

PADF-2. Data for stable isotopes of Cl, K, Sc, and Ti

A.Yu. Konobeyev¹, A. Stankovskiy², D. Leichtle¹, D. Koliadko¹, A. Klix¹

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¹ Institute for Neutron Physics and Reactor Technology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

² Belgian Nuclear Research Centre, SCK CEN, Boeretang 200, B-2400 Mol, Belgium

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Abstract

The cross-sections for proton interactions with stable isotopes of chlorine, potassium, scandium, and titanium were obtained for energies ranging from the reaction threshold up to 200 MeV. The study comprised model-based calculations, analysis of experimental data, and evaluation of resulting cross-sections.

For reactions lacking experimental data, the cross-sections were estimated based on calculated results, considering the accuracy and predictive capability of different models across various energy ranges.

The resulting data files can be accessed and downloaded from the KIT Cloud at <https://bwsyncandshare.kit.edu/s/YwCwKH5qSjBPjfx>

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1. INTRODUCTION

This work is a continuation of other published works [1-3] dedicated to the creation of the PADF-2 file.

The report describes the evaluation of cross-sections for stable isotopes of chlorine $^{35,37}\text{Cl}$, potassium $^{39,40,41}\text{K}$, scandium ^{45}Sc , and titanium $^{46,47,48,49,50}\text{Ti}$ at incident proton energies up to 200 MeV.

In this work, as in Refs. [1-3], all available experimental data for the targets under consideration were used - independent and cumulative measurements were utilized for individual target isotopes, as well as for natural isotopic mixtures.

The calculations were performed using advanced methods and the most recent releases of the computer codes applied also in Refs. [1-3].

The resulting files contain cross-sections of all observed reactions, provided and not provided by experimental data. They also include the total production cross-sections of neutrons, protons, deuterons, ^3He , α -particles, and heavy fragments.

Section 2 describes the cross-section calculation methods, Section 3 discusses the use of experimental data, Section 4 details the cross-section evaluation, and Section 5 presents the results.

2. CROSS-SECTION CALCULATION

As in works [1-3] the calculations were performed using current versions of the codes ALICE/ASH [4-6], CEM [7,8], PHITS [9,10], TALYS [11,12], and TALYS-G [13-15]. The calculations using TALYS-2.0 [12] were carried out using various models describing the level density of excited states and corresponding to the input code parameters *ldmodel* equal to 1, 2, and 3. The optimal parameters of the models obtained by the authors [12] were applied by including the value "fit y" for the parameters *ldmodel* equal to 1 and 2 in the input data file.

The spread of the calculation results and the use of different methods and codes in various ranges of energies and residual nuclei are discussed in work [3]. This includes an explanation of the use of a weighted sum of calculated cross-sections.

3. EXPERIMENTAL DATA

The experimental data were taken from EXFOR [16]. Auto-corrections, available on the website, were applied for the monitor cross-sections and decay data.

Before use, the experimental data were analysed by consulting the original publications and, in some cases, the results of theoretical calculations. The following considerations needed to be addressed, and the necessary cross-section corrections performed if required:

- Is the reaction cross-section independent or cumulative in the energy range under consideration? The results of calculations performed using CEM, PHITS, and TALYS were used as a basis for the answer.
- If comprehensive information on the used monitor reaction cross-sections is available, the measured cross-section should be corrected using the new monitor cross-sections, if exist. For some reactions, the automatic renormalization of cross-sections available on the EXFOR website was applied. For other reactions the corrections were made in this work.
- If a cross-section is presented in EXFOR as “partial” (PAR,SIG), can it be used as the total cross-section within a certain energy range of primary protons? The results of calculations using the TALYS code [12] were used to answer this question.

Below are comments explaining the use of measured data in specific cases.

Only publications, reactions, and nuclides for which changes have been made or the information about which is necessary for the explanations given below are considered here. If the changes were applied using the auto-correction feature on the EXFOR website or were not made at all, the measurement is not mentioned here. Experimental works [17-49] are cited mainly based on EXFOR entries and are listed in the bibliography alphabetically.

3.1 Chlorin

Following the analyses with TALYS, PHITS, and CEM, all available measurements of ^{22}Na and ^{24}Na yields were considered cumulative, due to potential contributions from their precursors, ^{22}Mg and ^{24}Ne , respectively.

R.Bimbot, H.Gauvin (1971) [19]. Data measured for ^{34m}Cl were corrected at 50 MeV using new cross-section [50] for the monitor reaction $^{27}\text{Al}(p,x)^{22}\text{Na}$.

R.G.Korteling, A.A.Caretto (1970) [31]. The cross-sections for the $^{\text{nat}}\text{Cl}(p,x)^{22}\text{Na}$ and $^{\text{nat}}\text{Cl}(p,x)^{24}\text{Na}$ reaction were adjusted based on the updated monitor reaction cross-section value for $^{27}\text{Al}(p,x)^{22}\text{Na}$ and $^{27}\text{Al}(p,x)^{24}\text{Na}$ from IAEA NDS at 100 MeV [50] and PADF-2 at 200 MeV [51-53]. The authors of Ref.[31] had used a monitor cross-section for $^{27}\text{Al}(p,x)^{22}\text{Na}$ at 100 MeV that is 20% lower than the updated value [50]. As a result, the cross-sections here are higher than those in Ref.[31].

The evaluated data for ^{22}Na production are based on the assumption that the $^{27}\text{Al}(p,x)^{22}\text{Na}$ reaction was used to determine the ^{22}Na yield for all target nuclei in Ref.[31], while the $^{27}\text{Al}(p,x)^{24}\text{Na}$ reaction was used for the ^{24}Na yield. This assumption is also reflected in the corresponding EXFOR file entries. However, the authors of Ref.[31] did not specify how exactly the $^{27}\text{Al}(p,x)^{22}\text{Na}$ and $^{27}\text{Al}(p,x)^{24}\text{Na}$ monitor reactions were applied. If the assumption is incorrect and both monitor reactions were actually used to determine the ^{22}Na yield, then the currently evaluated ^{22}Na production cross-section would be somewhat overestimated.

H.Lundqvist, P.Malmborg (1979) [35]. The measured ^{24}Na cross-sections using the monitor reaction cross-section $^{27}\text{Al}(p,x)^{24}\text{Na}$ of J.B. Cumming [22] were corrected using cross-section from Ref.[50] below 100 MeV and from Ref.[51] above 100 MeV.

The measurements of ^{28}Mg were treated as independent, based on an analysis of potential precursor contributions using nuclear modelling codes.

G.F.Steyn et al (2007) [48]. The yield of ^{28}Mg was considered as independent after the analysis using results of calculations.

3.2 Potassium

3.2.1 Natural potassium

M.Imamura et al. (1997) [28]. The data, originally obtained using $^{27}\text{Al}(p,x)^{22}\text{Na}$ monitor cross-sections from Ref.[47], were improved by applying IAEA monitor cross-sections [50].

R.G.Korteling, A.A.Caretto (1970) [31]. Based on the analysis using TALYS, PHITS, and CEM, the measurements of ^{22}Na and ^{24}Na were interpreted as cumulative, reflecting contributions from their respective precursors, ^{22}Mg and ^{24}Ne .

The cross-sections were adjusted based on the updated monitor reaction cross-sections for $^{27}\text{Al}(p,x)^{22}\text{Na}$ and $^{27}\text{Al}(p,x)^{24}\text{Na}$. See comments in Section 3.1.

H.Lundqvist, P.Malmborg (1979) [35]. The data for ^{24}Na were considered as cumulative and for ^{28}Mg as independent basing on codes calculations. All measurements were corrected using new values of monitor reaction cross-section, see comments in Section 3.1.

3.2.2 Potassium-39

M.Imamura et al. (1997) [28]. The data were improved by applying new monitor cross-sections [50].

3.2.3 Potassium-40

M.E.Sevior et al. (1986) [45]. Data for investigated reactions were transformed from the CM to the lab system.

Measured data for the (p,α) reaction for the ground state and first excited state of ^{38}Ar were summed to obtain the total (p,α) cross-section at proton energies up to 2.6 MeV.

Measured data for the (p,p') reaction for first five excited states were summed to obtain the total (p,p') cross-section at proton energies up to 1.86 to 2.6 MeV. The necessary correction was made using TALYS calculations with the input parameter *ldmodel* equal to 1 and 2.

M.E.Sevior et al. (1982) [44]. The data for all reactions were not used, as the authors of Ref. [45] stated that their work repeats the earlier measurements [44] with better statistics.

3.3 Scandium

L.Daraban et al. (2009) [23]. The measured data were normalized using new cross-section values [50] for the monitor reaction $^{\text{nat}}\text{Ti}(p,x)^{48}\text{V}$. The monitor cross-sections used in the Ref.[23] were taken from Refs.[54,55]

T.McGee et al. (1970) [27]. All measurements were normalized using PADF-2 cross-sections [51]. Old monitor data were taken from Table 2 [27]. The sum of two cross-sections $^{63}\text{Cu}(p,2n)^{62}\text{Zn}$ and $^{65}\text{Cu}(p,4n)^{62}\text{Zn}$ was calculated taken into account the contributions of ^{63}Cu and ^{65}Cu in natural copper mixture.

M.Lagarde-Simonoff et al. (1975) [33]. All measurements were normalized using cross-sections for monitor reaction $^{27}\text{Al}(p,x)^{22}\text{Na}$ from Ref.[50].

V.N.Levkovskij (1979) [34]. Data were corrected for ^{45}Sc target using the recommended value of 192.8 mb for the reaction $^{\text{nat}}\text{Mo}(p,x)^{96}\text{Tc}$ at 30 MeV [50].

For the other targets considered in this report, the cross-sections measured in Ref.[34] were normalized to the 190.8 mb value used in the auto-correction on the EXFOR page. At the same time, there is every reason to believe that the value of 192.8 mb is more accurate.

3.4 Titanium

Various works. All measurements of ^{43}K and ^{41}Ca production were considered as independent.

The calculated total contribution of ^{43}Ar and ^{43}Cl at proton energies up to 200 MeV does not exceed 0.21% (TALYS), 0.49% (PHITS), and 0.51% (CEM) of the production of ^{43}K . The contribution of ^{41}Sc in ^{41}Ca yield at proton energies up to 150 MeV, which is the maximum energy of measurements relevant for this work, is less than 0.45% (TALYS), 0.23% (PHITS), and 0.24% (CEM).

Based on the analysis of experimental data, all measurements of the ^{47}Sc yield were treated as independent for proton energies up to 200 MeV. This also includes the measurements labelled as “cumulative” in EXFOR.

All measurements of the ^{44}Ti production were considered as independent, including those which were marked as “CUM” or “(CUM)” in the reaction description in EXFOR. The reason is that the contribution of ^{44}V for natural titanium up to 200 MeV does not exceed 0.012% (TALYS), 0.16% (PHITS), and 0.15% (CEM) of the production of ^{44}Ti .

A. Azzam et al. (2020) [17]. The yield of ^{44}Sc presented in EXFOR file D0978003 was interpreted as ^{44g}Sc .

C.M.Bäcker et al (2021) [18]. Data for the reactions $^{\text{nat}}\text{Ti}(p,x)^{38}\text{Cl}$, $^{\text{nat}}\text{Ti}(p,x)^{39}\text{Cl}$, $^{\text{nat}}\text{Ti}(p,x)^{41}\text{Ar}$, and $^{\text{nat}}\text{Ti}(p,x)^{44}\text{K}$ were adopted as independent after the analysis of results of calculations.

R.L.Brodzinski et al. (1971) [20]. Data at 118 MeV were corrected using monitor cross-section for $^{27}\text{Al}(p,x)^{24}\text{Na}$ from PADF-2 [51] equal to 10.69 mb.

Data at 45 MeV were not changed due to the absence of information about monitor cross-section.

J.P.Cohen et al. (1965) [21]. The measured cross-sections were renormalized using the new value for the $^{12}\text{C}(p,pn)^{11}\text{C}$ reaction cross-section [51]. The data were multiplied by 1.22.

D. Fink et al. (1990) [24]. Data in file C0430004 were interpreted as referring to ^{44g}Sc . M.B.Fox et al. (2021) [25]. The measured cross-sections for ^{43}Sc reported in EXFOR as cumulative (C2702048) were treated as independent, since the contribution of ^{43}Ti for a natural titanium at proton energies up to 200 MeV does not exceed 0.30% (TALYS), 0.76% (PHITS), and 0.91% (CEM) of the ^{43}Sc production.

E.Gadioli et al. (1981) [26]. Measured data were normalized to new values of the monitor reaction cross-sections for the $^{63}\text{Cu}(p,n)^{63}\text{Zn}$ reaction below 20 MeV and the $^{65}\text{Cu}(p,x)^{64}\text{Cu}$ reaction above 25 MeV.

Data for ^{50}Ti , presented as "derived data" in EXFOR file D4060, were used for the evaluation. According to the authors, these constitute "recommended experimental data for the pure ^{50}Ti target", Table 5 [26].

M.U.Khandaker et al. (2009) [30]. The measured yields of ^{44g}Sc compiled in the EXFOR file D0569005 as "-G,M+,SIG"- data, were considered as not containing any contribution from ^{44m}Sc .

R.G.Korteling, A.A.Caretto (1970) [31]. After the analysis using TALYS, PHITS, and CEM the measurements for reactions $^{\text{nat}}\text{Ti}(p,x)^{22}\text{Na}$ and $^{\text{nat}}\text{Ti}(p,x)^{24}\text{Na}$ were treated as cumulative, due to possible contributions of precursors, ^{22}Mg and ^{24}Ne .

The measured cross-sections were normalized taking using new value of the monitor reaction cross-section for $^{27}\text{Al}(p,x)^{22}\text{Na}$ and $^{27}\text{Al}(p,x)^{24}\text{Na}$ [50,51].

It should be noted that the value of the monitor cross-section of the $^{27}\text{Al}(p,x)^{22}\text{Na}$ reaction used by the authors of Ref.[31] at an energy of 100 MeV is 20% lower than the new value [50]. Accordingly, the cross-sections used in the present work are noticeably higher than those presented by the authors of Ref.[31].

The present work proceeds from the fact that the $^{27}\text{Al}(p,x)^{22}\text{Na}$ reaction was used to get the yield of ^{22}Na for all target nuclei studied in Ref.[31] and the $^{27}\text{Al}(p,x)^{24}\text{Na}$ reaction was used for the yield of ^{24}Na . The compiler of the corresponding EXFOR files also assumes this. At the same time, it should be noted that the authors of Ref.[31] did not provide detailed information on how both monitor reactions $^{27}\text{Al}(p,x)^{22}\text{Na}$ and $^{27}\text{Al}(p,x)^{24}\text{Na}$ used in Ref.[31] were applied.

If the assumption made in this report is incorrect and both above mentioned monitor reactions were used to measure yield of ^{22}Na , the value of the ^{22}Na production cross-section should be somewhat lower.

M.S.Lafleur et al. (1966) [32]. Measured ^7Be yields were corrected using new monitor cross-sections from IAEA NDS [50].

L.F.Mausner et al.(1998) [36]. Data were corrected using monitor cross-sections [50].

Data from EXFOR file C2614003 (ratios) were applied to derive cross-sections for $^{44\text{m}}\text{Sc}$ and ^{46}Sc . Firstly the $^{\text{nat}}\text{Ti}(p,x)^{47}\text{Sc}$ cross-section was evaluated (Section 4) using available experimental data and then the $^{48}\text{Ti}(p,x)^{47}\text{Sc}$ cross-section, which was used to get values for $^{44\text{m}}\text{Sc}$ and ^{46}Sc by irradiation of ^{48}Ti .

R.Michel, R.Stück (1984) [39]. Data were corrected using IAEA NDS monitor cross-section for $^{27}\text{Al}(p,x)^{22}\text{Na}$ [50]. The monitor cross-sections used by the authors were taken from Ref.[38].

R.Michel et al. (1985) [38]. Data were corrected using new monitor cross-sections from Ref.[50].

R.Michel et al. (1997) [37]. All measured cross-sections were corrected using monitor cross-sections [37] and new data for $^{27}\text{Al}(p,x)^{22}\text{Na}$ reaction from IAEA NDS [50].

S. Neumann (1999) [40]. Measured data were corrected using monitor cross-section for $^{27}\text{Al}(p,x)^{22}\text{Na}$ from Ref.[50]. Monitor data used by author were taken from EXFOR file A0497002 [47].

S.M.Qaim et al. (2010) [41]. Data for the reaction $^{\text{nat}}\text{Ti}(p,x)^{45}\text{Ca}$ compiled in EXFOR as independent (D0608002) were considered as cumulative, because of the contribution of ^{45}K for natural titanium up to 200 MeV is up to 0.78% (TALYS), 2.25% (PHITS), and 2.42% (CEM) of the production of ^{45}Ca .

S.Regnier et al. (1977) [43]. Measured cross-sections for $^{\text{nat}}\text{Ti}(p,x)^{36}\text{Cl}$ were corrected as above.

Yields of ^{38}Cl , ^{39}Cl , ^{41}Ar , and ^{44}K were considered as independent. For the $^{\text{nat}}\text{Ti}(p,x)^{38}\text{Cl}$ cross-section, the contribution of ^{38}S up to 130 MeV does not exceed 0.42% (TALYS), 0.55% (PHITS), and 0.47% (CEM) of the production of ^{38}Cl . For $^{\text{nat}}\text{Ti}(p,x)^{39}\text{Cl}$ the part of ^{39}S in the production of ^{39}Cl up to 130 MeV is less than 0.05% (TALYS), 0.14% (PHITS), and 0.10% (CEM). For $^{\text{nat}}\text{Ti}(p,x)^{41}\text{Ar}$ contribution of ^{41}Cl in the yield of ^{41}Ar does not exceed 0.30% (TALYS), 0.61% (PHITS), and 0.56% (CEM). The contribution of ^{44}Ar for each titanium isotope up to 130 MeV does not exceed 0.13% (TALYS), 0.48% (PHITS), and 0.48% (CEM) of the production of ^{44}K .

The ^{44g}Sc yield from the EXFOR file O2560008 marked as “-G,(M),SIG”- data, was considered to be free of contribution from ^{44m}Sc .

S.Regnier (1979) [42]. The EXFOR entry O0095024 defines the data for the reaction $^{\text{nat}}\text{Ti}(p,x)^{36}\text{Ar}$ as “uncertain if cumulative”. In the present work, at least at 150 MeV, data were adopted as independent. The contribution of ^{36}K f up to 150 MeV does not exceed 0.021% (TALYS), 0.009% (PHITS), and 0.013% (CEM) of the production of ^{36}Ar . The contribution of ^{36}Ca is even much lower.

A similar situation occurs with measurements for the $^{\text{nat}}\text{Ti}(p,x)^{42}\text{Ar}$ reaction, which also were considered as independent. Here, the contribution of ^{42}Cl is no more than 0.059% (TALYS), 0.26% (PHITS), and 0.19% (CEM) of the production of ^{42}Ar .

Data for all reactions were corrected at 150 MeV using IAEA NDS monitor cross-section for $^{27}\text{Al}(p,x)^{22}\text{Na}$ [50].

M.Shahid et al. (2018) [46]. The measured ^{44g}Sc yields, presented in the EXFOR file D7033005 as “-G,M+,SIG”- data, were considered to be free of contribution from ^{44m}Sc .

L.Valentin (1965) [49]. Measured cross-sections were corrected using new values of cross-sections for monitor reaction $^{12}\text{C}(p,pn)^{11}\text{C}$ [51].

4. CROSS-SECTION EVALUATION

Using cross-section values obtained via various methods and codes, "average calculated values" were computed. These values were calculated using weights that reflect the applicability of the models across different energy ranges of primary particles and residual nuclei [3].

Where experimental data were available, the resulting average calculated values and measurement data were used to derive the final evaluated data.

In general, for each reaction, there is a noticeable spread in the values calculated using different models and codes.

To avoid creating a misleading impression regarding the quality of any specific model based on a limited number of illustrations, the Figures below present only the experimental data, the averaged curve derived exclusively from calculation results using various models, and the final evaluated data. The experimental data shown in the Figs.1-8 are taken from Refs. [17-20,23-25,27,29-31,34,35,37,39,40-42,46,48,56-88].

Figures 1-4 show data examples for chlorine, scandium, and titanium. Figures with calculation results obtained using all applied methods and computer codes for all reactions are available upon request [89].

When preparing the evaluated data in this work, information on reaction cross-sections used for medical applications from IAEA NDS [90] was utilized. For some reactions, the data from Ref.[90] were not adopted, and for such reactions a new evaluation of the cross-sections was carried out either over the full energy range or within a limited range. Examples of such evaluations for the reactions $^{45}\text{Sc}(p,n)^{45}\text{Ti}$ and $^{45}\text{Sc}(p,2n)^{44}\text{Ti}$ are shown in Figs. 5 and 6. The new evaluation reflects the availability of new measurements, the correction of the (p,n) reaction threshold, and was performed over the entire energy range up to 200 MeV.

Another example of a new evaluation is shown for the $^{\text{nat}}\text{Ti}(p,x)^{48}\text{V}$ reaction in Fig. 7. The cross-sections [90] are available in the range from 3.8 to 100 MeV. Significant differences between the present evaluation and the data [90] are observed below 4.9 MeV. The only contribution to the $^{\text{nat}}\text{Ti}(p,x)^{48}\text{V}$ reaction at such energies comes from the $^{47}\text{Ti}(p,\gamma)^{48}\text{V}$ reaction. The corresponding cross-section is shown in Fig. 8. The energy range covered by the experimental data [29] extends from 0.76 to 4.1 MeV. The evaluated values of the (p, γ) cross-section presented in Fig. 8 and the results of TALYS calculations support the lower evaluated cross-section values of the $^{\text{nat}}\text{Ti}(p,x)^{48}\text{V}$ reaction at energies up to 4.9 MeV compared with the evaluation [90], Fig. 7.

5. RESULTS

The evaluation was performed for the cross-sections of all energetically possible reactions.

The resulting data were written in ENDF format in two different ways: in the first case, the files were recorded with MF=10 and MT=5, and in the second case, some of prepared files were integrated into general-purpose JEFF-4.0 files using MF=6 and MT=5 section.

In the file description section (MF=1, MT=451) the experimental data employed are listed in detail, along with information on any cross-sections adopted from Ref.[90], if applicable.

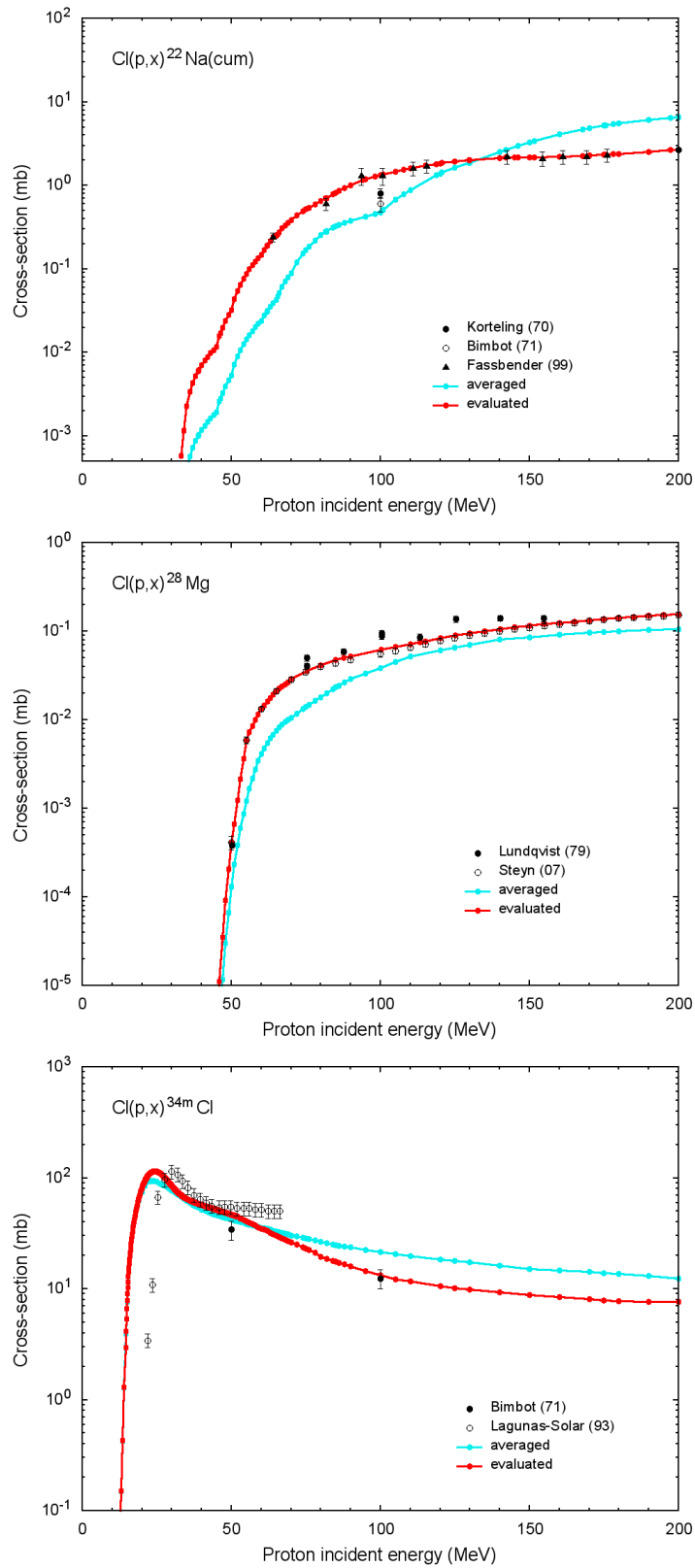


Fig.1 Example of cross-sections evaluated for natural chlorine. "Averaged" is the curve obtained by averaging the calculated data with weights corresponding to the applicability of the codes in different energy and residual nuclei ranges, "evaluated" is the final evaluation. See the explanations in the text.

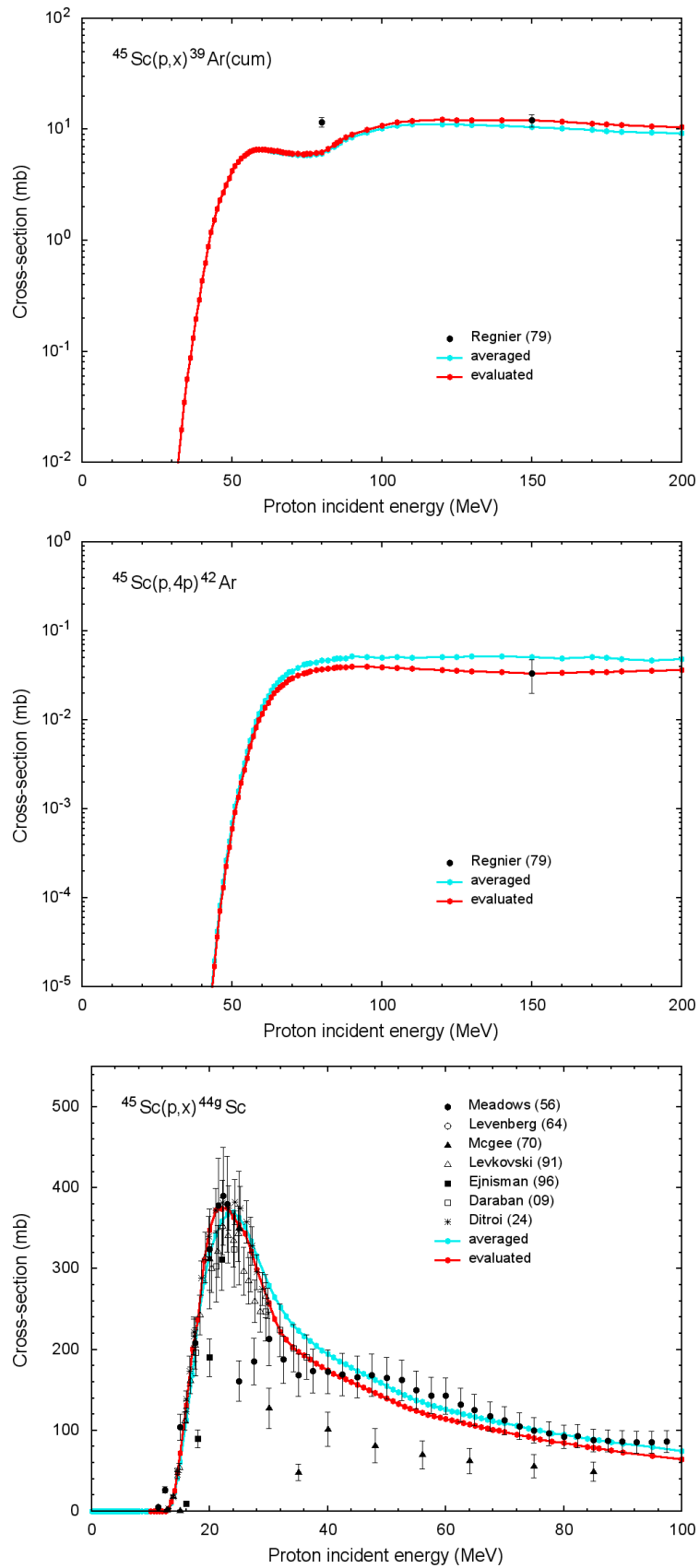


Fig.2 Example of cross-sections evaluated for ^{45}Sc . The data for the $^{45}\text{Sc}(p,x)^{44g}\text{Sc}$ reaction are presented on a linear scale and up to 100 MeV for clarity. See comments to Fig.1.

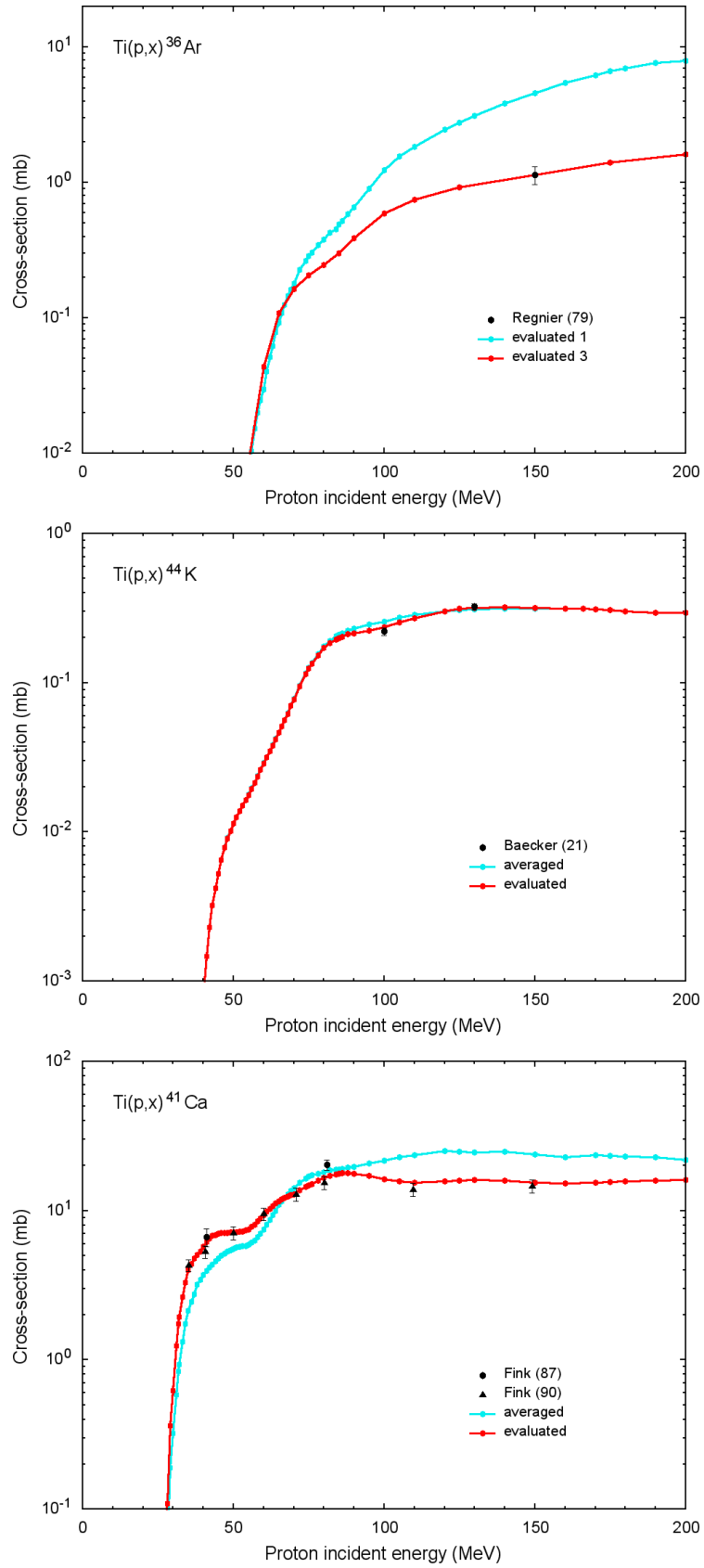


Fig.3 Example of cross-sections evaluated for titanium. See comments to Fig.1.

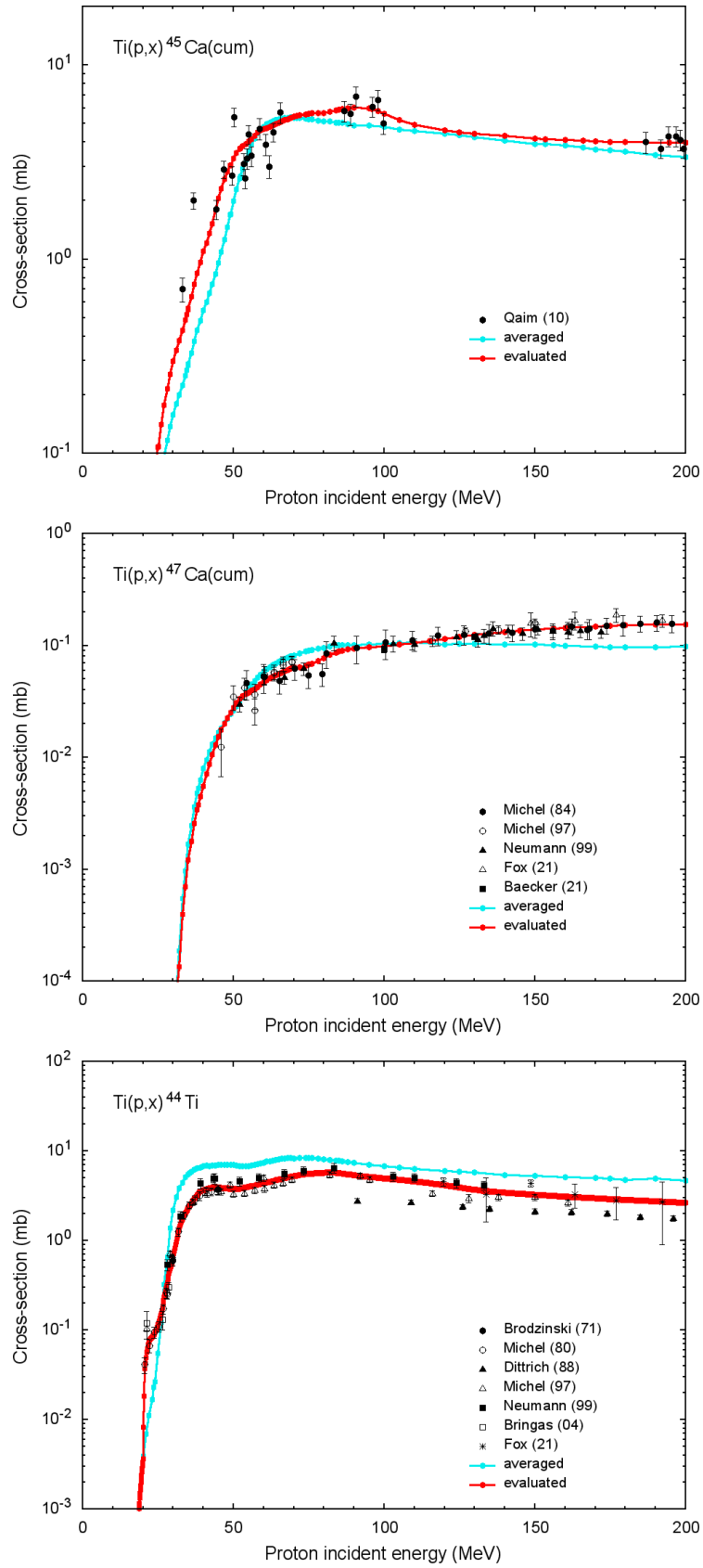


Fig.4 Example of cross-sections evaluated for titanium. See comments to Fig.1.

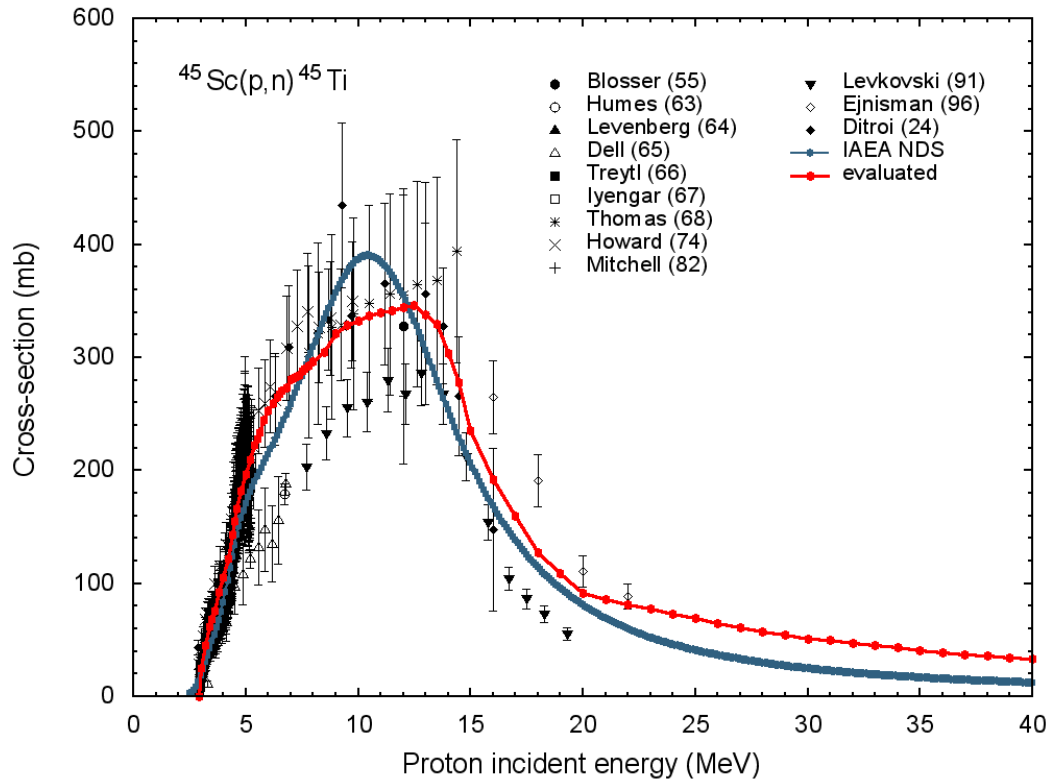


Fig.5 Cross-section for the $^{45}\text{Sc}(p,n)^{45}\text{Ti}$ reaction. See the explanations in the text.

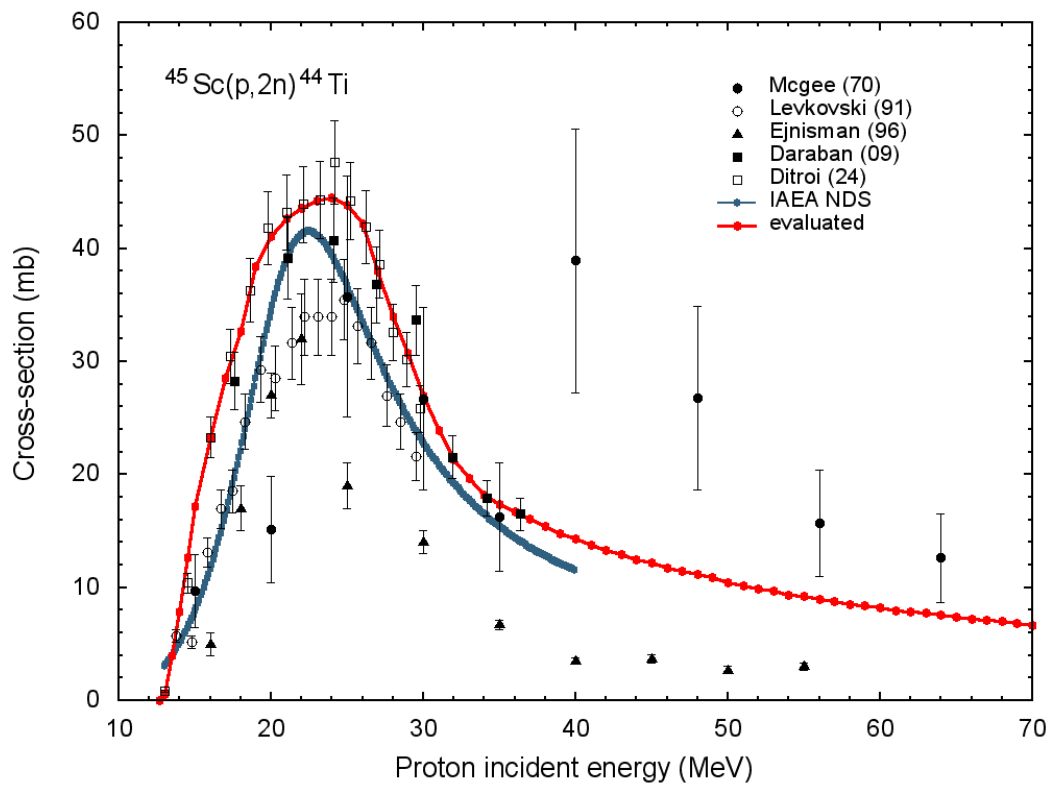


Fig.6 Cross-section for the $^{45}\text{Sc}(p,2n)^{44}\text{Ti}$ reaction.

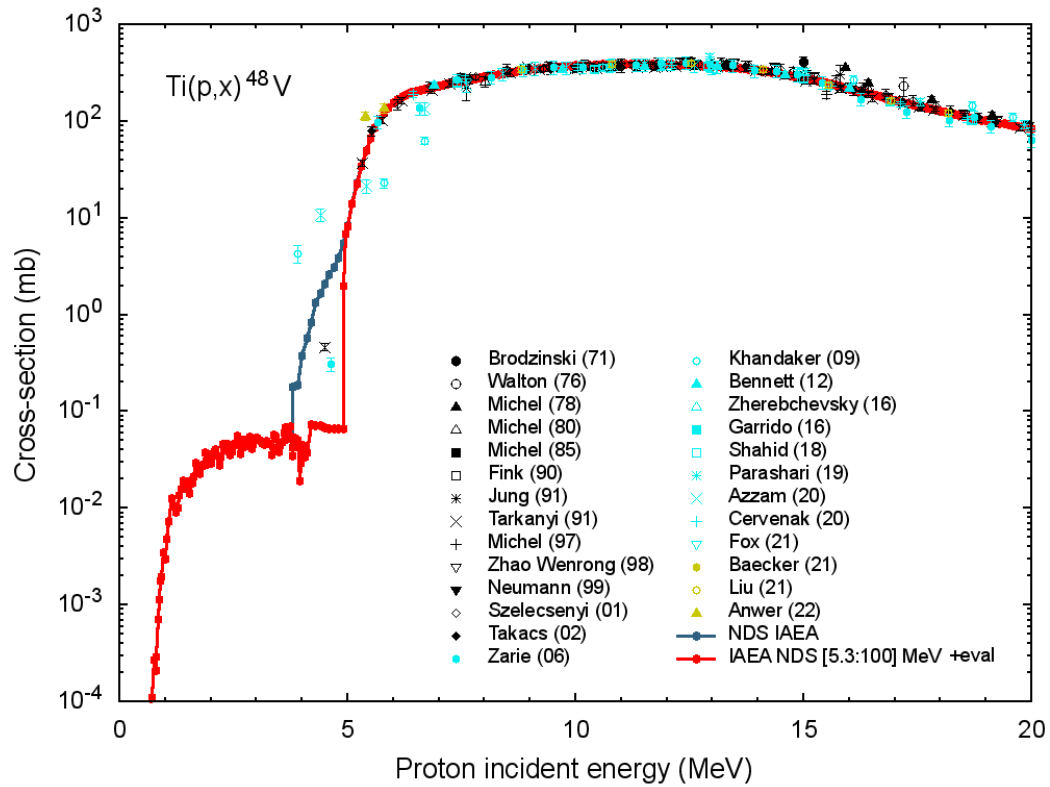
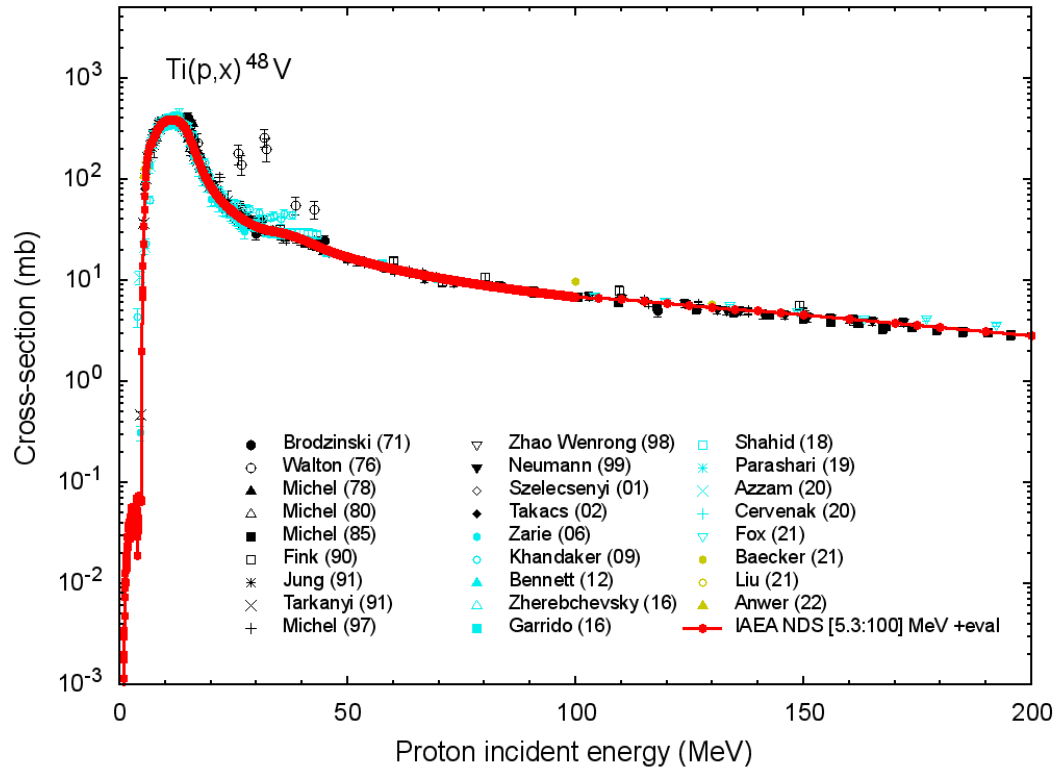


Fig.7 Cross-section for the $^{\text{nat}}\text{Ti}(p,x)^{48}\text{V}$ reaction. The bottom figure shows the cross-sections up to 20 MeV.

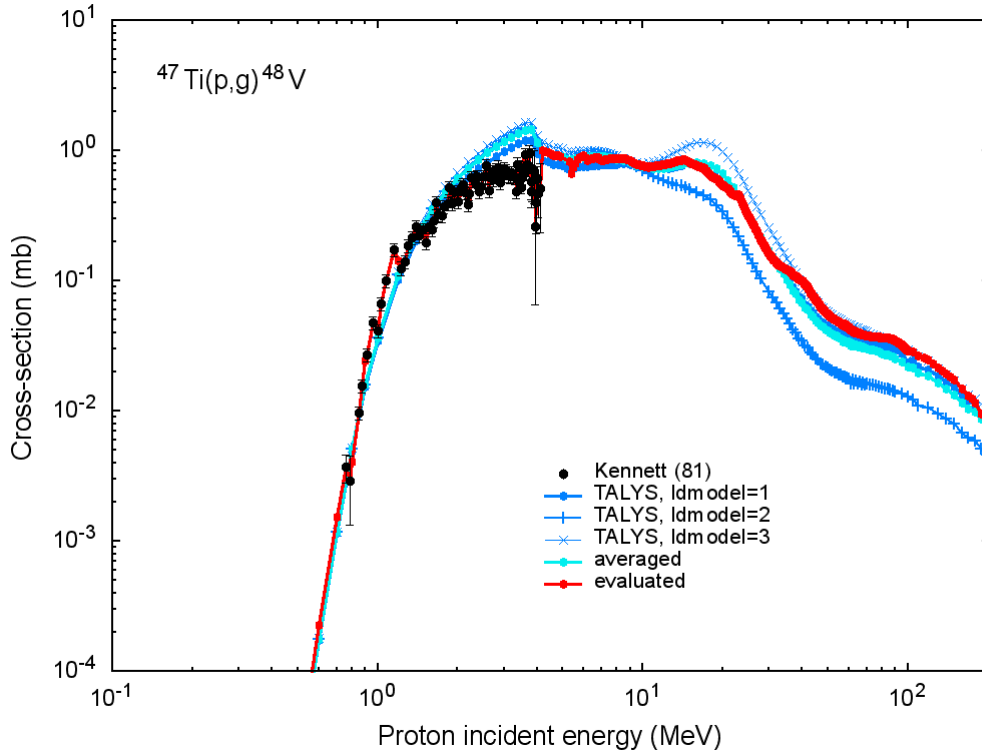


Fig.8 Cross-section for the $^{47}\text{Ti}(p,\gamma)^{48}\text{V}$ reaction.

The resulting data can be downloaded from the website [53].

Plots with the evaluated curves for all reactions for which experimental data exist and for gas production cross-sections are provided in the Appendix.

Detailed information on all steps of the evaluation is available upon request [89]. It includes calculation results obtained with different models and codes, the averaged sum corresponding to the calculated results, the experimental data, and the associated figures.

6. CONCLUSION

Proton-induced reaction cross-sections for stable isotopes of chlorine $^{35,37}\text{Cl}$, potassium $^{39,40,41}\text{K}$, ^{45}Sc , and titanium $^{46,47,48,49,50}\text{Ti}$ have been evaluated at energies up to 200 MeV.

The work involved calculations using various models and computer codes, as well as analysis of experimental data.

The resulting files, distributed under the name PADF-2, can be downloaded from Ref. [53].

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Chlorine

³⁵ Cl	A2
³⁷ Cl	A6
^{nat} Cl	A10

Potassium

³⁹ K	A13
⁴⁰ K	A18
⁴¹ K	A21
^{nat} K	A26

Scandium

⁴⁵ Sc	A28
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Titanium

⁴⁶ Ti	A37
⁴⁷ Ti	A43
⁴⁸ Ti	A50
⁴⁹ Ti	A61
⁵⁰ Ti	A67
^{nat} Ti	A76

