EFDA TECHNOLOGY WORKPROGRAMME 2005

TT-TRITIUM BREEDING AND MATERIALS
TTM – MATERIALS DEVELOPMENT

TASK: TW5-TTMN-001
NUCLEAR DATA: EFF/EAF data file upgrade, processing and benchmark analyses

***Deliverable*: Calculation of cross sections for Ta and Hf up to 50 MeV**

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1. Introduction

The long-life Hafnium isomers, which could be produced after a few reactions on W and Ta isotopes in the first-wall material of fusion reactors, are one of the most interesting cases which require accurate predictions for the fast-neutron reactions cross sections by using no normalization or free parameters but (i) the unitary use of the common model parameters for different mechanisms, (ii) consistent sets of input parameters which are determined by analyses of various independent experimental data, and (iii) the unitary account of a whole body of related experimental for isotope chains of neighboring elements. On the other hand, the needs of the evaluated neutron data for fusion devices concern the neutron energies up to 60 MeV.

In order to provide the results confidence and completeness, this analysis has concerned all activation data for the Hf, Ta and W stable isotopes. It continued the work carried out within the framework of the same EFDA task TTMN-001 between 2003-2004 up to the neutron energy of 20 MeV, and made use of also the computer codes EMPIRE-II [1] and TALYS [2] as well as a local parameter set within an updated version of STAPRE-H code [3]. The consistent input-parameter set made use of recent neutron total cross sections of Hf and Ta elements and the ^{182,183,184,186}W nuclei for analysis of deformed optical model (DOM) potential within the coupled-channels (CC) model, proton reaction cross sections, low-lying level and resonance data within the IAEA Reference Input Parameter Library (RIPL) [4], used for determination of level density parameters [5], and electric dipole γ-ray strength functions $f_{E1}(E_\gamma)$ used for calculation of the γ-ray transmission coefficients and related capture cross sections.

2. Total neutron cross section analysis for the Hf, Ta and W isotopes up to 60 MeV

In order to get confidence in the activation calculation, firstly a detailed analysis of a global neutron optical potential for the rare-earth nuclei and total neutron cross section analysis for the Hf, Ta and W stable isotopes up to actually 100 MeV has been carried out. The DOM potential parameter sets have been established by analysis of the low-energy neutron scattering properties (S_0, S_1, *R'*) and neutron total cross sections, following the 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. The CC calculations were carried out assuming the coupling bases ($7/2^+$, $9/2^+$, $11/2^+$, $13/2^+$, $15/2^+$) for ^{181}Ta 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 below the incident energy of 1-2 MeV (Figure 1, left) and being also consistent with the deformation parameters predicted by nuclear structure calculations. CC calculations were carried out by using the rare earth – actinide average DOM of Young [6] (Set A of Table II), and a version slightly modified in order to describe better the data well above 20 MeV. The main change concerns the real-potential depth V_R. Actually there have been three modified versions of increased number of V_R forms necessary for a better description of the total neutron cross sections in the incident energy range 10-20 MeV but with similar behavior between 20 and 100 MeV (well shown by using the linear energy scale in Figure 1, right).

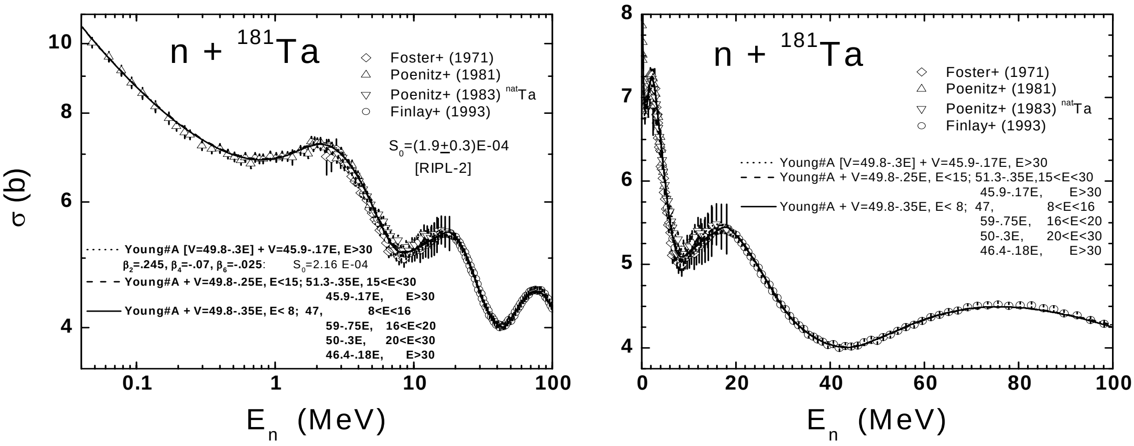


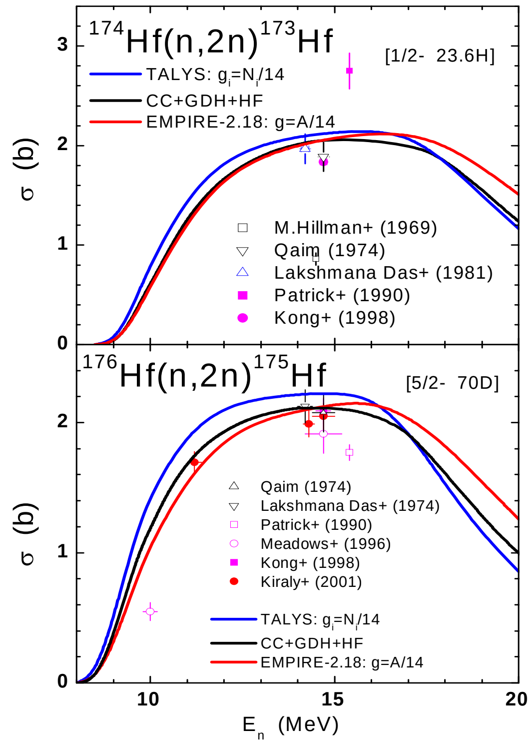
Figure 1. Comparison of calculated and experimental neutron total cross sections for the ^{181}Ta nucleus, with emphasis of the lower energy region (left).

Moreover, the simplest DOM modified version of the Set A have been used and found suitable also for stable isotopes of Hf, actually represented by the ^{178}Hf nucleus. There have been used in this respect the coupling bases (0^+, 2^+, 4^+) for ^{178}Hf with a quite good agreement with the experimental data in the whole energy range. However, since there are neutron total cross sections available only up to 20 MeV for the Hf element, the same analysis has been extended for the ^{182,183,184,186}W isotopes. Finally we may conclude that the modified extension up to 100 MeV of the global neutron optical potential for the rare-earth nuclei can be used with suitable confidence in further analysis of activation cross sections.

3. Activation including charged-particle emission analysis for the Hf stable isotopes

The above-mentioned global neutron optical potential for the rare-earth nuclei following the detailed analysis of total neutron cross section analysis for the Hf, Ta and W stable isotopes up to actually 100 MeV, adopted also previously [7] for W stable isotopes, has been used hereafter. Moreover, the neutron transmission coefficients provided by EMPIRE-II, already corrected for the direct inelastic scattering, were used also as input for TALYS and STAPRE-H calculations. The pre-equilibrium emission (PE) model Geometry-Dependent Hybrid (GDH) is used within the calculations by means of the code STAPRE-H, along with CC method and statistical Hauser-Feshbach model to analyze the fast-neutron interaction with ^{174,176,177,178,179,180}Hf isotopes. No free parameter was involved in the GDH calculations while the same common parameters of OMP and nuclear level density were used in the CC, GDH and HF model calculations. Thus, a proper description of a large body of data without free parameters may validate both the adopted nuclear model assumptions and parameter set.

The calculated activation cross sections are shown in Figs. 2-4, obtained with the STAPRE-H, EMPIRE-II and TALYS computer codes, are based on similar nuclear reaction models. The global predictions have been obtained by using the corresponding default single-particle level (s.p.l.) density values, i.e. $g=A/13$ MeV^{-1} by EMPIRE-II and $A/15$ MeV^{-1} by TALYS, respectively, as well as the alternate value $A/14$ MeV^{-1} which proved to be most suitable in the case of the W isotopes. Actually the present comparison with predictions of TALYS underlines the physical reason of some still existing discrepancies. Illustrative in this respect is the only large disagreement between the calculated and experimental data which exists for the reaction ^{178}Hf*(n,p)*^{178g}Lu. A quite similar disagreement is shown by the global EMPIRE-II and TALYS predictions.



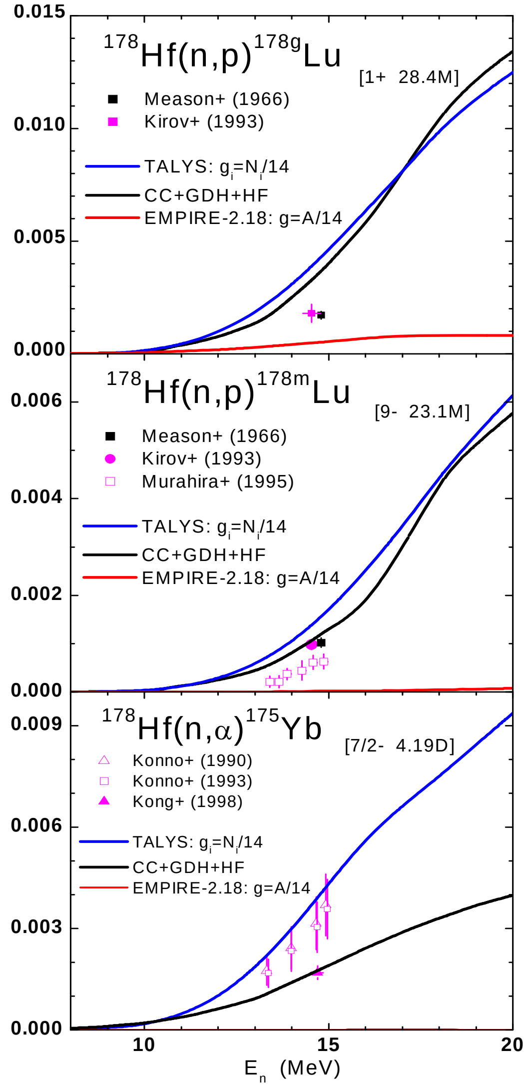
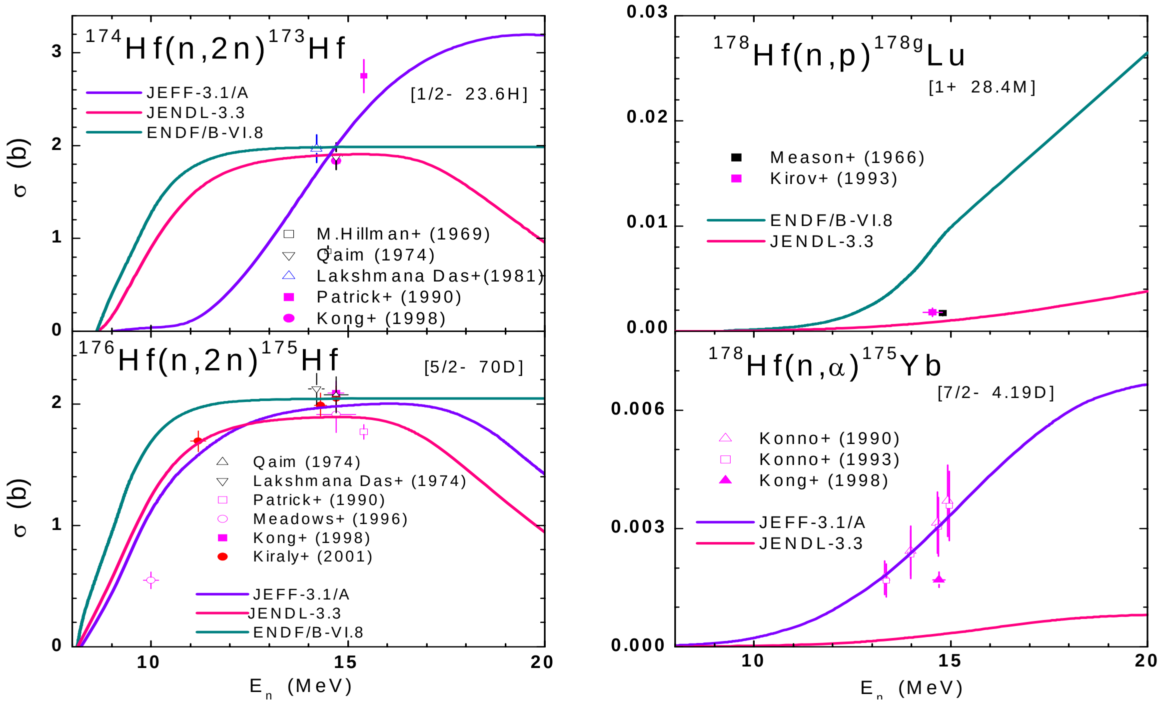


Figure 2. Comparison of calculated and measured neutron activation cross sections for ^{174,176,178}Hf nuclei (above and right) and available evaluated data (bottom).



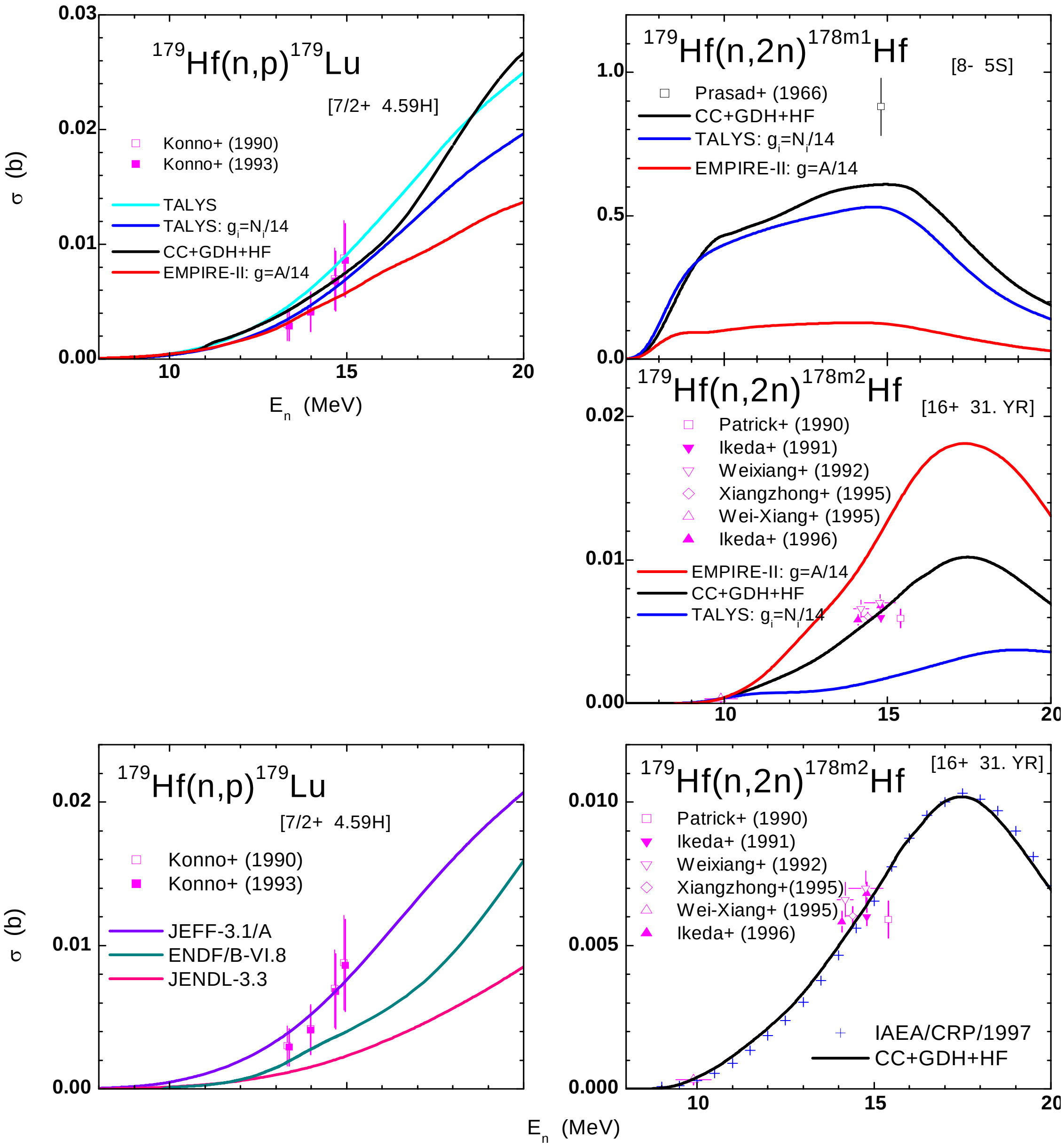


Figure 3. Comparison of experimental, calculated, and evaluated (bottom) reaction data of ^{179}Hf nucleus.

The agreement of STAPRE-H calculation results and measured low spin isomer data for the *(n,2n)* reaction on the ^{179,180}Hf target nuclei (Figs. 3,4) is decreased by the most probable missing known transitions between excited levels at higher energies and the related isomeric states ^{178m1,179m1}Hf. Thus it results a systematic underprediction of the corresponding isomeric cross sections. The same behavior was found earlier [8], while these schemes play a definite role also for the high-spin isomers ^{178m2,179m2}Hf at higher excitation. Thus, there are shown in Figure 5 the effects of various assumptions for the low-lying levels taken into account for the corresponding residual nuclei (on left) on the calculated high-spin isomeric cross sections (on right). The relative lack of sensitivity of the calculated activation of these low spin isomers ^{178m1,179m1}Hf with respect to the number of discrete levels taken into account is explained by the quite minor side feeding (i.e. by particle emission from the compound nucleus) of these levels, for incident energies E_n above ~12 MeV. Since it is even around 1% at E_n=15 MeV, the low-lying level population follows the continuum decay by γ-ray cascades. Therefore the observed lack of sensitivity is a proof of suitable level density and γ -ray strength function parameters.

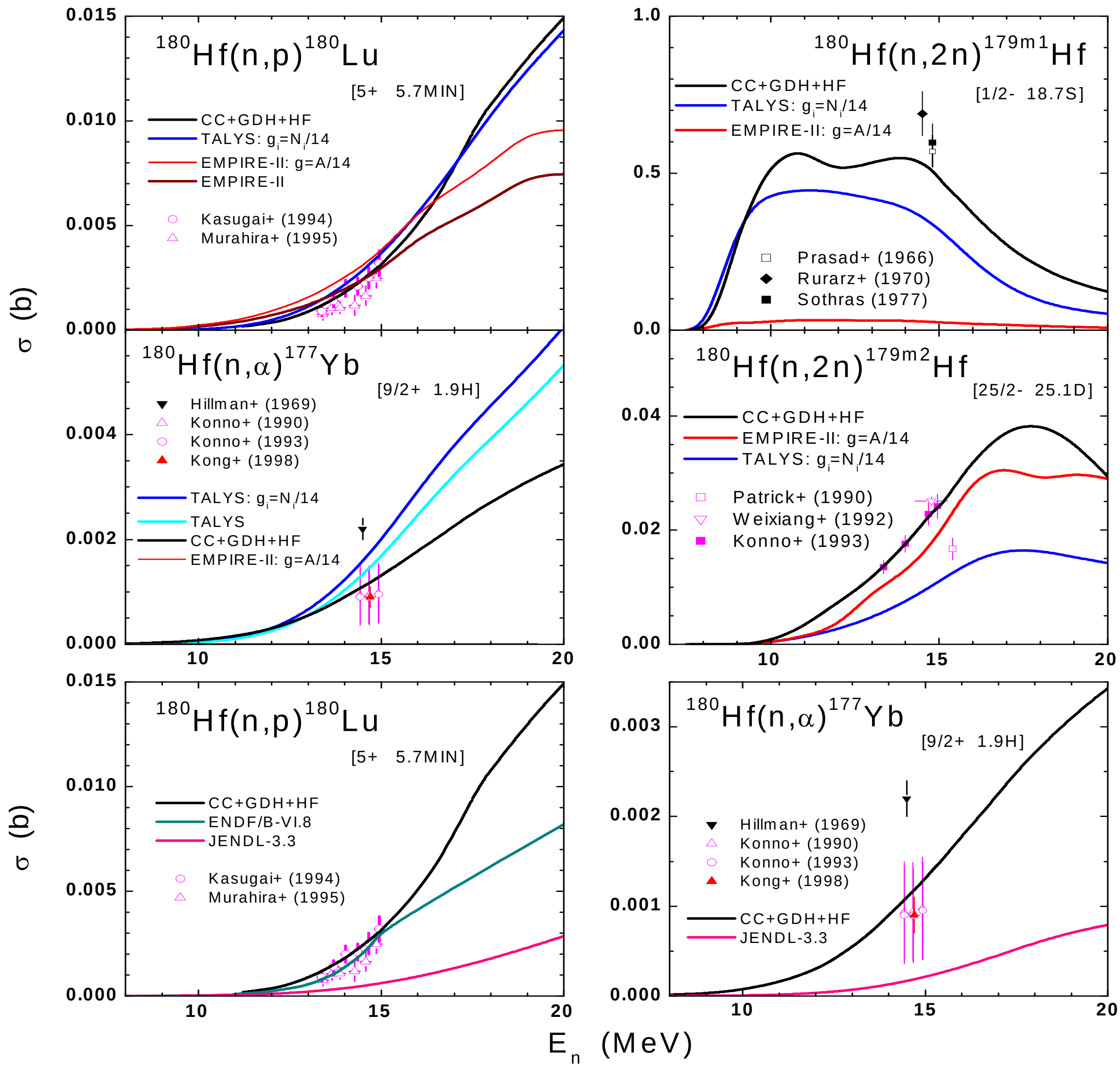


Figure 4. Comparison of experimental, calculated, and evaluated (bottom) reaction data of ^{180}Hf nucleus.

It results finally that the suitable consideration of the corresponding decay schemes is a definite need of the model calculations in order to provide accurate calculated cross sections without use of supplementary normalization. This has been shown also in the case of ^{179}Hf(n,2n)^{178m2}Hf reaction (Figure 3), which formed the object of an analysis [9] performed within an IAEA Coordinated Research Programme on activation cross sections for fusion reactor technology. However, the results obtained in the present work made use of no additional activation cross-section evaluation and complementary normalization of the calculated data to this evaluation, which was the case of the IAEA exercise. On the other hand, a detailed level scheme of the ^{178}Hf nucleus has become available only recently (e.g., Ref. [10]).

Finally, an overview of the calculated activation cross sections in the present work shows that differences between various evaluated data libraries are similar to those between model calculations using both global and local parameters, while the use of a consistent parameter set is able to provide a better general description of most of the reaction channels.

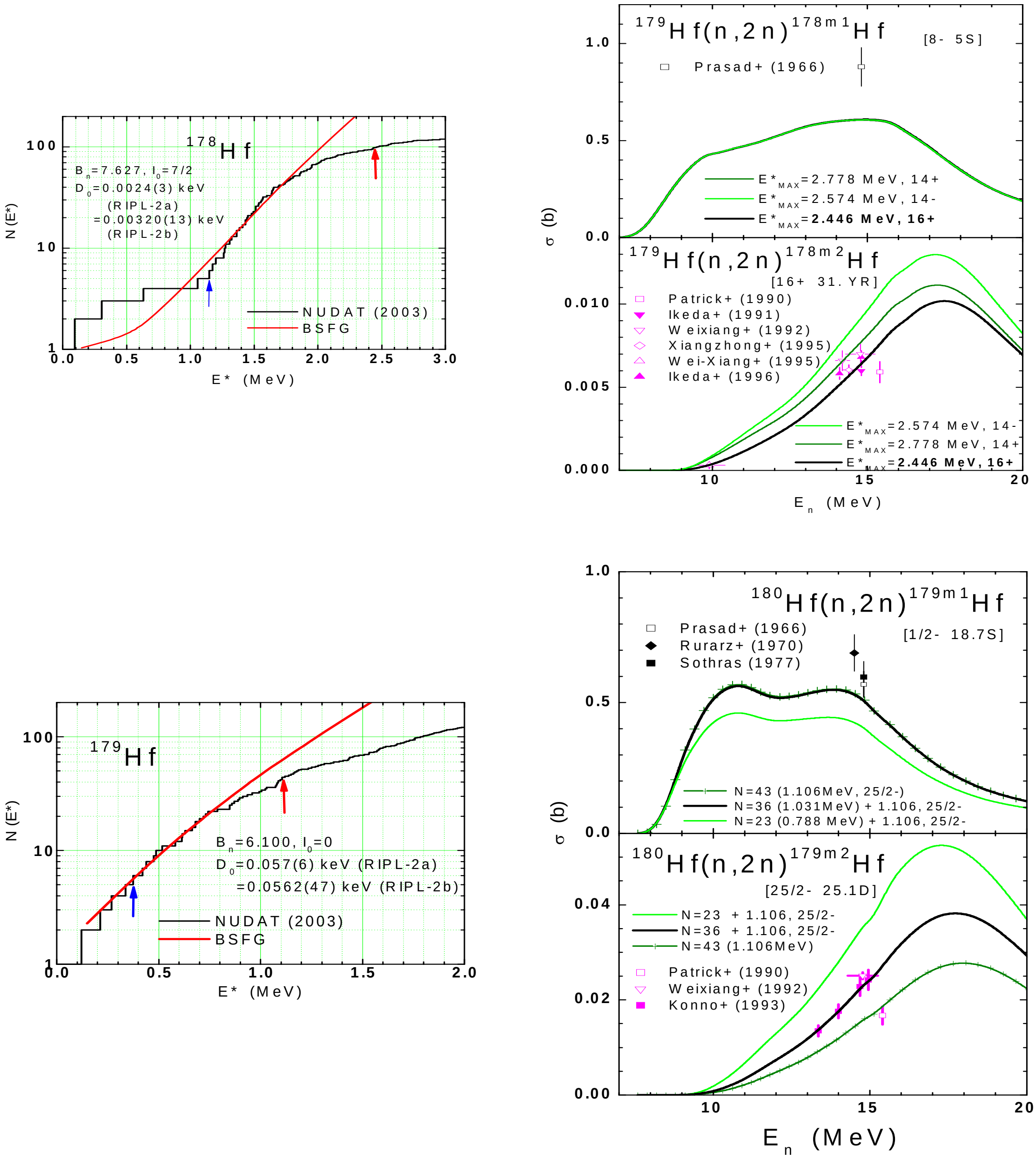


Figure 5. The effects of various assumptions taken into account for the low-lying levels taken into account for the corresponding residual nuclei (on left) on the calculated high-spin isomeric reaction cross sections, and the comparison(on right) of the latter to the experimental (n,2n) reaction cross sections of the ^{179,180}Hf nuclei.

4. The activation cross sections for the Hf and Ta stable isotopes up to 60 MeV

Following the former step of this work, devoted to comparison of the calculation results and experimental data available only up to E_n~20-24 MeV, it has been completed the main goal to obtain reliable cross section predictions for the stable Hf and Ta isotopes up to E_n=60 MeV. The results provided by the TALYS-0.64 and EMPIRE-II v.2.19 [11] codes are shown in Figs. 6-8, in comparison with the data at lower energies. This made possible also the comparison with the results obtained formerly with EMPIRE-II v.2.18, corresponding to the same input parameters excepting the Hybrid Monte-Carlo model for multiple PE which has to be taken into account for the neutron energies including those higher than 20 MeV. The last EMPIRE-II version has also taken the advantage of using the exciton PE model for cluster emission [11].

Finally, this comparison has supported both code predictions but especially the TALYS ones, in better agreement with the results of the local parameter analysis and the available experimental data up to 24 MeV as well. Therefore, the consistent results of the same computer code, i.e. TALYS-0.64, including the use of global as well as the two above-mentioned local parameter classes, were adopted in the whole energy range up to 60 MeV and for all reaction channels.

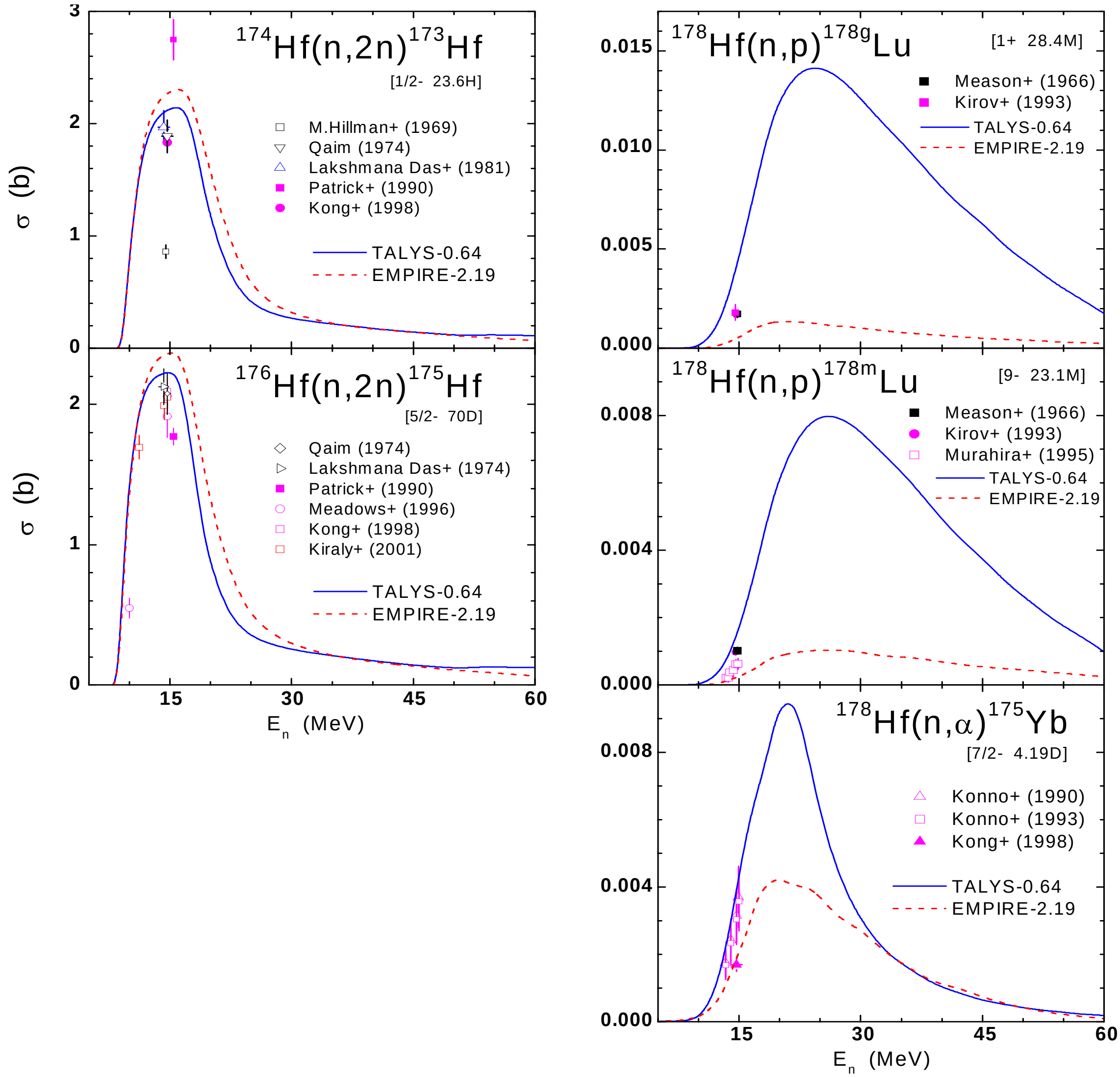


Figure 6. Comparison of experimental and calculated reaction cross sectons of ^{174,176,178}Hf nuclei for incident energies up to 60 MeV.

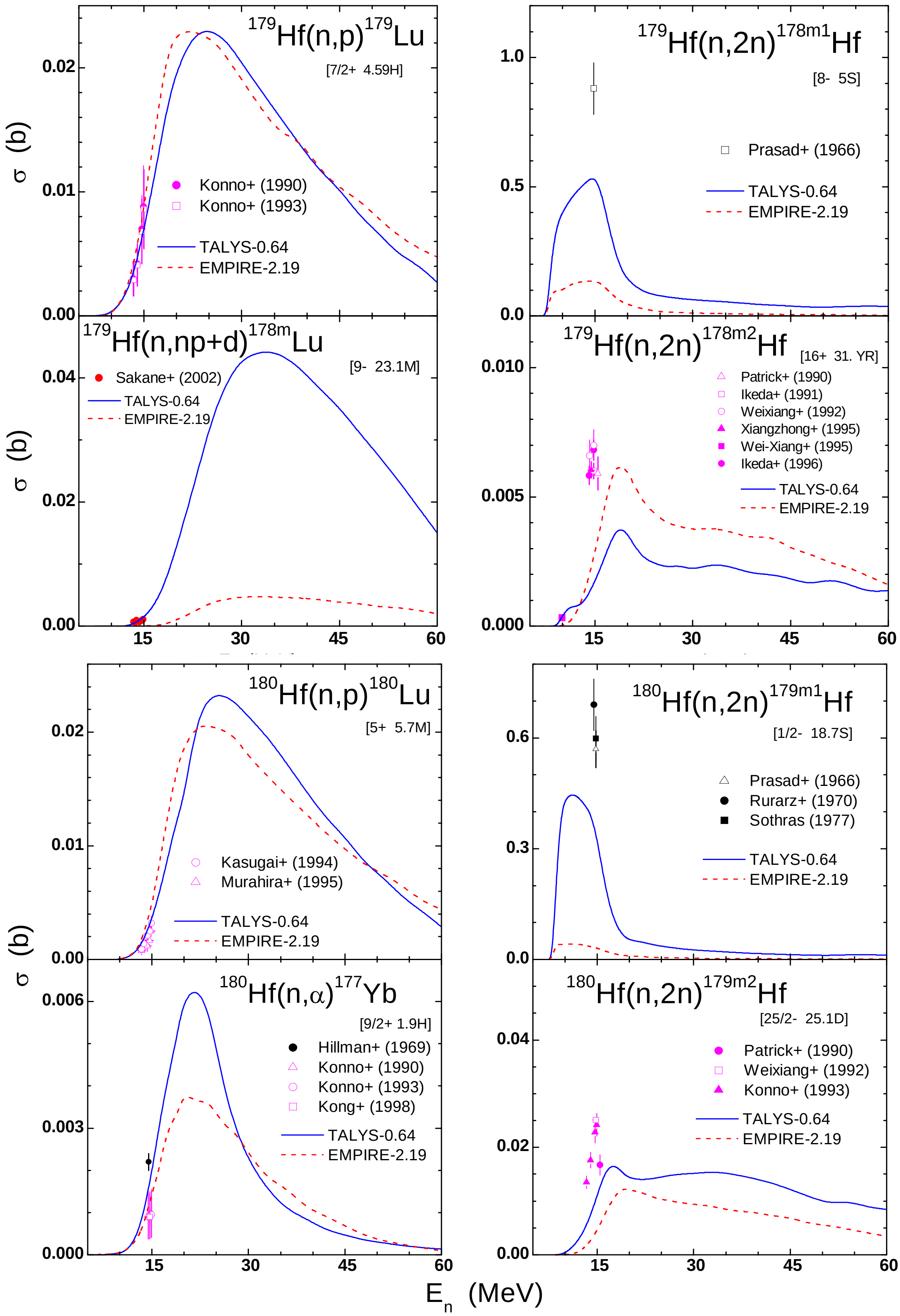


Figure 7. Comparison of experimental and calculated reaction cross sectons of ^{179,180}Hf nuclei for incident energies up to 60 MeV.

A particular point of these calculations concerned the optical potential for the emitted α-particles, which took into account the differences between the incident and emergent channels, respectively, based on a semi-microscopic double-folding (DF) model analysis [12].

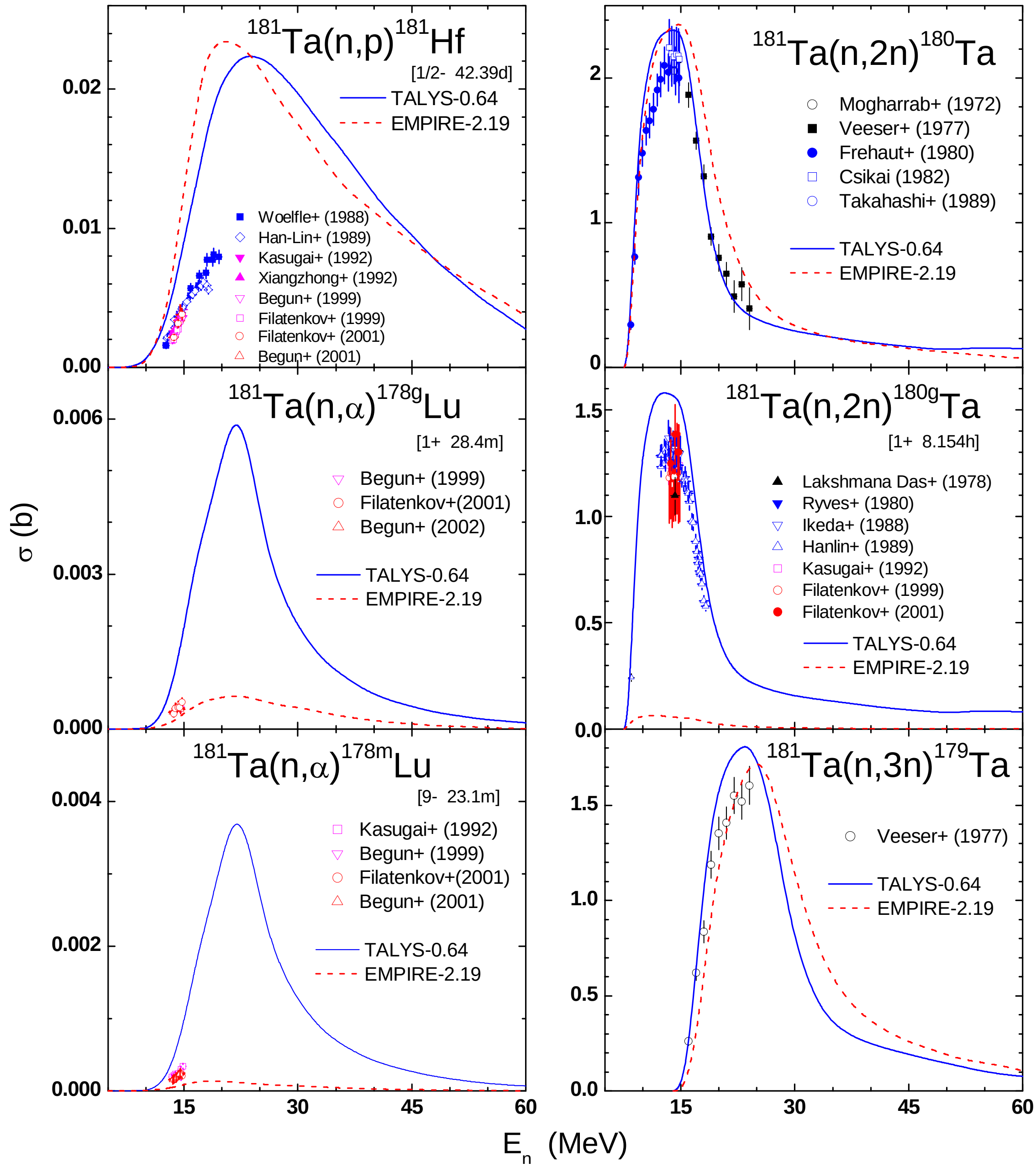


Figure 8. Comparison of experimental and calculated reaction cross sections of the ^{181}*Ta nucleus for incident energies up to 60 MeV.*

5. Conclusions

The present systematic analysis of the activation cross sections for all Hf, Ta, and W stable isotopes makes possible a closer look on the large disagreement between the calculated and experimental data for the reaction ^{181}Ta*(n,p)*^{181}Hf, which has been reported [13-15]. A rather similar disagreement is shown by the global TALYS and EMPIRE-II predictions as well as the local STAPRE-H analysis, while a general good agreement has been obtained for the rest of the Hf, Ta, and W stable isotopes. However, in the present case we may rely on the *isotopic effect* for the Hf and W isotopes, consisting in the experimental observation that the *(n,p)* reaction cross sections around E_n=15 MeV for a given element decrease with increasing mass number A of the isotope. The rather similar Q-values for the ^{179}Hf, ^{181}Ta, and ^{183}W odd-A target nuclei, having close asymmetry-parameter values too, suggest similar *(n,p)* reaction cross sections which are predicted by all three code calculations at variance with the consistent lower measured data. It is thus motivated the assumption of a longer-life isomer state of the ^{181}Hf nucleus, not yet observed but also in agreement with the related systematics of the Hf isotopes. Further measurements taking into account this possibility would be quite helpful in this respect.

6. Forecast progress for next year (2006)

Calculation of activation cross sections for the Mn and Cu stable isotopes up to 60 MeV, to be carried on within the EFDA task TW6-TTMN-001 (EFF/EAF data file upgrade, processing and benchmark analysis) as the deliverable No. 6, will be based on the same nuclear reaction models and related parameter sets. The calculated activation data will be used as input to both the *European Activation File* (EAF) and *European Fusion File* (EFF) libraries which are the well-qualified nuclear database and validated computational tools to provide the basis for reliable neutronics activation and transport calculations and the assessments of the associated uncertainties, within the EU-conducted unique effort on nuclear data for fusion application.

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