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Investigation of nuclear model predictions for proton induced reaction cross-sections up to 150 MeV

An extensive analysis of the accuracy in the theoretical reproduction of experimental proton induced reaction cross-sections up to 150 MeV is presented. The predictive capabilities of different models for the description of the nuclear level densities as implemented in the TALYS code and in the modified ALICE code have been assessed by means of a systematic comparison of the theoretical results with experimental EXFOR data relative to target nuclei from ^{24}Mg to ^{209}Bi. The results obtained give the possibility to find the best approaches for the cross-section calculation for nuclei from different mass ranges and for different channels.

Untersuchung von nuklearen Modellen für die Bestimmung von der Protonen induzierten Reaktionen bis 150 MeV. *Die extensive Analyse der Vollständigkeit in der theoretischen Reproduktion der experimentellen Wirkungsquerschnitte fuer Reaktionen induzierte durch Protonen mit einer Energie bis zu 150 MeV wird dargestellt. Die prädiktive Fähigkeit der verschiedenen Modellen fuer die Beschreibung die Kernniveaudichte verwendet in TALYS and ALICE/ASH Codes ist für Targets von ^{24}Mg bis ^{209}Bi festgesetzt. Die erhaltene Ergebnisse geben die Möglichkeit die besten Annäherungen für die Berechnung der Wirkungquerschnitten für Kerne der unterschiedlichen Massen zu finden.*

1 Introduction

The main purpose of this work is to investigate the uncertainty associated to the calculation of activation and transmutation cross-sections for proton induced reactions using nuclear models and codes having direct relation in the generation of nuclear data files. In a previous paper [1] the investigation of the uncertainty in the calculation of neutron induced reaction cross-sections was presented.

All the calculations have been performed using different nuclear models implemented in the TALYS code [2] and in the ALICE/ASH code [3–5], which are being extensively used nowadays within the international community for nuclear data evaluation [6–10]. The results of calculations are compared with experimental cross-sections from EXFOR [11] for proton induced reactions for nuclei from ^{24}Mg to ^{209}Bi. The comparison is done by means of different deviation factors which allow to define appropriate models for nuclear reaction cross-section calculation at different mass ranges of target nuclei.

2 Brief description of nuclear models applied for cross-section calculations

1.1 The TALYS code

The pre-equilibrium particle emission is described using the two-component exciton model [12]. The model implements new expressions for internal transition rates and new parameterization of the average squared matrix element for the residual interaction obtained using the optical model potential from [13]. The phenomenological model [14] is used for the description of the pre-equilibrium complex particle emission. The contribution of direct processes in inelastic scattering is calculated using the ECIS-97 code [15] incorporated in TALYS.

Table 1. The definition of symbols and code options used to perform cross-section calculations

Symbols	Model for nuclear level density calculation	Code	Input variable
IST (1)	Fermi gas model with the energy dependent nuclear level density parameter, *a(U)* [18] without explicit description of the collective enhancement[1]. The parameters are defined in Ref.[2]	TALYS	ldmodel = 1
IST-C	Fermi gas model with *a(U)* [18] with explicit description of the rotational and vibrational enhancement[1]	TALYS	ldmodel = 2
G	Microscopic calculations using the HF-BCS approach [21]	TALYS	ldmodel = 3
FG	Fermi gas model with a = A/9[1]	ALICE/ASH	ldopt = 0
IST (2)	Fermi gas model with the energy dependent nuclear level density parameter, *a(U)* [18][1]	ALICE/ASH	ldopt = 4
SF	Superfluid nuclear model [28, 29]	ALICE/ASH	ldopt = 5

[1] at low energy of the excitation the "constant temperature" model is used

The equilibrium particle emission is described using the Hauser-Feshbach model. In the present work the nuclear level density for equilibrium states is calculated using different nuclear models [16, 17], which are briefly described in Table 1.

The cross-sections for total neutron nonelastic interactions with nuclei have been calculated using the optical potential from [13].

1.2 The ALICE/ASH code

The ALICE/ASH code [3–5] is a modified and advanced version of the ALICE code [18].

The geometry dependent hybrid model [19] (GDH) is used for the description of the pre-equilibrium particle emission from nuclei. Intranuclear transition rates are calculated using the effective cross-section of nucleon-nucleon interactions in nuclear matter. Corrections are made to the GDH model for the treatment of effects in peripheral nuclear regions [5, 9]. The number of neutrons and protons for initial exciton state is calculated using realistic nucleon-nucleon interaction cross-sections in nucleus [5]. The exciton coalescence model [20, 21] and the knock-out model are used for the description of the pre-equilibrium complex particle emission.

The equilibrium emission of particles is described by the Weisskopf-Ewing model without detail consideration of angular momentum. Three models [16, 18, 22, 23], which are briefly described in Table 1, are used for the calculation of nuclear level density.

3 Experimental data and statistical criteria of comparison

The comparison of experimental data and calculations has been performed for nuclei from ^{24}Mg to ^{209}Bi. The experimental data were taken from EXFOR. Independent (non-cumulative) yields of radionuclides in (p, γ), (p, n) and other (p, xnypzα) reactions for target nuclei with atomic number from 12 to 83 in the energy range 0 $\div$ 150 MeV were selected for the comparison. The data were processed by the X4TOC4 code [24] and presented in the C4 format. The reaction list of the X4TOC4 code has been extended to include all possible reactions, which are available in EXFOR files.

The following data have been excluded from the consideration: i) out-dated and superceded measurements, ii) data for targets, which contain natural mixtures of isotopes; iii) data for reactions with metastable products, iv) data averaged for a wide range of proton incident energies, v) identical data and vi) data, which are referred in EXFOR as DATA-MIN or DATA-MAX. The last case required the change in the X4TOC4 code. If two or more data sets correspond to the identical reaction, the equal projectile energy, the same first author, and differ by the year of measurement, only the last measurement is left for the comparison with calculations. The total number of experimental points (Z, A, E) used for the comparison is in the order of 19000. The mass distribution and the energy distribution of the experimental data are shown in Fig. 1.

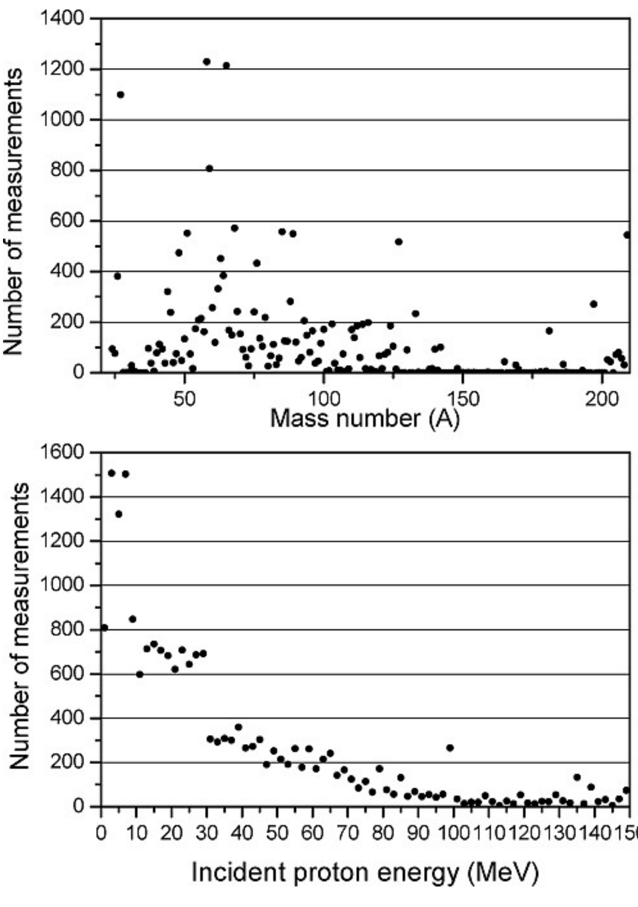

Fig. 1. The number of experimental points for (p, xnypzα) reaction cross-sections available in EXFOR with the proton incident energy up to 150 MeV for targets from ^{24}Mg to ^{203}Bi used for the comparison with calculations, depending upon the mass number of the target nucleus (upper figure) and the projectile energy (lower figure)

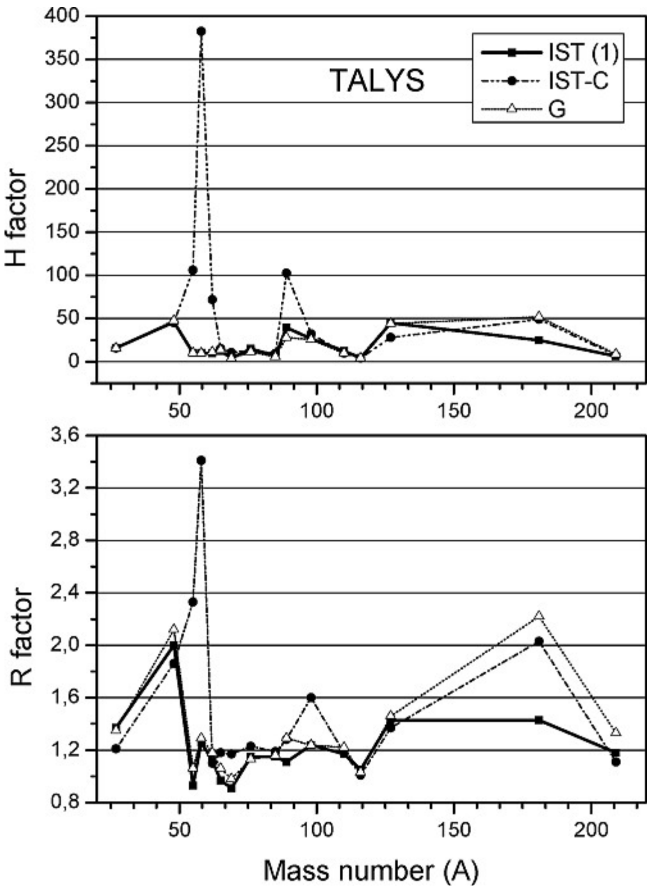

Fig. 2. The H- and R-deviation factors as functions of different groups of target nuclei mass numbers (A) calculated with the TALYS code using three different models for the nuclear level density calculation (Table 1). In each group of mass number the factors are averaged over a consistent number of experimental points, the difference being ±20 % at the maximum. Calculated points are linearly interpolated

The following deviation factors [25–28] were used for the comparison of the results of calculations with the measured data:

$$H = \left(\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\sigma_i^{\mathrm{exp}} - \sigma_i^{\mathrm{calc}}}{\Delta\sigma_i^{\mathrm{exp}}}\right)^2\right)^{1/2} \tag{1}$$

$$R = \frac{1}{N}\sum_{i=1}^{N}\frac{\sigma_i^{\mathrm{calc}}}{\sigma_i^{\mathrm{exp}}} \tag{2}$$

$$D = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\sigma_i^{\mathrm{exp}} - \sigma_i^{\mathrm{calc}}}{\sigma_i^{\mathrm{exp}}}\right| \tag{3}$$

$$F = 10^{\left(\frac{1}{N}\sum_{i=1}^{N}\left[\log(\sigma_i^{\mathrm{exp}}) - \log(\sigma_i^{\mathrm{calc}})\right]^2\right)^{1/2}} \tag{4}$$

$$L = (\delta u)^2 = \sum_{i=1}^{N}\left(\frac{\sigma_i^{\mathrm{calc}}}{\Delta\sigma_i^{\mathrm{exp}}}\right)^2\left(\frac{\sigma_i^{\mathrm{calc}} - \sigma_i^{\mathrm{exp}}}{\sigma_i^{\mathrm{calc}}}\right)^2 \Bigg/ \sum_{i=1}^{N}\left(\frac{\sigma_i^{\mathrm{calc}}}{\Delta\sigma_i^{\mathrm{exp}}}\right)^2 \tag{5}$$

where σ_i^{exp} and $\Delta\sigma_i^{\mathrm{exp}}$ are the measured cross-section and its uncertainty, σ_i^{calc} is the calculated cross-section, N is the number of experimental points.

4 Results and discussion

Deviation factors of Eqs. (2)–(5) calculated for target nuclei from ^{24}Mg to ^{209}Bi over the entire energy range (0 ÷ 150 MeV) and without distinction into reaction types are summarized in Table 2. Results are provided over the entire mass range and in the two atomic mass ranges below and above 120. The H factor (Eq.(1)) is given separately in Table 3. Data of Tables 2 and 3 have been calculated over a different number of experimental points. This is due to the fact that about 8 % of the total measurements considered for the calculation of the factors in Table 2 are provided in EXFOR without the associated experimental uncertainty $\Delta\sigma_i^{\mathrm{exp}}$ which is needed to compute the H factor of Eq. (1). Therefore these measurements have been excluded from the data treatment relative to Table 3. From the results one can observe that the TALYS code is globally performing better with respect to the ALICE code, particularly in the mass range below 120. The best results are obtained when using the Fermi gas model without the explicit description of the collective enhancement (IST(1) model) and the microscopic model of Goriely (G model). For target nuclei with mass numbers above 120 the ALICE/ASH calculations using the superfluid model (SF) for the nuclear level density determination provide the best results.

In Table 3 the results of the H factor calculated for different groups of reactions is also given. For target nuclei with mass number below 120 the IST (1) and G models in the TALYS code are the options providing the best accuracy in the reproduction of experimental data. In the mass number range above 120 the TALYS and ALICE/ASH codes are somehow in competition, particularly in the case of the (p, γ), (p, n), (p, p′), (p, 2n) and (p, np) reactions. Tables 4–6

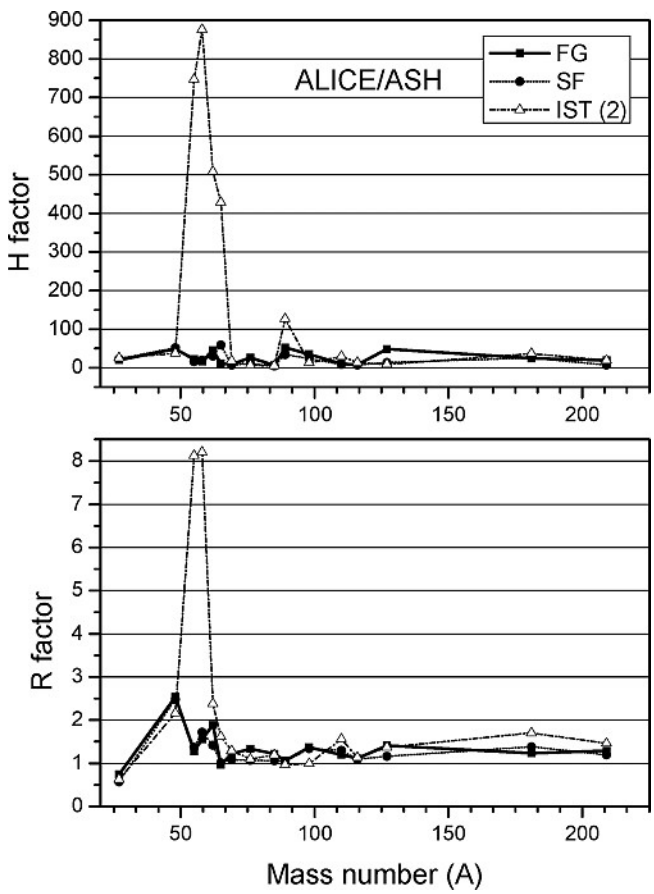

Fig. 3. The H- and R-deviation factors as functions of different groups of target nuclei mass numbers (A) calculated with the ALICE/ASH code using three different models for the nuclear level density calculation (Table 1). See comments to Fig. 2

Table 2. Deviation factors for nuclei from different mass number ranges calculated using the TALYS and ALICE/ASH codes. The best results are underlined. See Table 1 for symbols explanation. The H factor is shown in Table 3

Factors	TALYS			ALICE/ASH		
	IST (1)	IST-C	G	FG	IST (2)	SF
Target nuclei with atomic mass number 24 ≤ *A* < 120						
R	<u>1.76</u>	2.03	1.80	4.97	13.90	4.16
D	1.08	1.42	<u>1.07</u>	4.34	13.44	3.58
F	2.08	2.54	2.07	3.35	14.23	4.80
L	<u>0.91</u>	0.93	<u>0.91</u>	1.00	0.99	0.99
Number of points	16306	16269	16314	16030	15960	15995
120 ≤ *A* ≤ 209						
R	1.43	1.55	1.67	1.30	1.51	<u>1.21</u>
D	0.69	0.88	0.95	0.75	0.91	<u>0.63</u>
F	<u>2.25</u>	2.98	2.89	4.37	6.16	4.34
L	<u>0.91</u>	0.93	0.91	1.00	0.99	0.99
Number of points	2928	2927	2928	2907	2885	2905
All nuclei with 24 ≤ *A* ≤ 209						
R	<u>1.71</u>	1.96	1.78	4.40	12.00	3.71
D	<u>1.02</u>	1.34	1.05	3.79	11.52	3.13
F	<u>2.11</u>	2.61	2.20	3.51	12.74	4.73
L	<u>0.91</u>	0.93	0.91	1.00	0.99	0.99
Number of points	19234	19196	19242	18937	18845	18900

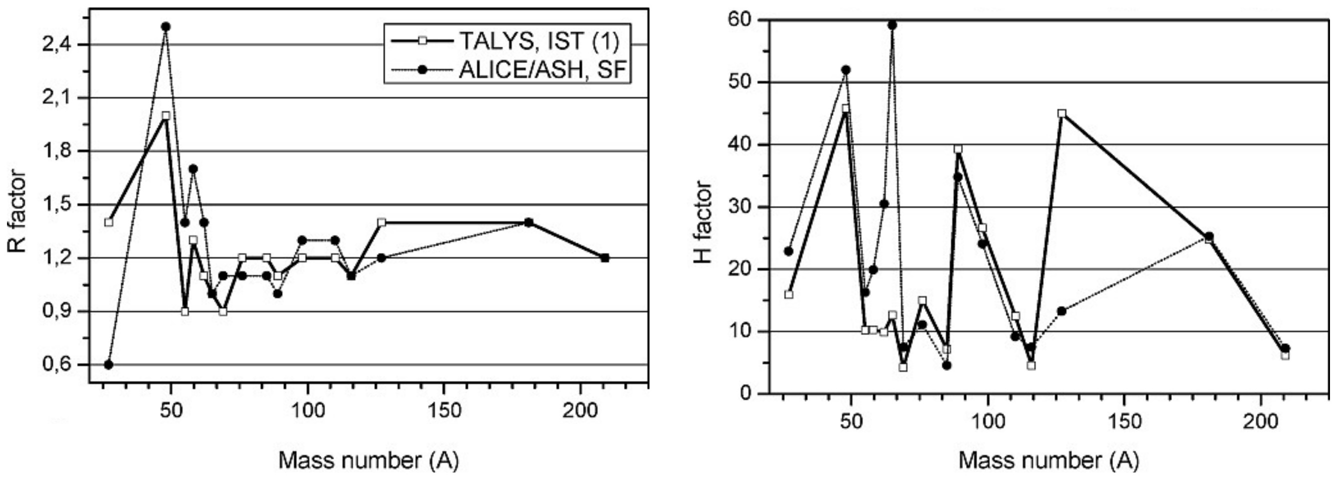

Fig. 4. The H- and R-deviation factors as functions of different groups of target nuclei mass numbers (A) calculated using the TALYS and ALICE/ASH codes. See comments to Fig. 2.

Table 3. The H factor for groups of reactions relative to target nuclei with mass number in the range 24 ≤ A < 120 and 120 ≤ A ≤ 209 calculated using the TALYS and ALICE/ASH codes. The best result is underlined for each group of reaction. See Table 1 for symbols explanation

Reaction	TALYS			ALICE/ASH		
	IST (1)	IST-C	G	FG	IST (2)	SF
Targets nuclei with atomic mass number 24 ≤ A < 120						
(p, γ) (Number of points)	32.2 (1653)	306.3 (1639)	31.4 1 (1664)	219.2 (1544)	3205.4 (1544)	320.4 (1544)
(p, n), (p, p′) (Number of points)	24.8 (5278)	27.0 (5278)	24.4 (5278)	1344.9 (5238)	54.1 (5238)	975.2 (5238)
(p, 2n), (p, np) (Number of points)	21.5 (2097)	61.2 (2097)	14.5 (2097)	24.5 (2070)	22.5 (2058)	14.9 (2058)
Others (Number of points)	11.2 (4380)	15.8 (4366)	10.6 (4376)	25.5 (4321)	12.8 (4271)	17.8 (4316)
All reactions (Number of points)	22.0 (13408)	111.6 (13380)	20.7 (13415)	851.6 (13173)	1100.6 (13111)	625.2 (13156)
120 ≤ A ≤ 209						
(p, γ) (Number of points)	25.5 (56)	25.9 (53)	25.7 (53)	78.2 (52)	87.8 (52)	6.3 (52)
(p, n), (p, p′) (Number of points)	36.6 (674)	50.4 (674)	39.3 (674)	22.3 (673)	37.4 (673)	26.0 (673)
(p, 2n), (p, np) (Number of points)	55.2 (650)	33.7 (649)	53.9 (650)	59.9 (645)	6.0 (645)	14.8 (645)
Others (Number of points)	10.5 (1233)	22.5 (1237)	35.2 (1237)	13.1 (1226)	7.3 (1210)	8.3 (1224)
All reactions (Number of points)	34.2 (2613)	34.5 (2613)	41.5 (2614)	35.0 (2596)	23.5 (2580)	16.2 (2594)
All nuclei with 24 ≤ *A* ≤ 209						
(p, γ)	32.0	301.5	31.21	216.1	3152.8	315.2
(p,n), (p,p')	26.4	30.5	26.54	1266.1	52.4	918.1
(p,2n), (p,np)	32.8	56.0	29.2	36.2	19.8	14.9
Others	11.1	17.5	19.0	23.3	11.8	16.2
All reactions	24.4	103.0	25.3	778.4	1006.1	571.4

Table 4. The H factor for groups of nuclei calculated using the TALYS and ALICE/ASH codes. The best result is underlined for each range of mass number. See Table 1 for symbols explanation

Factors	TALYS			ALICE/ASH		
	IST (1)	IST-C	G	FG	IST (2)	SF
24 ≤ A ≤ 27	15.9	15.9	15.6	20.4	26.0	22.9
28 ≤ A ≤ 48	45.8	45.3	47.6	49.1	37.2	52.0
49 ≤ A ≤ 55	10.2	105.9	10.4	22.4	747.2	16.3
56 ≤ A ≤ 58	10.3	382.4	9.9	17.2	875.9	19.9
59 ≤ A ≤ 62	9.9	72.0	11.5	45.9	508.1	30.5
63 ≤ A ≤ 65	12.6	15.4	13.6	11.6	428.9	59.2
66 ≤ A ≤ 69	4.2	10.8	3.9	9.2	18.1	7.5
70 ≤ A ≤ 76	15.0	13.7	11.4	26.6	6.4	11.1
77 ≤ A ≤ 85	7.2	9.5	5.7	6.4	5.9	4.6
86 ≤ A ≤ 89	39.3	102.5	28.1	53.1	126.4	34.8
90 ≤ A ≤ 98	26.6	32.3	25.4	35.0	13.3	24,1
99 ≤ A ≤ 110	12.5	10.0	9.8	10.3	29.6	9.2
111 ≤ A ≤ 116	4.6	4.3	4.1	7.9	14.0	7.5
117 ≤ A ≤ 127	45.0	28.0	44.1	48.9	9.2	13,3
128 ≤ A ≤ 181	24.8	49.2	52.0	24.6	36.6	25.3
182 ≤ A ≤ 209	6.2	7.0	9.0	19.0	19.1	7.3

summarize the H, R and F factors computed for different ranges of target nuclei mass numbers (A) selected in such a way to contain a number of experiments differing for a maximum of 20 %. This is motivated by the necessity to consistently compare deviation factors with similar statistics. Results in Table 4 are relative to the energy range 5 ÷ 150 MeV, corresponding to a total of 13407 experimental points.

In Fig. 1 the best performing model of TALYS (IST (1)) is compared with the best one of ALICE/ASH (SF) in the case of the treatment for different mass number ranges.

5 Conclusions

An investigation of the uncertainty associated to the calculation of proton induced reaction cross-sections in the energy range 0 ÷ 150 MeV relative to target nuclei from ^{24}Mg to ^{209}Bi has been presented. The study has been carried out by means of an extensive comparison between experimental data extracted from EXFOR and calculated results obtained with the TALYS and the ALICE/ASH codes.

The uncertainty on the theoretical prediction of proton cross-sections associated to the use of different models for the calculation of the nuclear level densities for equilibrium states (these being both phenomenological and microscopic ones) has been investigated and quantified by means of statistical deviation factors which can be used to provide recommendations on the best combinations of codes and models to optimize the accuracy of the simulations.

(Received on 2 April 2007)

Table 5. The R factor for groups of nuclei calculated using the TALYS and ALICE/ASH codes. The best result is underlined for each range of mass number. See Table 1 for symbols explanation

Factors	TALYS			ALICE/ASH		
	IST (1)	IST-C	G	FG	IST (2)	SF
24 ≤ A ≤ 27	1.4	1.2	1.4	0.7	0.6	0.6
28 ≤ A ≤ 48	2.0	1.9	2.1	2.5	2.2	2.5
49 ≤ A ≤ 55	0.9	2.3	1.1	1.3	8.1	1.4
56 ≤ A ≤ 58	1.3	3.4	1.3	1.6	8.2	1.7
59 ≤ A ≤ 62	1.1	1.1	1.2	1.9	2.4	1.4
63 ≤ A ≤ 65	1.0	1.2	1.1	1.0	1.6	1.0
66 ≤ A ≤ 69	0.9	1.2	1.0	1.2	1.3	1.1
70 ≤ A ≤ 76	1.2	1.2	1.1	1.3	1.1	1.1
77 ≤ A ≤ 85	1.2	1.2	1.2	1.2	1.2	1.1
86 ≤ A ≤ 89	1.1	1.3	1.3	1.1	1.0	1.0
90 ≤ A ≤ 98	1.2	1.6	1.2	1.4	1.0	1.3
99 ≤ A ≤ 110	1.2	1.2	1.2	1.2	1.6	1.3
111 ≤ A ≤ 116	1.1	1.0	1.0	1.1	1.1	1.1
117 ≤ A ≤ 127	1.4	1.4	1.5	1.4	1.4	1.2
128 ≤ A ≤ 181	1.4	2.0	2.2	1.2	1.7	1.4
182 ≤ A ≤ 209	1.2	1.1	1.3	1.3	1.5	1.2

Table 6. The F factor for groups of nuclei calculated using the TALYS and ALICE/ASH codes. The best result is underlined for each range of mass number. See Table 1 for symbols explanation

Factors	TALYS			ALICE/ASH		
	IST (1)	IST-C	G	FG	IST (2)	SF
24 ≤ A ≤ 27	1.85	2.27	1.9	5.29	26.24	78.44
28 ≤ A ≤ 48	2.35	2.99	2.6	4.1	6.4	6.07
49 ≤ A ≤ 55	2.19	2.97	2.04	2.75	2.99	5.09
56 ≤ A ≤ 58	1.8	3.23	1.86	2.38	2.71	3.41
59 ≤ A ≤ 62	1.98	3.39	1.97	3.1	2.8	3.9
63 ≤ A ≤ 65	1.64	2.09	1.58	1.75	1.76	2.81
66 ≤ A ≤ 69	1.72	2.16	1.68	2.1	2.23	3.74
70 ≤ A ≤ 76	1.76	1.89	1.71	1.94	1.92	2.8
77 ≤ A ≤ 85	1.65	1.76	1.72	1.85	1.83	2.48
86 ≤ A ≤ 89	1.73	2.01	1.72	1.95	2	12.4
90 ≤ A ≤ 98	1.94	2.22	1.81	2.79	2.6	10.62
99 ≤ A ≤ 110	2.01	2.25	1.82	2	1.77	7.55
111 ≤ A ≤ 116	1.28	1.33	1.26	1.39	1.29	2.33
117 ≤ A ≤ 127	2.11	2.71	2.27	2.33	2.98	4.42
128 ≤ A ≤ 181	2.13	2.65	2.7	2.46	2.6	4.92
182 ≤ A ≤ 209	2.17	2.22	2.38	3.99	3.51	6.2

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