EFDA TECHNOLOGY WORKPROGRAMME 2004

TT-TRITIUM BREEDING AND MATERIALS
TTM - MATERIALS DEVELOPMENT

TASK: TW4-TTMN-001
NUCLEAR DATA: EFF/EAF data file upgrade, processing and benchmark analyses

Deliverable: *Evaluation of cross sections for Ta for the EAF and the EFF files*

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1. Introduction

Following a benchmark experiment with pure W irradiated by 14 MeV neutrons which showed radionuclide ratios of calculated-to-experimental activity (C/E) significantly above unity for several of the dominantly produced nuclides [1,2], when calculated with the European Activation System [3] (EASY), and the detailed analysis of the activation cross sections of the W stable isotopes carried out by using the computer codes EMPIRE-II [4] and TALYS [5], as well as fully local parameter sets within the STAPRE-H [6,7] code, the sensitivity of these calculated cross sections to various model parameters has been discussed. Since the final aim is to improve the C/E of the benchmark experiment, this discussion has concerned the main model parameters and assumptions. Thus, the optical model potentials, corresponding neutron-resonance data within the IAEA Reference Input Parameter Library (RIPL) [8], neutron total cross sections [9,10], proton reaction cross sections, low-lying level and resonance data involved for determination of the level density parameters within a realistic approach recently developed [11] are presented and discussed. A similar discussion concerns the electric dipole γ-ray strength functions $f_{E1}(E_{\gamma})$ which are used for the calculation of the γ-ray transmission coefficients and the corresponding capture cross sections.

The same consistent parameter set or a similar one has been involved for the calculation of the activation cross sections for the ^{181}Ta nucleus (standing actually for the whole Ta natural element) and their comparison with all available experimental data; This concerned especially the same residual nuclei which are, in this case, in the neutron channel but have been also in the charged-particle channel for the neutron-induced reactions on the target nuclei ^{180,182,183,184186}W.

2. Calculated cross-section sensitivity to nuclear reaction mechanisms and parameters

In order to study the effects of various pre-equilibrium emission (PE) models on the calculated cross sections (Figure 1), we have also used in the EMPIRE-II calculations the statistical Multi-step Direct (MSD) and Multi-step Compound (MSC) theory for neutron emission prior to equilibration, while the proton PE was still given by the exciton (DEGAS) model with the standard value of single-particle level (s.p.l.) density parameter g=A/13 MeV^{-1}.

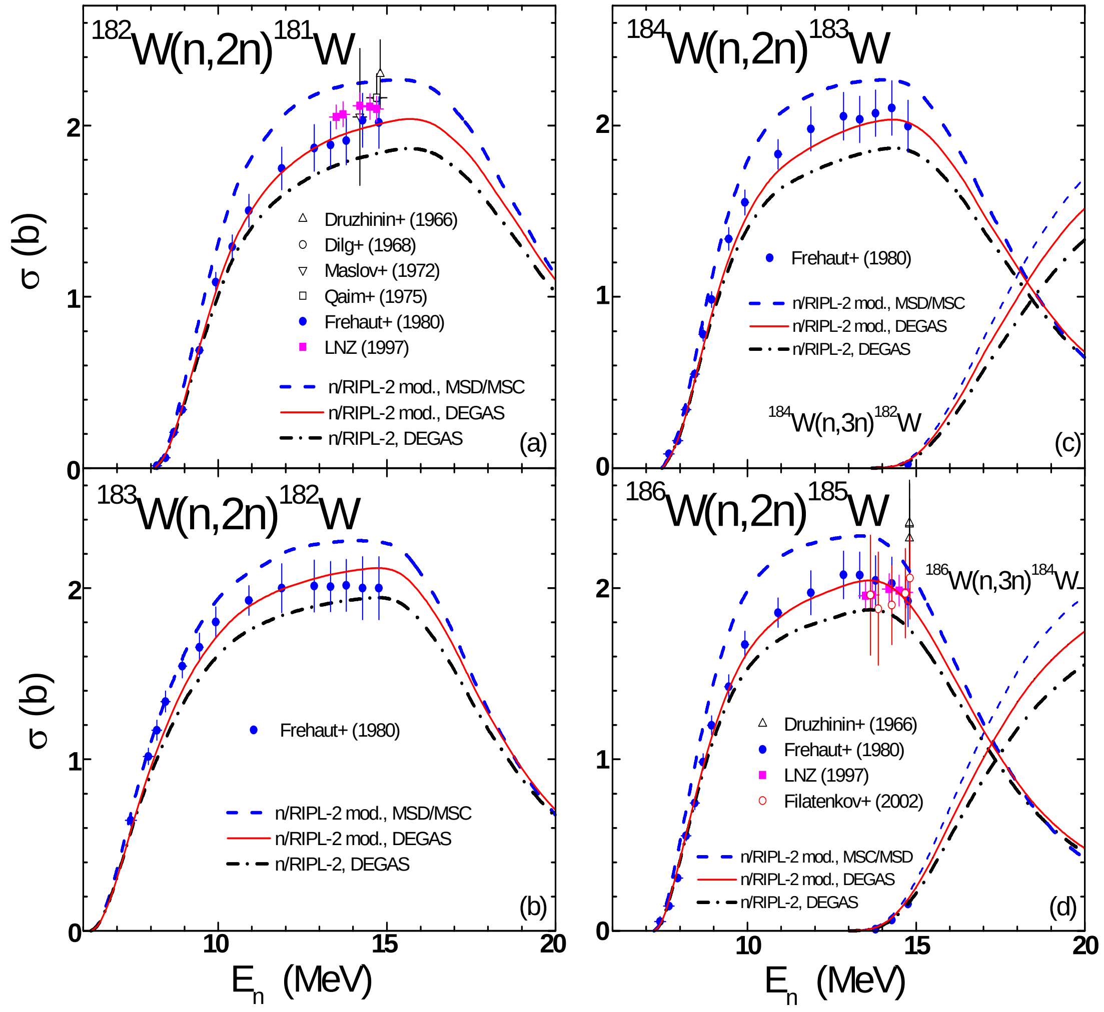

Figure 1. Sensitivity of calculated (n,2n) reaction cross sections vs. reaction mechanisms and model parameters.

It is useful to compare the sensitivity of the calculated cross sections with respect to reaction mechanisms, and the sensitivity to model parameters. The neutron optical model potential (OMP) and single-particle level (s.p.l.) density values are particularly important due to their key role in activation reactions. Firstly, we have chosen two rather close neutron OMP parameter sets, i.e. the LANL deformed OMP available in EMPIRE-II from RIPL-2, and its modified version used in this work.

Secondly, we compared the cross sections of the *(n,p)* reaction on ^{182,183,184,186}W obtained with the code EMPIRE-II using the default value g=A/13 MeV^{-1} as well as the values A/14 and A/15 MeV^{-1} (Figure 2). The last value is also the default value within the TALYS code, making possible a comparison with its results. It can be seen that the EMPIRE-II calculations also describe well the experimental data for the *(n,p)* reaction on the even-even W isotopes, if the s.p.l. value *g*=A/14 MeV^{-1} is adopted. The underestimation still present in the case of the target nucleus ^{183}W seems to be due to the use of a particle-hole level density without an advanced pairing correction in the DEGAS model. A similar analysis for the ratios C/E is shown in Figure 3, the model uncertainties fully supporting the EASY-03 results.

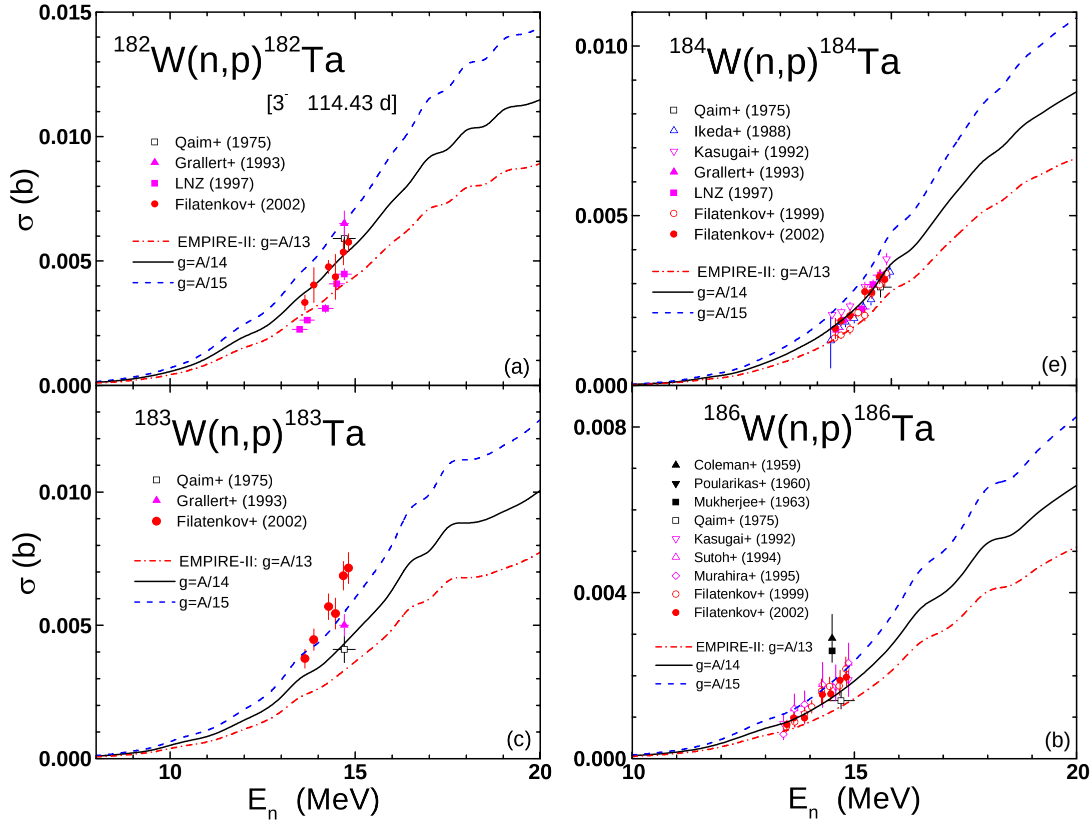

Figure 2. Sensitivity of calculated (n,p) reaction cross sections vs. model parameters.

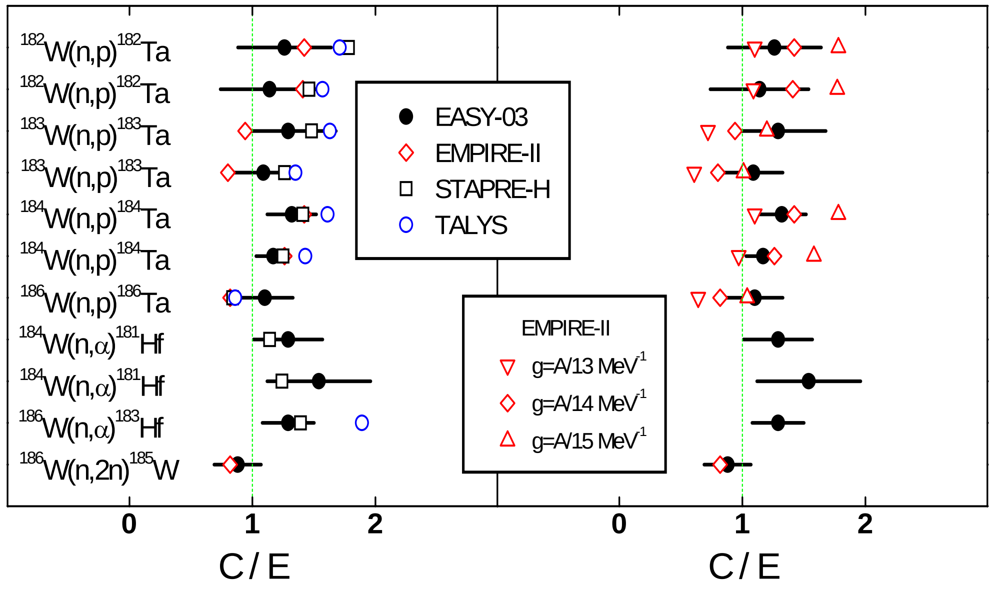

Figure 3. Sensitivity of C/E ratios vs. reaction mechanisms and model parameters.

3. Nuclear model parameters for calculation of ^{181}Ta activation cross sections

3.1. The neutron optical potential analysis

Since the heavy deformed nuclei are quite different from other mass regions, a series of various specific points have to be considered in addition to the recent analyses that use the Geometry-Dependent Hybrid (GDH) semi-classical model for pre-equilibrium emission (PE) and the Hauser-Feshbach (HF) statistical model for nuclei with A<100. Thus the coupled-channels (CC) model should replace the spherical optical model potential (OMP) for modeling reactions on deformed nuclei as within the last version of the EMPIRE-II statistical model code for nuclear reaction calculations, now installed [12] at IFIN-HH. Moreover, the neutron optical potentials for both cases of the ^{181}Ta and stable isotopes of Hf (actually the ^{178}Hf nucleus) have been analyzed at the same time in order to find a systematic trend of the OMP parameters.

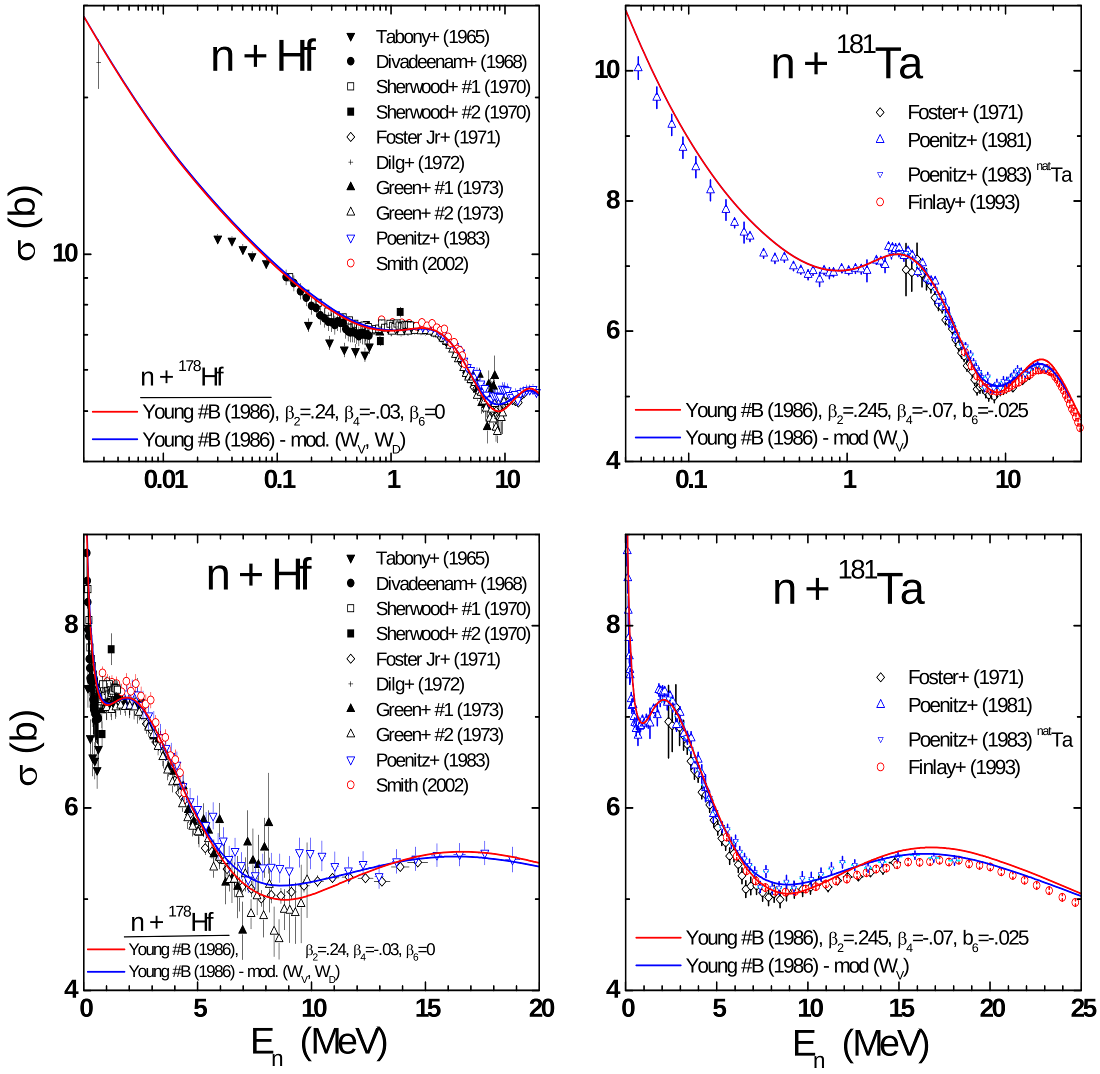

Figure 4. Comparison of calculated and experimental neutron total cross sections for ^{178}Hf and ^{181}Ta isotopes, with emphasis of the lower energy region (upper side).

The CC calculations were carried out assuming the coupling bases ($7/2^+$, $9/2^+$, $11/2^+$, $13/2^+$, $15/2^+$) for ^{181}Ta and (0^+, 2^+, 4^+) for ^{178}Hf and using the values of the β_2, β_4, and β_6

deformation parameters which provided the best description of the corresponding total neutron cross sections (Figure 4) and being also consistent with the deformation parameters found by Delaroche [13] for the ^{182,183,184,186}W isotopes and nuclear structure calculations [14]. Our analysis concerned the deformed phenomenological optical potential available in EMPIRE-II from RIPL-2, the specification [15] of the NEA-DB intercomparison for n+^{184}W at 25.7 MeV, and the rare earth–actinide average potential of Young [16] (Set B of Table II). Finally [17] we adopted a slightly modified version of the rare earth–actinide average potential, by using some features (e.g., the real potential radius and the surface imaginary well depth) of the NEA-DB potential in order to describe better the latest ANL total neutron cross sections [18]. Moreover, check of the OMP parameter sets by analysis of the low-energy neutron scattering properties (S_0, S_1, R') and neutron total cross sections (SPRT method [19]) has followed inclusion of the calculated *s*- and *p*-wave neutron strength functions S_0, S_1 and potential scattering radius R' in the EMPIRE-II output and the comparison with the corresponding recent average resonance data RIPL-2 recommendations [20]. Comparison of calculated data and measurements [18] of the neutron total cross sections for the ^{178}Hf and ^{181}Ta isotopes are shown in Figure 4.

3.2. The γ-ray strength functions

The electric dipole γ-ray strength functions $f_{E1}(E_\gamma)$ which are used for the calculation of the γ-ray transmission coefficients, have been obtained by means of a modified energy-dependent Breit-Wigner (EDBW) model [21,22]. Moreover, systematic EDBW correction factors F_{SR} were obtained by using the experimental [20] average radiative widths $\Gamma_{\gamma\,0}^{exp}$ of the *s*-wave neutron resonances, and assuming that $F_{SR}= \Gamma_{\gamma\,0}^{exp}/\ \Gamma_{\gamma\,0}^{EDBW}$. Next, the $f_{E1}(E_\gamma)$ thus obtained have been checked within calculations of capture cross sections. The calculated and experimental cross sections of the reactions ^{176}Hf*(n,γ)*^{177}Hf, ^{177}Hf*(n,γ)*^{178}Hf, ^{178}Hf*(n,γ)*^{179}Hf, ^{179}Hf*(n,γ)*^{180}Hf, ^{180}Hf*(n,γ)*^{181}Hf, and ^{181}Ta*(n,γ)*^{182}Ta were compared in the neutron energy range from keV to 2-3 MeV. The RIPL values for $\Gamma_{\gamma\,0}^{exp}$ lead to $f_{E1}(E_\gamma)$ strength functions are sometime too large, so that more appropriate values have been established in these cases, leading to a systematical behavior (Figure 5) based on capture cross-section analysis (Figure 6), to be used in further activation calculations.

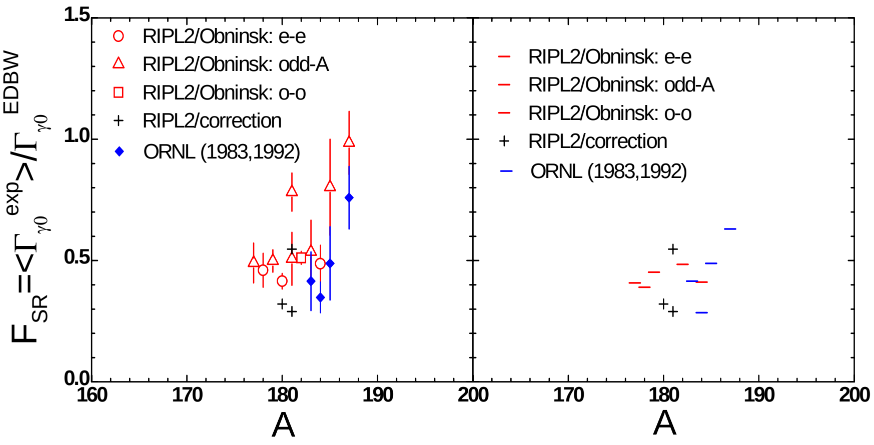

Figure 5. The EDBW-model correction factors (left) and limits (right) provided by the ratio of experimental [20,23] and EDBW-predicted $\Gamma_{\gamma\,0}^{exp}$ values for the Hf, Ta, and W stable nuclei.

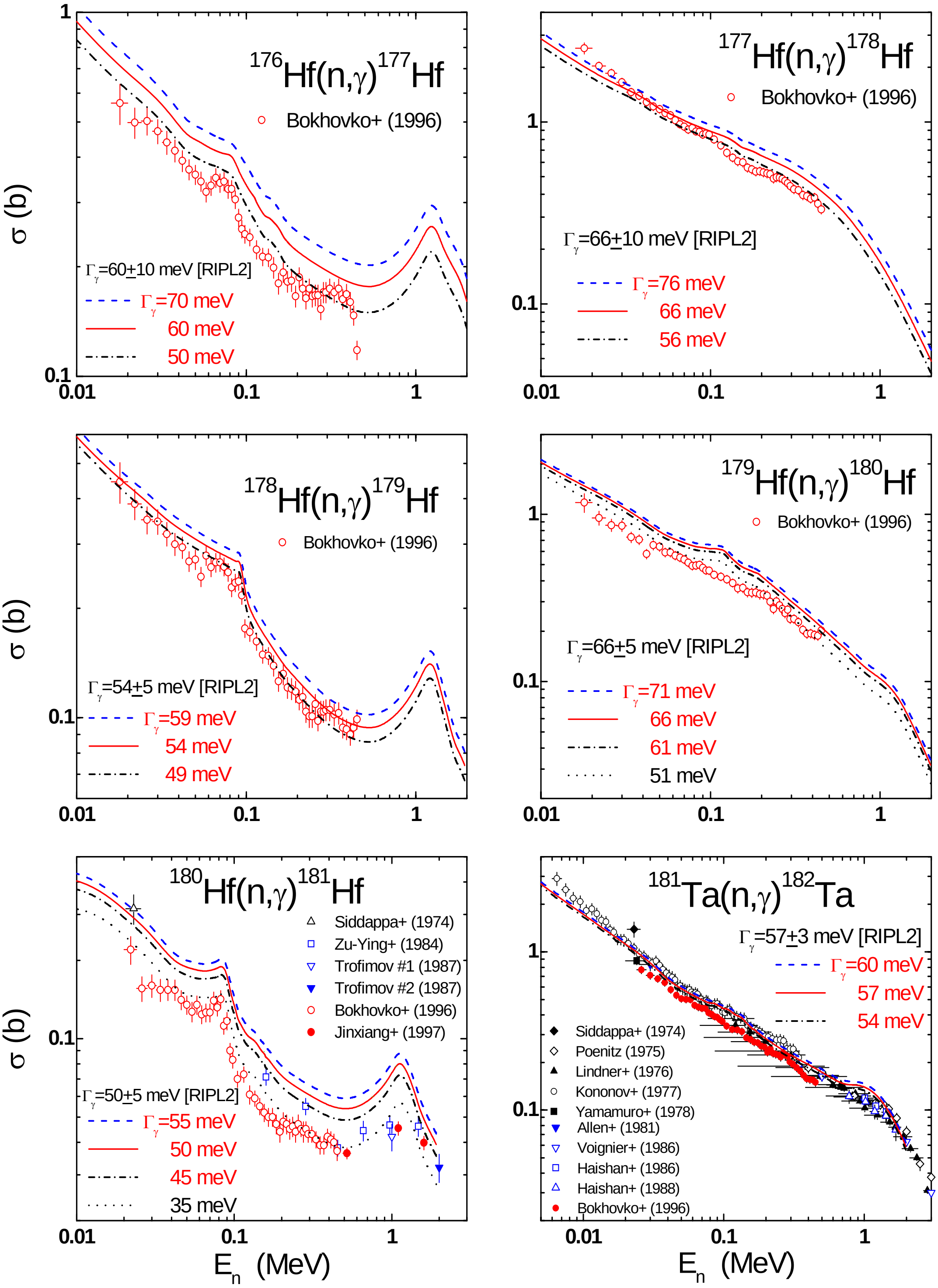

Figure 6. Comparison of calculated and measured neutron capture cross sections of $^{176-180}$Hf and ^{181}Ta nuclei, with respect to experimental [20] average radiative widths $\Gamma_{\gamma\ 0}^{exp}$ of the s-wave neutron resonances.

4. Activation cross section results

In order to understand the particular points of various target nuclei and reaction channels we have used the code STAPRE-H and a consistent local parameter set. The neutron transmission coefficients provided by the code EMPIRE-II, already corrected for the direct inelastic scattering, have been taken as input in the STAPRE-H calculations. The PE model

Geometry-Dependent Hybrid has been used along with the CC method and statistical Hauser-Feshbach models to analyze data of fast-neutron interaction with the ^{181}Ta isotope (Ta element).

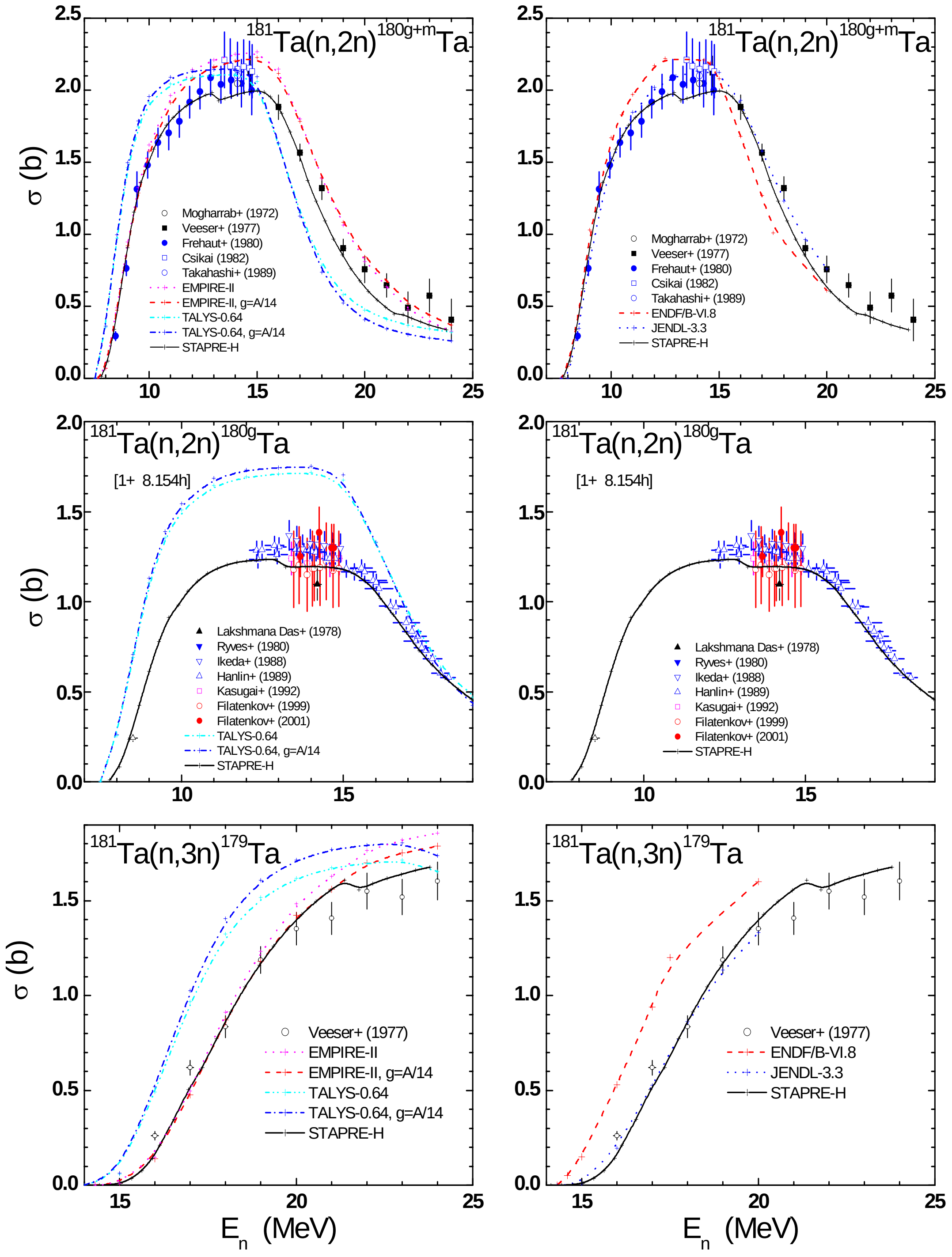

Figure 7. (Left) Comparison of measured reaction cross sections for the target nucleus ^{181}Ta and calculated values by using EMPIRE-II and TALYS codes with default global parameters (except local OMPs and the s.p.l. value g=A/14 MeV^{-1}) and STAPRE-H with the local parameter set given in this work. (Right) Comparison of measured, calculated and evaluated reaction cross sections available within the libraries ENDF/B-VI.8 [24] and JENDL-3.3 [25]. A normalization factor of 1.078 was applied to the data of Frehaut et al. [26], according to Vonach et al. [18].

The calculated activation cross sections are shown in Figures 7 and 8, as obtained by means of the STAPRE-H, EMPIRE-II and TALYS computer codes, based on similar nuclear reaction models.

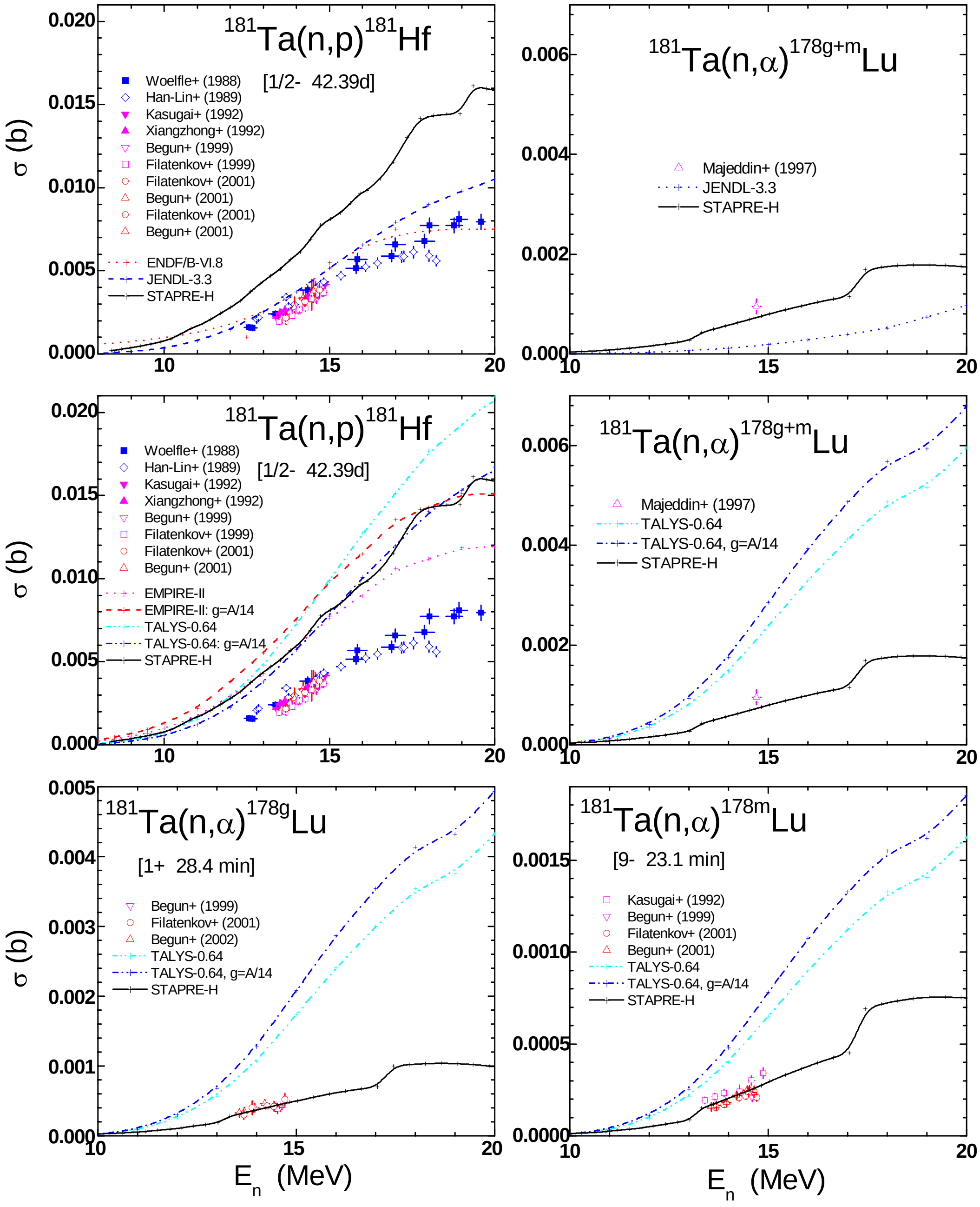

Figure 8. Same as Figure 7, for charged-particle emission induced by fast neutrons on the target nucleus ^{181}Ta and (Center/Bottom) calculated values by using STAPRE-H, EMPIRE-II, and TALYS codes, and (Top) evaluated cross sections available within the libraries ENDF/B-VI.8 and JENDL-3.3.

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References:

[1]. **Seidel K., Forrest R. A., Freiesleben H., Goncharov S. A., Kovalchuk V. D., Markovskij D. V., Maximovich D. V., Unholzer S., and Weigel R.**, Report TUD-IKTP/02-01, Dresden, Germany, 2002.

[2]. **Eichin R., Forrest R.A., Freiesleben H., Goncharov S.A., Kovalchuk V.D., Markovskij D.M., Seidel K., and Unholzer S.**, Int. Workshop on Fast Neutron Physics, Sept. 5-7, 2002, Dresden, Germany.

[3]. **Forrest R.A. and Sublet J-Ch.**, Reports UKAEA FUS-450,-451, Culham Science Centre, Abingdon, UK.

[4]. **Herman M.**, EMPIRE-II v.2.18 dated 2002-09-27; http://www-nds.iaea.org/empire/ .

[5]. **Koning A.J.**, in Nuclear Model Parameter Testing for Nuclear Data Evaluation, M. Herman (Ed.), Report INDC(NDS)-431, IAEA, Vienna, 2002, p. 117.

[6]. **Avrigeanu M. and Avrigeanu V.**, *“STAPRE-H95 Computer Code”*, IPNE Report NP-86-1995, Bucharest, 1995, and references therein;

News NEA Data Bank **17**, 22 (1995).

[7]. **Avrigeanu M. and Avrigeanu V.**, Comp. Phys. Comm. 112, 191 (1998); **Harangozo A., Stetcu I., Avrigeanu M. and Avrigeanu V.**, Phys. Rev. C 58, 295 (1998).

[8]. **Herman M.**, *“Nuclear Model Parameter Testing for Nuclear Data Evaluation (Reference Input Parameter Library)”,* Report INDC(NDS)-431, IAEA, Vienna, 2002; http://www-nds.iaea.or.at/ripl/

[9]. **Abfalterer W.P., Bateman F.B., Dietrich F.S., Finlay R.W., Haight R.C., and Morgan G.L.**, Phys. Rev. C 63, 044608 (2001); **F.S. Dietrich et al.**, Phys. Rev. C 67, 044606 (2003).

[10]. **Dietrich F.S. et al.**, Phys. Rev. C 67, 044606 (2003).

[11]. **Avrigeanu V., Glodariu T., Plompen A. J. M., and Weigmann H.**, J. Nucl. Sci. Tech. Suppl. 2, 746 (2002).

[12]. **Avrigeanu V., et al.**, Report CERES No. 66 /2003-10-01, IFIN-HH, Bucharest, 2003.

[13]. **Delaroche J.P.,** Phys. Rev. C 26, 1899 (1982).

[14]. **Nilsson S.G. et al.**, Nucl. Phys. A131, 1 (1969).

[15]. **Delaroche J. P.**, private communication to H.K. Vonach and P. Nagel, Report NEANDC-253”U”, OECD/NEA Data Bank, Gif-sur-Yvette, 1989.

[16]. **Young P. G.,** Report NEANDC-222"U", OECD/NEA Data Bank, Gif-sur-Yvette, 1986, 127.

[17]. **Avrigeanu V.**, EFFDOC-906, EFF/EAF Meeting, Paris, Nov. 24-26, 2004.

[18]. **Smith A.B.**, Argonne Natonal Laboratory, Argonne, Report ANL/NDM-153, June 2001.

[19]. **Delaroche J. P., Lagrange Ch., and Salvy J.**,

IAEA-190 (IAEA, Vienna, 1976), vol. 1, 251.

[20]. **Ignatyuk A.V.**, at http://161.5.7.5/RIPL-2/resonances/ .

[21]. **Gardner D. G. and Dietrich F. S.**, Report UCRL-82998, LLNL-Livermore, 1979.

[22]. **Avrigeanu M., Avrigeanu V., Cata G., and Ivascu M.**,

Rev. Roum. Phys. 32, 837 (1987).

[23]. **Macklin R.L., Drake D.M., and Arthur E.D.**, Nucl. Sci. Eng. 89, 98 (1983).

[24]. Evaluated Nuclear Data File (ENDF), available at http://www.nndc.bnl.gov/exfor1/endf00.htm.

[25]. Japanese Evaluated Nuclear Data Library JENDL-3.3, http://wwwndc.tokai.jaeri.go.jp/jendl/j33/j33.htm

[26]. **Frehaut J., Bertin A., Bois R., and Jary J.**, in Proc. Symp. Neutron Cross Sections from 1-50 MeV, Upton, New York, May 12-14, 1980, Report BNL-NCS-51245, BNL, 1980, vol. I, 399.