-}$ states), indicating that there are still large Shift functions in this formulation. The data sets were well fitted, though the 135 degree Spiger data for ^{3}He+^{4}He scattering was difficult to fit, itself contributing 0.21 to the total χ^2/dof.

2.5. SAMMY, Marco Pigni, Oak Ridge National Laboratory

An important part of Test2 involved the generation of a resonance parameter covariance matrix by fitting a set of selected experimental data. We used SAMMY-8.2b with the following assumptions. The initial set of resonance parameters used to start the Bayesian fitting procedure was converted to the laboratory system together with the fitted experimental data (energy and angle). Additional transformation from ^{6}Li(p,^{3}He)^{4}He to ^{4}He(^{3}He,p)^{6}Li were performed on the experimental data sets since SAMMY-8.2b does not have the capability to include multiple incident channels. Therefore, it was not possible to include in the fitting the measured data for the ^{6}Li(p,p)^{6}Li reaction channel. The initial and fitted resonance parameters are listed below.

In Tables 1 and 2 below the parameters selected for the fit are shown in red.

Table 1. The values of the initial (or prior) set of parameters assumed with an uncertainty of 1.5% on the reduced-widths and a very small uncertainty (<1%) on the resonance energies.

$J^\pi = 0.5^+$				
E	photon+Be7	He4+He3	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 0, 1/2	LS: 0, 1/2	LS: 2, 3/2
5922.0	0.00	−4029.75	−3888.61	−1795.41
$J^\pi = 0.5^-$				
E	photon+Be7	He4+He3	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 1, 1/2	LS: 1, 1/2	LS: 1, 3/2
−5364.6	0.00	−1672.23	4184.76	952.28
5922.0	0.00	1722.53	27.54	−1717.81
$J^\pi = 1.5^-$				
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 1, 1/2	LS: 1, 1/2	LS: 1, 3/2	LS: 3, 3/2
−3089.7	0.00	−1159.43	−15.23	−1835.88	1414.13
4907.1	0.00	−224.63	−1843.84	−3002.46	−1360.26
5922.0	0.00	2147.40	921.92	251.53	1000.41
$J^\pi = 1.5^+$					
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 2, 1/2	LS: 0, 3/2	LS: 2, 1/2	LS: 2, 3/2
4726.0	0.00	39.62	2657.94	616.23	3568.10
5922.0	0.00	2364.12	−545.56	2125.04	−1156.48
$J^\pi = 2.5^+$					
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 2, 1/2	LS: 2, 1/2	LS: 2, 3/2	LS: 4, 3/2
5213.7	0.00	−498.62	1716.45	85.00	−8571.08
5922.0	0.00	−2247.98	−1601.60	140.41	166.88

$J^\pi = 2.5^-$					
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 3, 1/2	LS: 1, 3/2	LS: 3, 1/2	LS: 3, 3/2
3306.8	0.00	653.10	1165.68	841.94	−1587.23
3518.1	0.00	−794.67	1468.36	1268.93	−2620.69
5922.0	0.00	−3045.22	−74.69	−3598.78	1979.46
$J^\pi = 3.5^-$					
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 3, 1/2	LS: 3, 1/2	LS: 3, 3/2	LS: 5, 3/2
−4681.5	0.00	4539.33	−1377.53	−12626.16	4580.28
5922.0	0.00	3747.30	−1151.01	−4907.61	239.24

Initial R-matrix parameters in the B_c=-L_c basis. Pole energies in the lab. frame of ^{3}He (projectile)+^{4}He (target) reaction. Energies $E^{1/2}$ and reduced widths γ_c in units of eV$^{1/2}$ (lab). The fitted parameters are displayed in red.

Table 2. The values of the fitted (or posterior) set of parameters.

$J^\pi = 0.5^+$				
E	photon+Be7	He4+He3	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 0, 1/2	LS: 0, 1/2	LS: 2, 3/2
5922.0	0.00	−4029.75	−3888.61	−1795.41
$J^\pi = 0.5^-$				
E	photon+Be7	He4+He3	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 1, 1/2	LS: 1, 1/2	LS: 1, 3/2
−5364.6	0.00	−1710.22	4184.76	952.28
5922.0	0.00	1722.53	27.54	−1717.81
$J^\pi = 1.5^-$					
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 1, 1/2	LS: 1, 1/2	LS: 1, 3/2	LS: 3, 3/2
−3089.7	0.00	−1176.21	−15.23	−1835.88	1414.13
4907.1	0.00	−224.63	−1843.84	−3002.46	−1360.26
5922.0	0.00	2147.40	921.92	251.53	1000.41
$J^\pi = 1.5^+$					
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 2, 1/2	LS: 0, 3/2	LS: 2, 1/2	LS: 2, 3/2
4726.0	0.00	39.62	2657.94	616.23	3568.10
5922.0	0.00	2364.12	−545.56	2125.04	−1156.48
$J^\pi = 2.5^+$					
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 2, 1/2	LS: 2, 1/2	LS: 2, 3/2	LS: 4, 3/2
5213.7	0.00	−498.62	1716.45	85.00	−8571.08
5922.0	0.00	−2247.98	−1601.60	140.41	166.88

$J^\pi = 2.5^-$					
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 3, 1/2	LS: 1, 3/2	LS: 3, 1/2	LS: 3, 3/2
3306.8	0.00	623.63	1187.30	1000.27	−1790.23
3518.1	0.00	−852.87	1402.31	1537.21	−2522.59
5922.0	0.00	−3045.22	−74.69	−3598.78	1979.46
$J^\pi = 3.5^-$					
E	photon+Be7	He4+He3	H1+Li6	H1+Li6	H1+Li6
(eV$^{1/2}$)	LS: 0, 0	LS: 3, 1/2	LS: 3, 1/2	LS: 3, 3/2	LS: 5, 3/2
−4681.5	0.00	4548.36	−1377.53	−12626.16	4580.28
5922.0	0.00	3747.30	−1151.01	−4907.61	239.24

Fitted R-matrix parameters in the B_c=-L_c basis. Pole energies in the lab. frame of ^{3}He (projectile)+^{4}He (target) reaction. Energies $E^{1/2}$ and reduced widths γ_c in units of eV$^{1/2}$ (lab). The fitted parameters are displayed in red.

The correlation matrix and standard deviations (STD. DEV.) and relative uncertainties (REL.) of the selected 16 parameters (listed in red in the previous tables) is reported below. In the correlation matrix the parameter uncertainties are ordered consecutively such as the values -5364.6, -1710.22, -3089.7, … are the 1st, 2nd, 3rd, …parameters.

***** CORRELATION MATRIX FOR INPUT PARAMETERS

	STD.DEV.	(REL.)	CORRELATION*100														
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1.8640E−02	.000	100														
2	0.2446	.000	3	100													
3	3.2363E−02	.000	0	0	100												
4	0.1162	.000	0	−8	8	100											
5	3.0174E−02	.000	0	0	0	0	100										
6	0.3152	.001	0	8	0	15	29	100									
7	0.7302	.001	0	3	0	−8	−6	−66	100								
8	4.578	.005	0	−2	0	−3	0	−43	38	100							
9	3.638	.002	0	5	0	2	−3	−6	33	76	100						
10	2.8405E−02	.000	0	0	0	0	0	9	−6	0	3	100					
11	0.3843	.000	0	9	0	14	20	98	−67	−42	−5	3	100				
12	0.9802	.001	0	8	0	10	15	71	−18	−20	−5	11	72	100			
13	4.513	.003	0	−2	0	−10	4	23	−11	62	61	1	27	35	100		
14	2.771	.001	0	0	0	−14	−5	−37	60	74	78	−12	−34	−4	64	100	
15	2.0334E−02	.000	0	−10	0	−15	0	−5	2	1	−2	0	−5	−4	0	1	100
16	4.0477E−02	.000	0	−4	0	−9	0	−3	1	1	0	0	−3	−2	2	3	90	100

2.6. The Primary Global fitting for ^{7}Be System, Zhenpeng Chen, Tsinghua University

This report provides the results obtained for the project “R-matrix Codes for Charged-particle Induced Reactions in the Resolved Resonance Region” held by the IAEA, using the evaluation method: RAC-CERNGEPLIS. In fact this method has been used in the evaluation of the neutron-induced reactions n+^{6}Li and n+^{10}B, which were included in the IAEA Neutron Standards (2006 and 2017 release), and in the evaluation of (n+p, n+n, p+p), α+^{12}C, n+^{2}H, n+^{3}H, n+^{3}He, n+^{7}Li, n+^{9}Be, n+^{11}B. The main characteristics of RAC are the inclusion of the eliminated channel width, and the use of the Generalized-Least Square method in the fitting procedure. In a more detailed report, currently in preparation, the different views on R-matrix fitting within the nuclear data evaluation community are discussed. The implementation and results obtained with the RAC-CERNGEPLIS method demonstrate that it is a reasonable, scientific, useful and powerful tool for description of nuclear data.

A global database including all available experimental data for the ^{7}Be system was created. In this database, the ^{6}Li(p, p)^{6}Li and ^{4}He(^{3}He, ^{3}He)^{4}He channels are the most complete and most accurate experimental datasets, which play a dominant role in the fitting; the fitting of ^{6}Li(p, ^{3}He)^{4}He and ^{4}He(^{3}He, p)^{6}Li reactions depends on the ^{6}Li(p, p)^{6}Li and ^{4}He(^{3}He, ^{3}He)^{4}He, of course ^{6}Li(p, ^{3}He)^{4}He and ^{4}He(^{3}He, p)^{6}Li are to a certain extent in competition. For each of the reactions ^{6}Li(p, p_1)^{6}Li*, ^{6}Li(p, p_2)^{6}Li**, ^{6}Li(p, g)^{7}Li, ^{4}He(^{3}He, p_1)^{6}Li, ^{4}He(^{3}He, g)^{7}Li, there is a free parameter, so most of the shape factors are kept as 1.00.

The figures show the results obtained in this work. The comparisons with data have been shown in detail in the previous meeting report (INDC(NDS)-0767). A more comprehensive publication of this evaluation is in preparation (INDC(NDS)-0791).

The evaluation has been performed at incident energies from Ep=0.01 to 20 MeV and for E_{3He}=1 to 20 MeV. The angular distributions DA are calculated from 0.1 degree to 180 degree with step=1 degree.

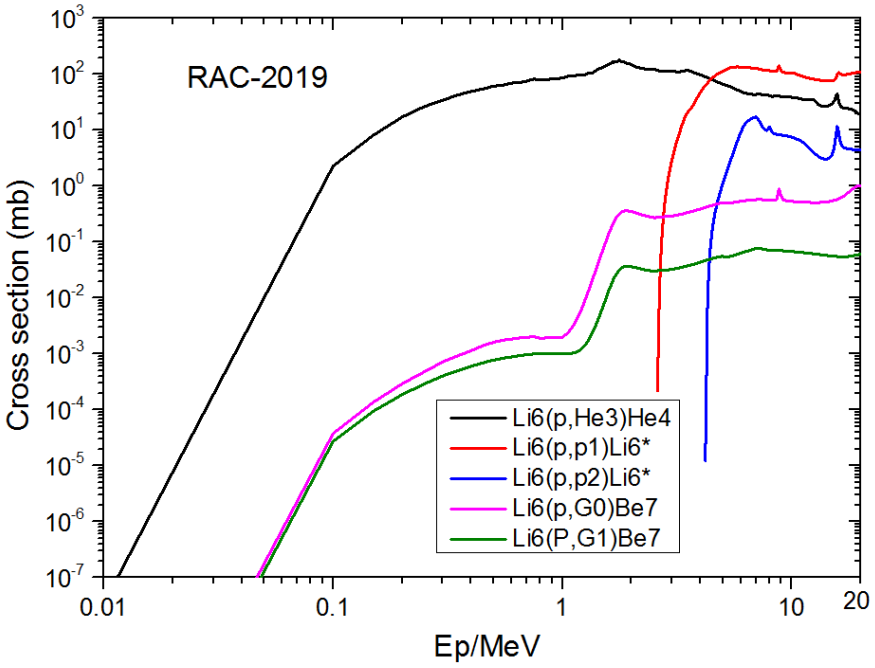

FIG. 1. The CS for p+^{6}Li

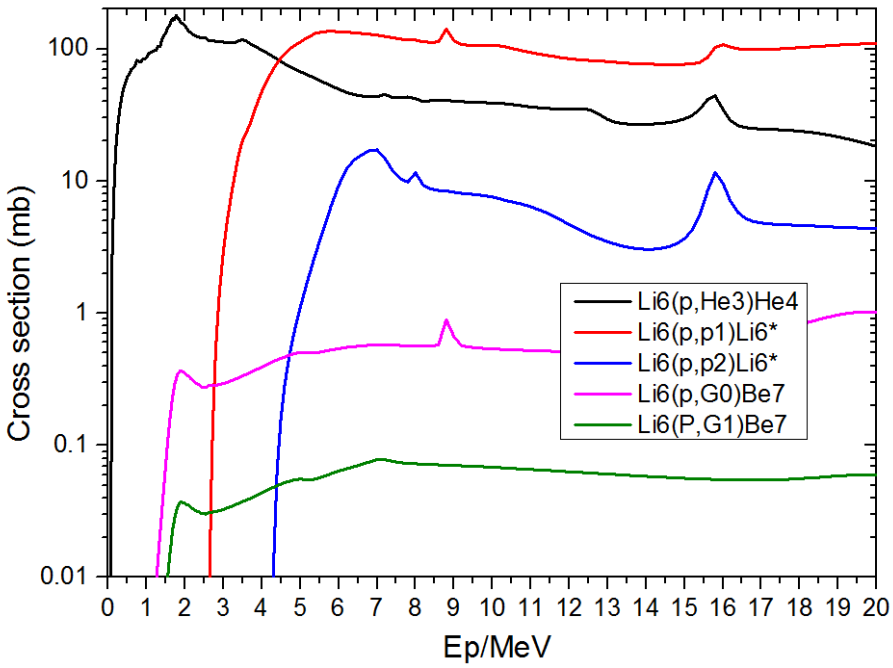

FIG. 2. The CS for p+^{6}Li

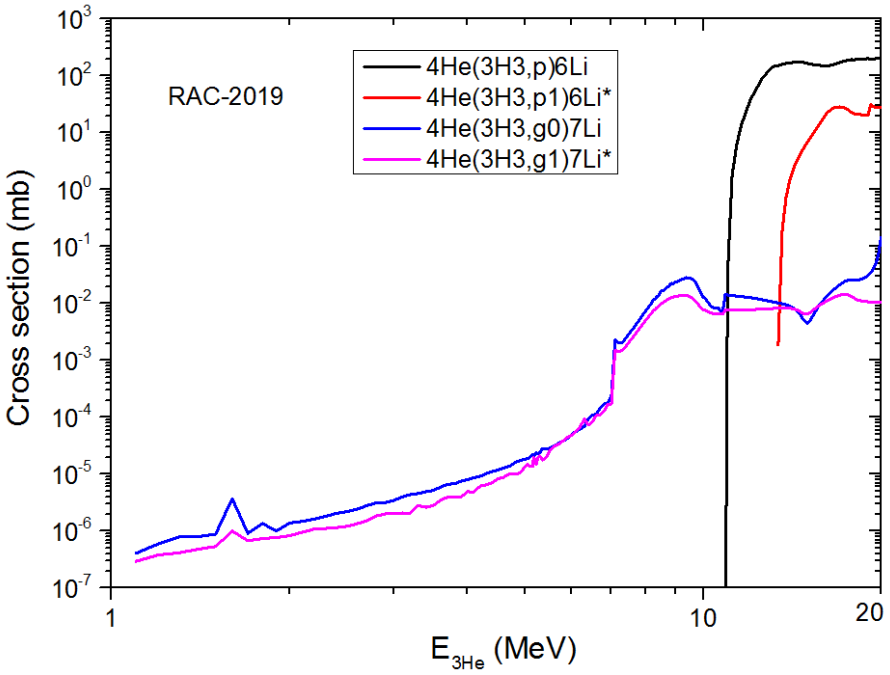

FIG.3. The CS for $^{3}He+^{4}He$

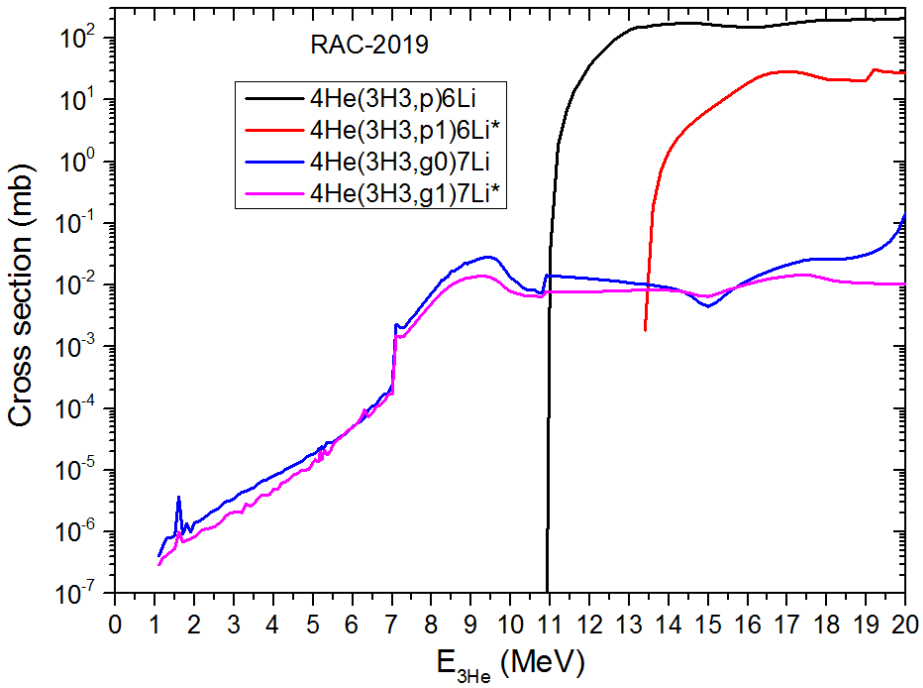

FIG. 4. The CS for $^{3}He+^{4}He$

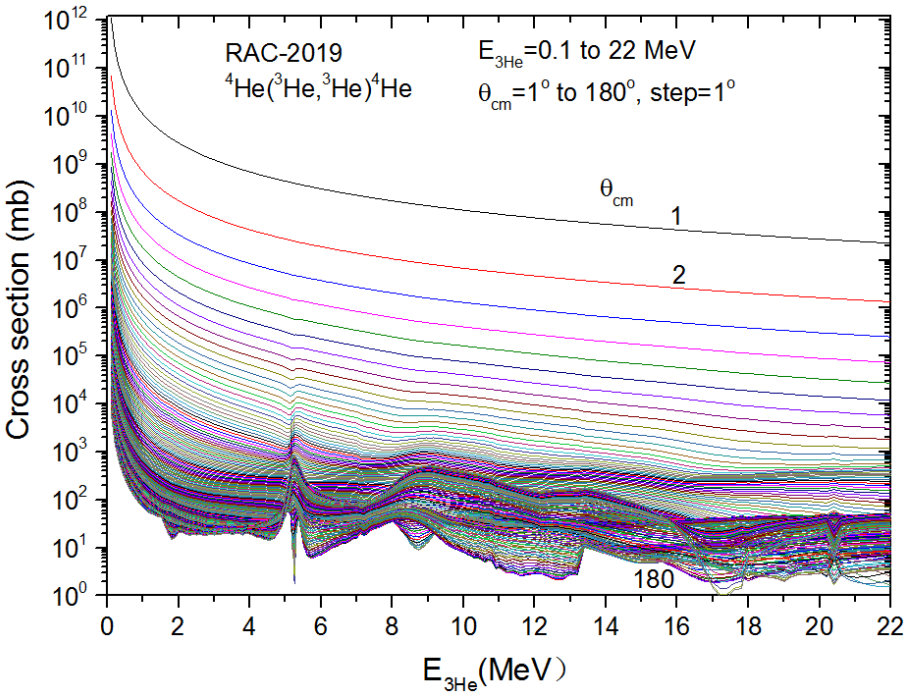

FIG. 5. The DA for p+^{6}Li

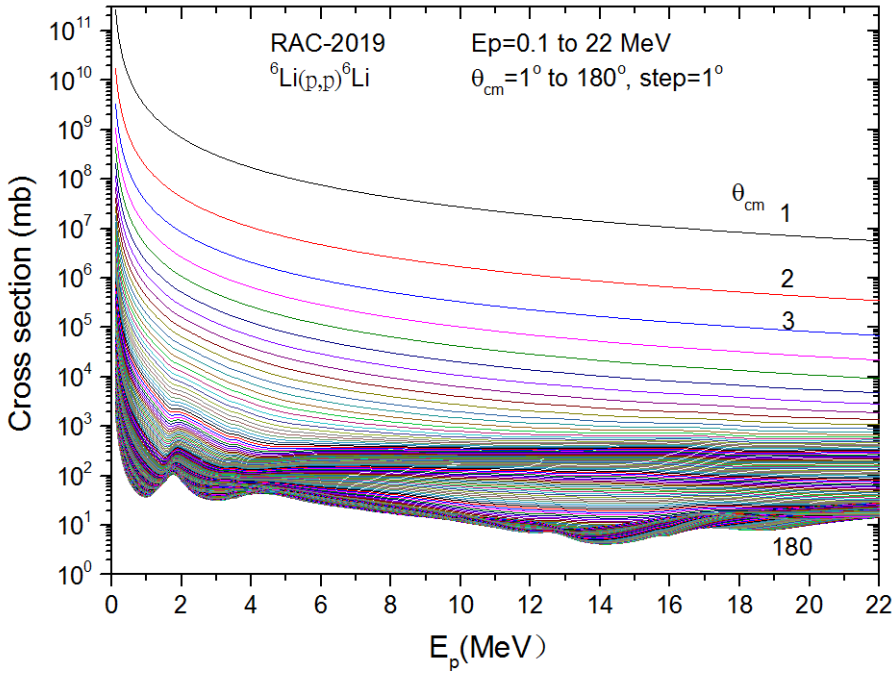

FIG. 6. The DA of ^{3}He+^{4}He

3. Technical discussions

3.1. Finalization of Test 2

In order to finalize Test 2 and to draw conclusions, it was realized that certain quantities and terms need to be defined so as to be used uniformly by the code developers and allow the comparison of the results obtained with the different codes:

- Degrees of freedom: number of experimental points - number of R-matrix parameters - number of unconstrained normalization (unconstrained = no measurement of normalization error)
- Total χ^2-value per data set: sum of χ^2 for each data set + χ^2 for normalization for each data set
- Number of iterations: those with analytical derivatives should estimate their iterations by also taking into account the number of free parameters
- Uncertainties of initial parameters should be specified (without correlations)
- Apart from normalizations, only statistical experimental uncertainties are assumed in Test 2

Comparison of the results of Test 2:

Ian Thompson will collect the input files with final R-matrix parameters and covariances – and will produce File 32. Note to code developers: the covariance matrix should be accompanied by labels! Normalisation should not be considered so a covariance matrix for 16 free parameters should be provided (16x16 matrix). Order of parameters in correlation matrix: should agree with the order of R-matrix parameters provided.

Action on all (AZURE2, CONRAD, EDA, SFRESCO, SAMMY): send the above results of Test 2 to I. Thompson. Deadline: End of October 2019.

Action on I. Thompson: repeat Test 2 using non-rel. and rel. kinematics

The results of Test 2 will be published in an INDC(NDS) report.

3.2. Extension to higher energies

The extension of the R-matrix algorithm to higher energies where more and more channels are open is challenging. Especially if one also considers the break-up channels. Zh. Chen has implemented the Reduced R-matrix theory (A.M. Lane, R.G. Thomas, Rev. Mod. Phys. 30, 257 (1958)) that treats eliminated channels as flux that is absorbed by an imaginary width in the denominator that resembles the role of the imaginary term in the optical potential. In the RAC implementation of the reduced R-matrix theory, this imaginary term is an adjustable parameter for each channel.

Participants have acknowledged the usefulness of the reduced R-matrix theory for treating large number of open channels, but the implementation and consequences for unitarity are still debated. Zh. Chen demonstrated that he can perform a global fit of all available experimental data relevant to the ^{7}Be compound system up to 20 MeV, however, the question remains whether the other codes can reproduce his results using the same input parameters.

I. Thompson has also developed an optical R-matrix model along the lines of the reduced R-matrix but with an eye on keeping unitarity satisfied. A summary of his work is given in INDC(NDS)-0788.

3.3. Test 3 - Evaluation of ^{7}Be

The evaluation of ^{7}Be consists of two separate evaluations: p+^{6}Li for lab projectile energies up to 20 MeV and ^{3}He+^{4}He for lab projectile energies up to 30 MeV. One should use all the available observables: cross sections, differential cross sections, polarisation observables.

For all code developers:

- The R-matrix representation will be applied – up to the highest energy possible: the energy of validity of R-matrix theory needs to be defined. A smooth transition from resonance to statistical regime needs to be established.
- Inclusion of photon channels: (p,γ) and (p,pγ) if data are available.
- Breakup reactions need to be considered in the evaluation
- Relativistic kinematics should be used, if the code allows this option

Problem of breakup reactions

^{3}He+^{4}He, p+^{6}Li: G. Hale has some ideas using hyperspherical harmonics. I. Thompson will use optical R-matrix and also reaction break-up models.

Retrieval of experimental data:

Zh. Chen will provide the EXFOR entries he used in his evaluation. The provided EXFOR entries will be checked and this information will be shared in an IAEA OneDrive repository. All experimental data will be uploaded onto GitHub.

Not specified in this exercise: channel radii, partial waves to be included: these quantities are up to the evaluator – boundary conditions should be chosen depending on the problem (bound states).

Final data files will be produced in the ENDF-6 format: definitely point-wise cross sections (File 3) and covariances (File 33, 34 and 35). If possible resonance-parameter files (File 2) and covariances (File 32) will also be provided.

All evaluated data files will be uploaded onto the GitHub repository that has been created for sharing information on this data development project. The GitHUb repository is called “Be7 Rmatrix Analysis” and is available at

https://github.com/RMACPR/Be7_Rmatrix_Analysis.

A shared folder has also been created by the IAEA on OneDrive so that all participants in the project can access the experimental database and share their R-matrix input and output files, as well as their ENDF-6 files.

Organisational matters

Technical coordinator: Ian Thompson.
Evaluations will be performed by: P. Tamagno, M. Pigni, I. Thompson, H. Leeb, Zh. Chen, G. Hale, J. deBoer, P. Dimitriou.

Duration of ^{7}Be Evaluation: Estimated about 2 years. An interim meeting to discuss issues with data and evaluation: in one year, back-to-back with INDEN.

Action on I. Thompson and G. Hale: to submit proposal to include relativistic kinematics option in ENDF6 format (File 2) to CSEWG.

Action on Zh. Chen: to provide the EXFOR entries he used in his ^{7}Be evaluation.

Action on all: to submit problems with EXFOR entries to IAEA EXFOR contact person (Naohiko Otsuka).

4. Conclusions and Recommendations

The project on R-matrix codes for charged-particle reactions in the resolved-resonance region is in the last stage of verification and validation which consists in performing an evaluation of ^{7}Be. The results of this evaluation will be discussed in a forthcoming meeting and will be published in a peer-reviewed journal.

The meeting participants recommend that this group continues the effort to exchange technical expertise and ideas on the development of R-matrix codes, evaluation methodologies and how to implement them to deliver evaluated data ready for dissemination and use in applications.

The IAEA staff confirmed the commitment on behalf of the IAEA to continuing this project in parallel with INDEN.

5. List of Actions

Item #	Action	Responsible	Deadline
1	Send the final results of Test 2 to Thompson.	All	End of October 2019
2	Repeat Test 2 using non-relativistic and relativistic kinematics	Ian Thompson	tbd
3	Submit proposal to include relativistic kinematics option in ENDF6 format (File 2) to CSEWG	Ian Thompson and Gerry Hale	US Nuclear Data week Nov. 2019
4	Provide the EXFOR entries he used in his ^{7}Be evaluation	Zhenpeng Chen	End of September 2019
5	Submit problems with EXFOR entries to IAEA EXFOR contact person (Naohiko Otsuka).	All	Continuous

Annex 1

Consultants' Meeting on

R-matrix Codes for Charged-particle Reactions in the Resolved Resonance Region (5)

IAEA, Vienna, Austria

13 to 14 May 2019
Meeting Room VIC MOE

ADOPTED AGENDA

Monday, 13 May

08:30 – 09:00 **Registration** (IAEA Registration Desk, Gate 1)

09:00 – 09:30 **Opening Session**

Welcoming address (Arjan Koning, NDS Section Head)
Administrative matters

Election of Chairman and Rapporteur

Adoption of the Agenda

09:30 – 17:30 **Presentations by participants**

Test2 results

1) AZURE2, R. deBoer (Univ. Notre Dame)
2) SFRESCO, I. Thompson (LLNL)
3) SAMMY, M. Pigni (ORNL)
4) EDA, G. Hale (LANL)
5) CONRAD, P. Tamagno (CEA Cadarache)

Discussion-conclusions for Test 2

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

Annex 1

Tuesday, 14 May

09:00 – 17:00 **Evaluation of ^{7}Be**

6) RAC, Z. Chen (Tsinghua Univ.)

Discussion:

- How to proceed
- Timeframe
- Publication of results

Drafting of Summary Report

17:00 – 17:30 **Closing of Meeting**

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

Annex 2

Consultancy Meeting on

R-Matrix Codes for Charged-particle Reactions in the Resolved Resonance Region (5)

13 – 14 May 2019
IAEA, Vienna

Meeting Room VIC MOE

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Annex 2

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Annex 3

Consultancy Meeting on

R-Matrix Codes for Charged-particle Reactions in the Resolved Resonance Region (5)

13 – 14 May 2019

IAEA, Vienna

Meeting Room VIC MOE

Participants' Presentations

#	Author	Title	Link
1	R.J. deBoer	TEST2	PDF
2	I.J. Thompson	Fitting R-matrix models to Test-2 data for A=7 systems	PDF
3	M.T. Pigni	R-Matrix Evaluation for the 7Be compound nucleus	PDF
4	G.Hale	EDA 7Be R-matrix fit for Test-2	PDF
5	P. Tamagno	On the way to ^{7}Be CN evaluation, Test2 results with CONRAD	PDF

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