Statistical analysis of cross-section data for $^{12}C(^{4}He,^{4}He)^{12}C$ backscattering

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Abstract

A statistical analysis of experimental and theoretical SigmaCalc 1.6 data for the $^{12}C(^{4}He,^{4}He)^{12}C$ cross-section was performed in the energy range 1600–8200 keV at backscattering angles in the range 149°–172°. In the vicinity of sharp resonances experimental data show a very large scatter, in energy ranges with sufficiently smooth cross-section the overall uncertainty of a single measured cross-section data set is 10.3%. SigmaCalc allows averaging of experimental data at different angles, resulting in an averaged experimental cross-section with an accuracy of 2.1–6.6%. While SigmaCalc-2000 showed some systematic deviations from the experimental data, the improved SigmaCalc-2012 shows agreement with the average experimental cross-section within its error bars over most of the energy range. SigmaCalc and the average cross-section were compared to benchmark measurements at 2000–6000 keV. The deviations between SigmaCalc-2000 and experimental data were confirmed in the benchmark. Both SigmaCalc-2012 and the average cross-section agree with the benchmark over almost the whole energy range.

Keywords: Data analysis, Ion beam analysis, Scattering cross-section

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1. Introduction

The accuracy of ion beam analysis (IBA) methods is mainly limited by the limited accuracy of basic input data, with stopping power and non-Rutherford scattering or nuclear reaction cross-section data being the most important [1]. A large number of cross-section data for non-Rutherford scattering and nuclear reactions were determined experimentally during the last six decades and are available through the IBANDL data base provided by the Nuclear Data Section of the International Atomic Energy Agency (IAEA) [2, 3, 4]. Gurbich has developed the program SigmaCalc, which allows to calculate cross-sections at any angle for many ion-target combinations [2, 5]. These SigmaCalc cross-sections are also available via the IBANDL data base [4] and are widely used within the IBA community.

A large number of different data has been published for the ^{12}C(^{4}He,^{4}He)^{12}C cross-section: IBANDL [4] lists 110 data sets, of which 37 are at the practically important range of backscattering angles $\geq 150°$. Despite this large number of available data a quantitative comparison of the different data sets has not been performed up to now, because the data sets were usually measured at different scattering angles: This makes a direct comparison difficult. However, the use of SigmaCalc allows a quantitative comparison of the data and an estimate of the uncertainty of cross-section measurements. Averaging of multiple data sets allows to derive more accurate experimental cross-section data together with their associated uncertainties. Finally, this allows also an estimate of the largest deviations of the theoretical SigmaCalc cross-section.

Given a set of data $\{d_i\} = \vec{d}$ with associated uncertainties σ_i, $i = 1 \dots N$, the well known weighted arithmetic mean $\bar{d}$ is obtained from

$$\bar{d} = \sigma_{\bar{d}}^2 \sum_{i=1}^{N} \frac{d_i}{\sigma_i^2}, \quad \text{with} \quad \sigma_{\bar{d}}^2 = \frac{1}{\sum \frac{1}{\sigma_i^2}}. \tag{1}$$

$\sigma_{\bar{d}}^2$ is the uncertainty (variance) of the weighted mean. The weighted arithmetic mean is used for example by the international CODATA committee to determine the numerical values of basic physical constants and their associated uncertainties.

The uncertainties of cross-section data measurements, as estimated by their authors, can be roughly divided into the following categories:

1. Some measurements do not provide any uncertainties at all.
2. Many measurements provide only the statistical uncertainty of data points due to count statistics, typically in the range 2–4%. Estimates of systematic errors due to uncertainties of incident beam current integration, layer thickness determination, sample inhomogeneities, systematic changes of sample composition during the measurements (for example by beam-induced build-up of a carbon layer in poor vacuum) etc. are not given. Because the statistical error is only one (and, as will be shown, usually a small) contribution to the total error, the given uncertainty may be much too small.
3. Some measurements provide an overall estimate of the uncertainty, typically about 5%. This number takes statistical and systematic errors into account, but does not provide any details how it was obtained: This type of error estimate is therefore not traceable, and its reliability is hard to judge.

4. Only very few measurements provide a full error estimate, where individual contributions of different statistical and systematic uncertainties are quantified. The resulting total uncertainty is typically 5–10%.
5. Some measurements were published only in graphical form, with hand-drawn graphs in the 50's and 60's. Besides drawing inaccuracies digitizing of the graphs introduces additional digitizing errors.

This heterogeneous quality of uncertainty estimates found in the literature renders the use of eq. 1 difficult: If uncertainty estimates provided by authors are used for σ_i, then measurements providing only statistical uncertainties (category 2. above) would receive the highest statistical weight due to their lowest stated error, while the most thorough measurements (category 4. above) would receive the lowest statistical weight due to their largest stated errors. Such a procedure would be absurd. The use of the weighted mean with author-provided uncertainties as weight factor is therefore not possible for cross-section measurements due to the much too heterogeneous quality of cross-section uncertainty estimates. This is a fundamental difference to measurements of basic physical constants, where usually a large effort is used to determine not only the numerical value of the constant, but also its associated uncertainty.

Dose [6] has shown that author-provided estimates of the uncertainty σ_i can be replaced by the real uncertainties s_i according to $s_i^2 = \alpha \sigma_i^2$. The scale factor α is determined from the data. However, while this approach is generally able to handle incorrect uncertainty estimates σ_i, it still requires identical quality of the author-provided uncertainty estimates σ_i. As discussed above, this is generally not the case for cross-section data.

At the other hand it is possible to determine the uncertainty σ^2 of cross-section data measurements by a statistical analysis of the data with the implicit assumption that all data sets have identical uncertainty σ. Because cross-section measurements use comparable methods and comparable count statistics, this assumption is reasonable. It is also implicitly used in the statistical analysis of stopping power data where all data sets receive identical weights, see for example [7].

The series of cross-section measurements d_i then are assumed to have fluctuations ϵ_i, with the ϵ_i obeying a Gaussian distribution with variance σ^2 around the real cross-section value θ. θ and its uncertainty (variance) $\Delta\theta^2$ then can be simply obtained from

$$\theta = \frac{1}{N}\sum_{i}^{N} d_i, \tag{2}$$

$$\Delta\theta^2 = \frac{\sigma^2}{N}. \tag{3}$$

The uncertainty of the mean therefore can be decreased by increasing the number of independent measurements N. As has been already pointed out in [6], eqs. 2 and 3 give reasonable results only, if the $\{d_i\}$ are samples from Gaussian distributions with mean θ and with the real variance σ^2, i.e. the *real* uncertainty of experimental cross-section measurements. The handling of non-Gaussian distributions is beyond the scope of the present work, a discussion can be found e.g. in [6].

2. Data selection and renormalization

Theoretical curves were calculated with SigmaCalc 1.6 [8, 4]. The version described in [8] was available at IBANDL before 12.1.2012 and will be called

SigmaCalc-2000. An improved version became available on 12.1.2012 and is called SigmaCalc-2012.

We limit ourselves to backscattering angles suitable for RBS, and to incident energies below 7.3 MeV for SigmaCalc-2000 and 8.2 MeV for SigmaCalc-2012: At higher energies SigmaCalc values are not available.

The following measurements were used as published:

Cheng et al. [9] at a scattering angle of 170°;
Berti et al. [10] at 170°;
Yonezawa et al. [11] at 169°;
Wetteland [12] at 167°;
Bittner [13] at 167°;
Hill [14] at 166.6°;
Zhou [15] at 165°;
Plaga et al. [16] at 163° and 157°;
Bogdanović-Radović et al. [17] at 150°;
Tong et al. [18] at 150°;
Marvin and Singh [19] at 149°.

Leavitt et al. [20] measured at a scattering angle of 170.5°, and absolute cross-section values were determined by assuming the Rutherford cross-section at energies from 1.6–2 MeV. However, according to SigmaCalc-2000 [8] the cross-section is below Rutherford by about 5% at these energies. Consequently, for comparison to SigmaCalc-2000 the published Leavitt data were renormalized to a ratio-to-Rutherford (RR) value of 0.947 at energies below 2 MeV, which is the mean SigmaCalc-2000 value in the range 1.6–2 MeV. With SigmaCalc-2012 the ratio-to-Rutherford (RR) value is 0.986 at energies below 2 MeV, which was used for renormalization and comparison to SigmaCalc-2012.

Feng et al. [21] published an extensive set of cross-section data at 165° over a wide energy range. Absolute cross-section values were determined by assuming the Rutherford cross-section at 2 MeV. However, according to SigmaCalc-2000 [8] the cross-section is below Rutherford by 8% at this energy. The published Feng data therefore have been renormalized to a ratio-to-Rutherford (RR) value of 0.92 at 2 MeV for comparison to SigmaCalc-2000. SigmaCalc-2012 gives a ratio-to-Rutherford (RR) value of 0.979 at 2 MeV, which was used for renormalization and comparison to SigmaCalc-2012.

Somatri et al. [22] published a data set at 172°. While most data points agree well with other data sets, the four data points in the range 4310–4440 keV deviate by almost 100% from all other data. These four data points therefore have been excluded as outliers, all other Somatri data points were included.

Miller Jones et al. [23] published a data set at 160°. While the data above about 3200 keV agree well with all other data sets, the data points below 3200 keV show a large scatter and deviation up to 100% from all other data. The Miller Jones data were published only in graphical form, and the large scatter is most likely due to digitizing inaccuracies: The cross-section is small below 3200 keV, so that digitizing errors can get large. Consequently the Miller Jones data below 3200 keV were excluded, while the data at higher energies were taken into account.

The original data by Jiang et al. [24] at 150° showed large discrepancies to all other data sets, both with respect to the energy of the 4.27 MeV resonance and to the absolute cross-section values [25]. The energies of all data points were readjusted by the authors [26], but the discrepancy by about 50% of the cross-section values to all other data was not solved. The whole data set is therefore considered as a systematic outlier and excluded.

Davies et al. [27] measured in the energy intervals 4.1–4.5 MeV and 5.5–5.875 MeV, i.e. in the vicinity of two large resonances. The Davies' energy of both resonances disagrees with all other data by about 50 keV, indicating a systematic error of the initial beam energy. The Davies' data are therefore considered as outliers and were excluded.

The data of Ferguson and Walker [28] belong to the oldest measured cross-sections and were published already in 1940. The data are sparse, have large error bars, and show systematic deviations to all other data, both with respect to energy and to the absolute cross-section values. The data are therefore considered as too inaccurate and were excluded.

The data of Clark et al. [29] and of Morris et al. [30] at several angles have a too sparse energy spacing to be useful for our purposes.

3. Statistical analysis of cross-section data

Experimental cross-section data are shown in Fig. 1a)–1c) together with the SigmaCalc-2000 values, the difference to SigmaCalc-2000 is shown in Fig. 1d). At energies below about 4200 keV all experimental data sets show good agreement, except for the region around the 3570 keV resonance. At about 2500 keV the experimental data deviate from SigmaCalc-2000 by about 20%, and in the cross-section minimum around 2950 keV by up to 50%. In the range 3200–3500 keV experimental data and SigmaCalc-2000 show good agreement, while the experimental data exceed the SigmaCalc-2000 values by 10–15% in the range 3600–4100 keV. From 4400 keV to about 7000 keV the experimental data show a large scatter, and SigmaCalc-2000 follows about the middle of the data cloud. The Marvin data are below all other data from 4400–5700 keV, but show good agreement to the other data at higher energies. It is difficult to see any systematics in this energy range or to exclude any data set as outlier. Around the cross-section minimum at 7100 keV SigmaCalc-2000 deviates from the experimental data by up to 30%.

Systematic deviations between experimental data and SigmaCalc-2000 with varying scattering angle are not observed in this angular range, and the scatter of different data sets at about the same angle (for example Feng, Wetteland and Bittner) is identical to the scatter of data sets at different angles. The angular dependence of the cross-section therefore seems to be correctly reproduced by SigmaCalc-2000 within the experimental error bars.

The agreement of experimental data in the vicinity of the sharp resonances at 3570, 4270 and 5840 keV is generally poor, and large outliers are observed here, see Fig. 1d): This is partly due to inaccuracies of the incident ion energy, where already small errors result in a large scatter of cross-section data, and partly due to poor energy resolution by a large incident beam energy spread or a too thick carbon layer.

As a result of the systematic deviations between the experimental data and SigmaCalc-2000 especially at energies below about 4200 keV the SigmaCalc model was improved in SigmaCalc-2012, and the energy range was extended to 8140 keV. The comparison of experimental data with SigmaCalc-2012 is shown in Fig. 2a)–2d). Systematic deviations between all experimental data and SigmaCalc are not observed any more at all energies below about 7000 keV. Only at energies above about 7200 keV the experimental data are systematically above the SigmaCalc-2012 values.

As discussed above, the agreement of experimental data in the vicinity of the sharp resonances is poor, see Figs. 1d) and 2d), and the energy ranges 3573–3610, 4184–4353, 5780–5872, and $\geq$ 7750 keV containing resonances were therefore excluded from further data processing.

In order to obtain a quantitative comparison of data sets measured at different angles the difference to SigmaCalc-2012 according to

$$d_i = \frac{d_{\mathrm{exp}} - d_{\mathrm{SC}}}{d_{\mathrm{SC}}}, \tag{4}$$

with the experimental data d_{exp} and the SigmaCalc-2012 values d_{SC}. The mean value of all experimental data sets available in the corresponding energy range was derived using linear interpolation between the individual data points. 2–9 different data sets were available at each energy. Identical weights were assigned to all data sets, see section 1.

As can be seen already in Fig. 2 the cross-section data show a larger scatter in regions with fast variation of the cross-section with energy (i.e. the regions 2700-3200, 4800-6000, 6700-8000 keV) than in regions with slow variation (i.e. $\leq$ 2700, 3200-4800, 6000-6700, $\geq$ 8000 keV): Inaccuracies of the energy, introduced either by an inaccurate accelerator energy calibration or by digitizing errors, have only a small influence on the cross-section in regions with slow variation of the cross-section with energy, but may have a larger influence in regions with fast variation. In order to take not only the cross-section error, but also the energy error into account, the whole energy range is therefore roughly divided in regions with slow variation and with fast variation, see above. The frequency distributions of the difference to the mean value are shown in Fig. 3. As discussed above, energy ranges in the vicinity of sharp resonances were excluded. The frequency distribution for the slow varying regions has a standard deviation $\sigma = 6.3\%$ and is close to a Gaussian, see Fig. 3 bottom. The frequency distribution in the fast varying regions has a standard deviation $\sigma = 13.1\%$ and shows some deviations from a Gaussian distribution. Nevertheless, according to the Kolmogorov-Smirnov test at a level of 0.05 both distributions shown in Fig. 3 are still significantly drawn from Gaussian distributions. The combined standard deviation for both regions is $\sigma = 10.3\%$. Provided that SigmaCalc-2012 describes the angular dependence correctly, then the standard deviation $\sigma = 10.3\%$ is the real uncertainty of a cross-section measurement. This uncertainty is considerably larger than stated in most publications: Berti [10] states an accuracy of 2.5%, Somatri [22] 5%, Feng [21] 2–3%, Plaga [16] 3–4%, and Miller Jones [23] 2.6%. Jiang [24, 26] gives an uncertainty of 4%, while his data deviate by about 50% from all other data [25] and were excluded as outliers. But the uncertainty of 10.3% is very close to the error estimates of 10% presented by Bogdanovic-Radovic [17] and Morris [30].

Errors are mainly systematic and therefore affect either the whole data set (i.e. all data points presented in one publication), or at least groups of data points of one data set within some energy range (for example the Marvin data at 149°, which agree with all other data above about 6000 keV, but are systematically lower than all other data below about 5800 keV). The number of independent data points in Fig. 3 is therefore somewhere between the number of data sets and the number of data points.

If SigmaCalc-2012 would contain systematic errors in the angular dependence, then the standard deviation $\sigma = 10.3\%$ would be the combined uncertainty of measurements and SigmaCalc. However, because the scatter of different data sets at about the same angle (for example Feng, Wetteland and Bittner in Fig. 1d)) is identical to the scatter of data sets at different angles, a possible error contribution of SigmaCalc seems to be small compared to the experimental error.

By averaging all available experimental data at a given energy the average cross-section and its associated uncertainty are obtained from eq. 2 using linear interpolation between the measured data points. The uncertainties $\sigma = 6.3\%$ and $\sigma = 13.1\%$ were used for experimental data in the slow varying and fast varying regions, respectively. The number of available measurements N is in the range 3–9, resulting in uncertainties of 2.1–6.6% for the averaged cross-section value. The averaged cross-section is shown as black line in Fig. 2d), the uncertainty range is shown as gray area. The SigmaCalc-2000 and SigmaCalc-2012 values and the averaged cross-section are compared in Fig. 4 at a scattering angle of 165°. The energy ranges 3573–3610, 4184–4353, 5780–5872, and ≥ 7750 keV in the vicinity of resonances were excluded from the averaging process due to the much larger uncertainty of experimental data in these ranges.

SigmaCalc-2000 is systematically lower than the average cross-section at energies around 2500 keV by up to 18%, systematically higher by up to 40% around 2950 keV and by up to 30% around 7090 keV, and it deviates by typically 10% in the range 3600-4050 keV. At all other energies SigmaCalc-2000 agrees with the average cross-section within the given uncertainties.

SigmaCalc-2012 agrees with the average cross-section at all energies below about 4200 keV within the error bars, with the only exception around the minimum at 2950 keV, where a 10% discrepancy is observed. SigmaCalc-2012 agrees with the average cross-section in the range 4500–5000 keV within the error bars, but is smaller than the mean cross-section by up to 10% from 5000–5700 keV. Agreement is almost within the error bars at 6000–7200 keV. At 7300–7600 keV a systematic disagreement by about 15% is observed: As stated in [8] SigmaCalc-2012 follows the data of Bittner [13], which are somewhat lower than all other data at these energies.

4. Benchmark measurements

Benchmark measurements were performed at the 3 MV tandem accelerator of IPP Garching at a scattering angle of 165° in Cornell geometry. The incident beam energy was calibrated using the 4267 keV resonance and the 5842 keV dip in the $^{12}C(^{4}He,^{4}He)^{12}C$ cross-section and the 2751 keV resonance in the $^{13}C(^{4}He,^{4}He)^{13}C$ cross-section [31]. It is accurate within about 5 keV, the incident beam energy spread is below 1 keV.

The detector solid angle was (1.15 ± 0.03) msr. It was determined with certified targets from IRMM GEEL (48.3 ± 1.0 μg/cm^2 Rh on C and 35.1 ± 1.1 μg/cm^2 Pd on C) and with SRIM 2010 stopping powers [32] from Al, Co, Rh, and Au bulk targets at 2 MeV ^{4}He. The above error already includes the error due to the beam current measurement. A polished pyrolylitic graphite (PG) bulk target was used for the benchmark measurements at an incident angle of 5°. The PG target had a density > 2.2 g/cm^3, which is close to the theoretical density of graphite: The porosity of the target and any potential porosity-induced straggling is therefore assumed to be small. The PG target was coated with a $(1.47 \pm 0.03) \times 10^{16}$ Au-atoms/cm^2 layer as beam fluence reference. The thickness of the Au layer was determined with 1.6 MeV ^{4}He backscattering: At this energy the scattering cross-section from the carbon substrate is Rutherford within about 1%. The thickness of the Au layer was determined by two different methods:

1. From the known detector solid angle and the measured beam fluence. This measurement is accurate within about 3%.
2. By adjusting the product of solid angle and beam fluence to the backscattering spectrum from the bulk PG using SRIM 2010 stopping powers [32] and the Rutherford cross-section with Andersen screening [33]. The accuracy of this measurement of the Au thickness is determined by the accuracy of the SRIM 2010 stopping power, which is about 3.5% [32].

Both Au thickness determinations agreed within 4%, which is within the error bars of both methods. The mean thickness value was used, which therefore has an absolute error of about 2%.

Simulation calculations were performed using SIMNRA 6.70 [34] using SRIM 2010 stopping powers [32]. The accuracy of the simulation calculations is mainly determined by the accuracy of the stopping power, which is about 3.5% [32]. Other inaccuracies of the simulation, such as inaccuracies of the algorithms of the simulation code, are much smaller [35, 36] and can be neglected, at least outside of the vicinity of sharp resonances. The absolute uncertainty of the benchmark measurements due to uncertainties of the stopping power and Au thickness determination is therefore about 4%.

The experimental data together with simulation calculations using SigmaCalc-

2000 and SigmaCalc-2012 cross-section data and the average cross-section are shown in Figs. 5 and 6. Towards larger energy losses, i.e. at smaller channel numbers, simulated spectra are always systematically lower than the measured ones. This discrepancy is always observed for ^{4}He backscattered from carbon and independent of the simulation program. The reason for this discrepancy is unknown and may be due to inaccuracies in the stopping power data, or a higher contribution of plural scattering [37]. Consequently, experimental spectra and simulations can be compared only in channels originating from particles backscattered close to the surface.

At 2386 keV incident energy the spectrum calculated with the SigmaCalc-2000 cross-section is too low by about 10%, while the averaged and the SigmaCalc-2012 cross-sections show very good agreement with the experimental data. At 2783 keV and 3181 keV all cross-sections are compatible with the data, with a slightly better agreement for SigmaCalc-2012 and the averaged cross-section. At 2783 keV incident energy the 2751 keV resonance in the ^{13}C(^{4}He,^{4}He)^{13}C cross-section [31] is visible. At 3578 keV only SigmaCalc cross-sections are available due to the vicinity to the 3570 keV resonance. Both have a tendency to be too high. At 3976 keV the spectra calculated with the average cross-section and with SigmaCalc-2012 are about 7% higher than the experimental data. At 4373 keV again only SigmaCalc cross-sections are available due to the vicinity to the 4270 keV resonance. Both simulations are too high, indicating that the SigmaCalc cross-section values for the resonance are too high by about 5%. At 4771 keV, 5169 keV and 5566 keV the spectra calculated with the averaged cross-section are about 6% higher than the experimental data, while SigmaCalc-2012 is in perfect agreement and SigmaCalc-2000 slightly too low. The small hump in the 5566 keV data in channels 60–90 is due to the resonance in the cross-section at 5262 keV, see Fig. 4. This hump is missing in the SigmaCalc-2000 data. At 5964 keV the spectrum calculated with the SigmaCalc-2000 cross-section is up to 9% too high in channels 215–235, while the average cross-section is close to the experimental data and SigmaCalc-2012 shows perfect agreement.

The benchmark measurements therefore prove the correctness of the SigmaCalc-2000 cross-section in the energy range 4400–5600 keV with an accuracy of about 4%. In the range 3600-4000 keV the SigmaCalc-2000 cross-section is about 5% too low, and about 10% too low at about 2400 keV. SigmaCalc-2012 is accurate within the benchmark accuracy of 4% over almost the whole energy range, only in the range 3600–4000 keV it may be somewhat too high. The average cross-section agrees with the benchmark measurements within the benchmark accuracy of 4% at all energies below 3200 keV. At around 4000 keV and at 4800–5600 keV it is too high by about 5%.

5. Conclusions

A statistical analysis was performed for the ^{12}C(^{4}He,^{4}He)^{12}C cross-section data in the energy range 1600–8100 keV at backscattering angles in the range 149°–172°. The analysis included 15 different data sets with 1270 cross-section data points. SigmaCalc allows the comparison of data sets measured at different angles assuming that the angular dependence is correctly described by SigmaCalc.

In the vicinity of sharp resonances experimental data show a very large scatter: The use of experimental cross-section data in resonance regions therefore may result in large uncertainties. Experimental data from resonance regions were excluded from further data processing, leaving 1045 data points. Inaccuracies of the energy, either during the measurement or by digitizing data published only in graphical form, introduce an additional error. In energy ranges with slow variation of the cross-section with energy the real uncertainty of experimental cross-section data is 6.3%, but increases to 13.1% in energy ranges with faster variation of the cross-section with energy due to the additional influence of the energy error. The overall uncertainty is 10.3%. These numbers are based on the scatter of the data points and are considerably larger than usually stated by the authors. Theoretical SigmaCalc-2000 values agree with the available experimental data at energies in the range 4400–6900 keV, but show systematic deviations from all experimental data in the range 2200–4000 keV and from 6900–7200 keV. SigmaCalc-2012 shows an improved agreement with the experimental data. A weighted average of all experimental data from sufficiently smooth areas gives an average cross-section with an accuracy in the range 2.1–6.6%: The uncertainty depends on the number of available data sets at a specific energy. At most energies SigmaCalc-2012 agrees with the average experimental cross-section within the uncertainty of the average.

Benchmark measurements were performed in the range 2000–6000 keV and show the correctness of the SigmaCalc-2012 cross-section over almost the whole energy range with an accuracy of about 4%. Only in the range 3600–4000 keV it may be somewhat too high. The average cross-section agrees with the benchmark measurements within the benchmark accuracy of 4% at all energies below 3200 keV. At around 4000 keV and at 4800–5600 keV it is too high by about 5%.

Cross-section data are being measured since almost 60 years. Measurements are usually performed at different scattering angles, rendering a direct comparison of different data sets difficult. The accuracy of individual data sets is mainly limited by systematic errors which affect several or all data points in the same way. The real uncertainty of experimentally determined cross-section data is much higher than usually stated by the experimentalist, and unless a break-trough in experimental techniques is discovered it is not expected that new measurements will gain a higher accuracy than already performed ones. Consequently, the accuracy of experimental cross-section data can be only improved by averaging multiple data sets. The application of SigmaCalc allows to average cross-section measurements performed at different angles. The averaged cross-section has a higher accuracy than individual measurements and allows the assignment of uncertainties using established statistical methods. This average experimental cross-section can be used for a comparison to theoretical SigmaCalc cross-section data.

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[1] M. Mayer, W. Eckstein, H. Langhuth, F. Schiettekatte, and U. von Toussaint. Nucl. Instr. Meth. B 269 (2011) 3006.

[2] A. Gurbich, I. Bogdanovic-Radovic, M. Chiari, C. Jeynes, M. Kokko-

ris, A.R. Ramos, M. Mayer, E. Rauhala, O. Schwerer, Shi Liqun, and I. Vickridge. Nucl. Instr. Meth. B 266 (2008) 1198.

[3] D. Abriola, A.F. Gurbich, N.P. Barradas, I. Bogdanovic-Radovic, M. Chiari, C. Jeynes, M. Kokkoris, M. Mayer, A.R. Ramos, L. Shi, and I. Vickridge. Nucl. Instr. Meth. B 269 (2011) 2972.

[4] Ion Beam Analysis Nuclear Data Library (IBANDL). http://www-nds.iaea.org/ibandl/.

[5] A. Gurbich. Nucl. Instr. Meth. B 268 (2010) 1703.

[6] V. Dose. Meas. Sci. Technol. 18 (2007) 176.

[7] H. Paul. Nucl. Instr. Meth. B in press (2012) .

[8] A.F. Gurbich. Nucl. Instr. Meth. B 161-163 (2000) 125.

[9] H.-S. Cheng, H. Shen, J. Tang, and F. Yang. Acta Phys. Sinica 43 (1994) 1569.

[10] M. Berti, D.De Salvador, A.V. Drigo, F. Romanato, A. Sambo, S. Zerlauth, J. Stangl, F. Schäffler, and G. Bauer. Nucl. Instr. Meth. B 143 (1998) 357.

[11] H. Yonezawa, K. Shikano, and T. Shigematsu. Nucl. Instr. Meth. B 88 (1994) 207.

[12] C.J.Wetteland. Tech. Rep. LA-UR-98-4867, 1998.

[13] J.W. Bittner and R.D. Moffat. Phys. Rev. 96 (1954) 374.

[14] R.W. Hill. Phys. Rev. 90 (1953) 845.

[15] Z. Zhou. In *Proceedings of the International Conference on High Energy Beams in Materials Analysis* (1989), p. 153.

[16] R. Plaga, H.W. Becker, A. Redder, C. Rolfs, H.P. Trautvetter, and K. Langanke. Nucl. Phys. A 465 (1987) 291.

[17] I. Bogdanović Radović, M. Jakšić, O. Benka, and A.F. Gurbich. Nucl. Instr. Meth. B 190 (2002) 100.

[18] S.Y. Tong, W.N. Lennard, P.F.A. Alkemade, and I.V. Mitchell. Nucl. Instr. Meth. B 45 (1990) 30.

[19] T.P. Marvin and P.P. Singh. Nucl. Phys. A 180 (1972) 282.

[20] J.A. Leavitt, L.C. McIntyre Jr., P. Stoss, J.G. Oder, M.D. Ashbaugh, B. Dezfouly-Arjomandy, Z.M. Yang, and Z. Lin. Nucl. Instr. Meth. B 40-41 (1989) 776.

[21] Y. Feng, Z. Zhou, Y. Zhou, and G. Zhao. Nucl. Instr. Meth. B 86 (1994) 225.

[22] R. Somatri, J.F. Chailan, A. Chevarier, N. Chevarier, G. Ferro, Y. Monteil, H. Vincent, and J. Bouix. Nucl. Instr. Meth. B 113 (1996) 284.

[23] C. Miller Jones, G.C. Phillips, R.W. Harris, and E.H. Beckner. Nucl. Phys. 37 (1962) 1.

[24] W. Jiang, V. Shutthanandan, S. Thevuthasan, D.E. McCready, and W.J. Weber. Nucl. Instr. Meth. B 222 (2004) 538.

[25] A.F. Gurbich. Nucl. Instr. Meth. B 229 (2005) 157.

[26] W. Jiang, V. Shutthanandan, S. Thevuthasan, D.E. McCready, and W.J. Weber. Nucl. Instr. Meth. B 227 (2005) 450.

[27] J.A.Davies, F.J.D.Almeida, H.K.Haugen, R.Siegele, J.S.Foster, and T.E. Jackman. Nucl. Instr. Meth. B 85 (1994) 28.

[28] A.J. Ferguson and L.R. Walker. Phys. Rev. 58 (1940) 666.

[29] G.J. Clark, D.J. Sullivan, and P.B. Treacy. Nucl. Phys. A 110 (1968) 481.

[30] J.M. Morris, G.W. Kerr, and T.R. Ophel. Nucl. Phys. A 112 (1968) 97.

[31] B.K. Barnes, T.A. Belote, and J.R. Risser. Phys. Rev. 140 (1965) B616.

[32] J.F. Ziegler, M.D. Ziegler, and J.P. Biersack. Nucl. Instr. Meth. B 268 (2010) 1818.

[33] H.H. Andersen, F. Besenbacher, P. Loftager, and W. Möller. Phys. Rev. A21, 6 (1980) 1891.

[34] M. Mayer. SIMNRA user's guide. Tech. Rep. IPP 9/113, Max-Planck-Institut für Plasmaphysik, Garching, 1997.

[35] N.P. Barradas, K. Arstila, G. Battistig, M. Bianconi, N. Dytlewski, C. Jeynes, E. Kótai, G. Lulli, M. Mayer, E. Rauhala, E. Szilágyi, and M. Thompson. Nucl. Instr. Meth. B 262 (2007) 281.

[36] N.P. Barradas, K. Arstila, G. Battistig, M. Bianconi, N. Dytlewski, C. Jeynes, E. Kótai, G. Lulli, M. Mayer, E. Rauhala, E. Szilágyi, and M. Thompson. Nucl. Instr. Meth. B 266 (2008) 1338.

[37] W. Eckstein and M. Mayer. Nucl. Instr. Meth. B 153 (1999) 337.

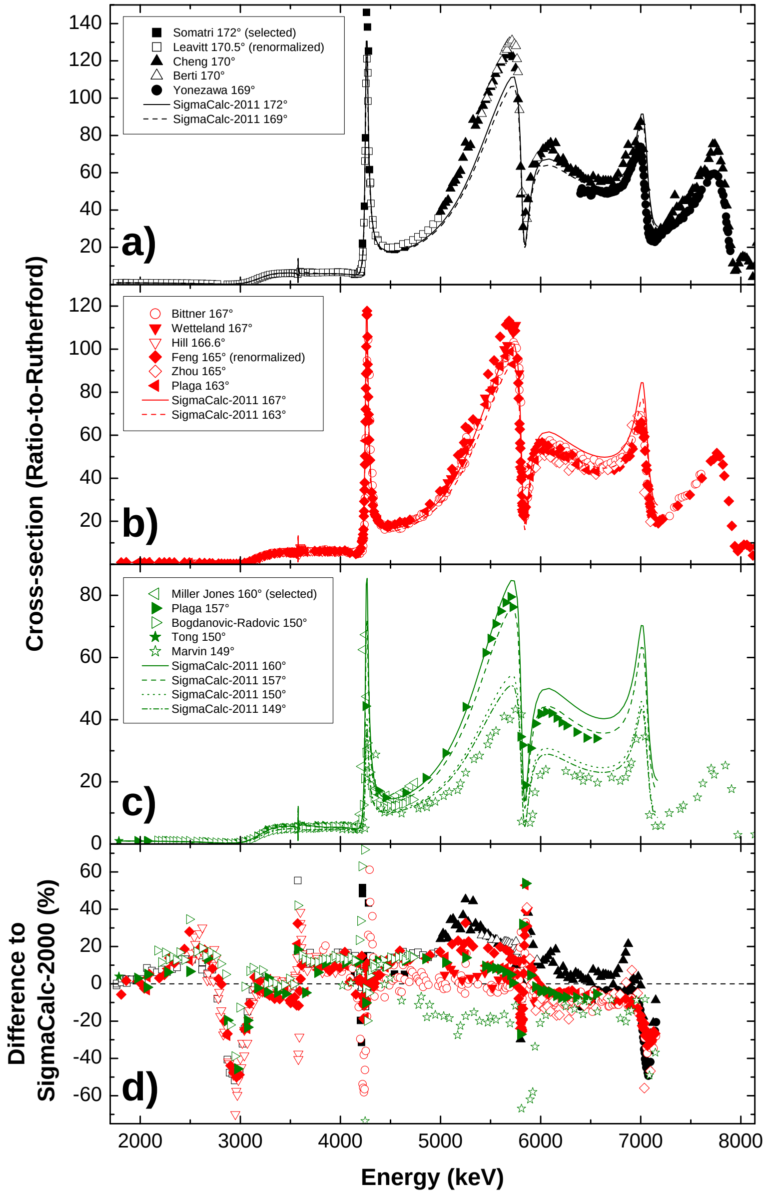

Figure 1: Experimental cross-section data together with SigmaCalc-2000 theoretical data. a) Scattering angle 169–172°; b) Scattering angle 163–167°; c) Scattering angle 149–160°. See text for renormalization and data selection. d) Difference of the experimental data to the corresponding SigmaCalc-2000 values. Note that outliers larger than ±75% are not visible.

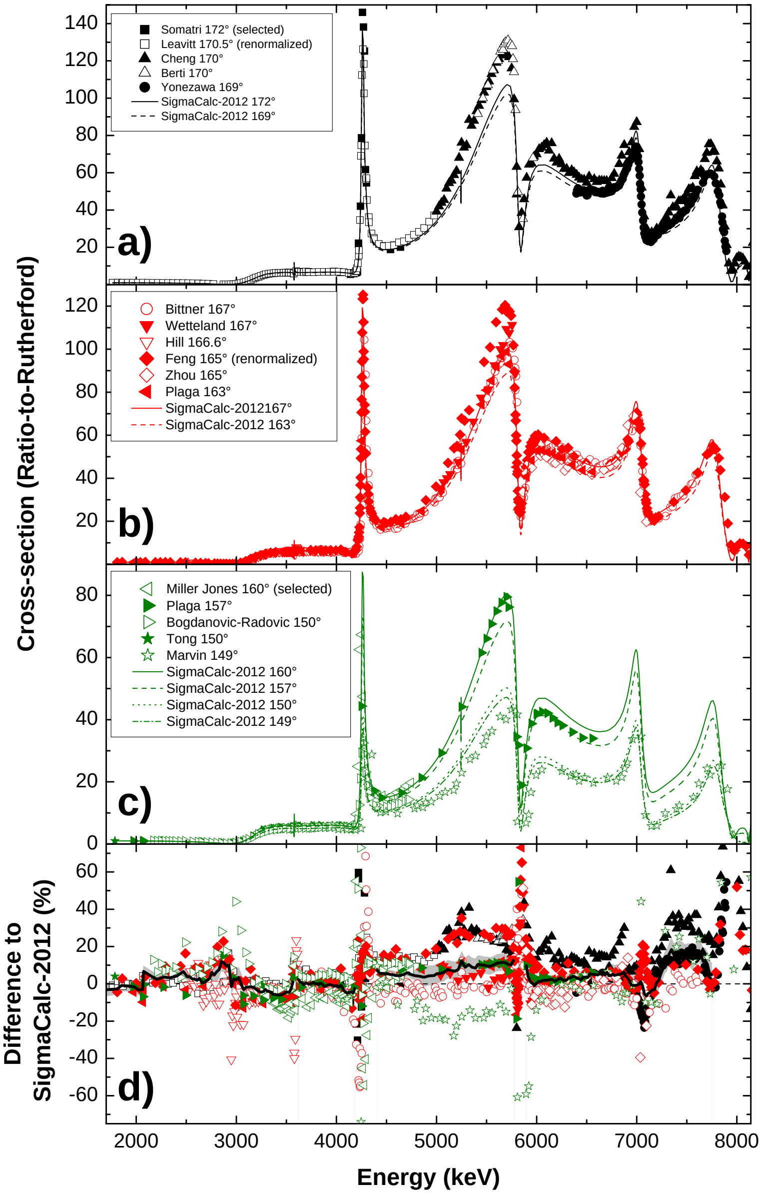

Figure 2: Experimental cross-section data together with SigmaCalc-2012 theoretical data. a) Scattering angle 169–172°; b) Scattering angle 163–167°; c) Scattering angle 149–160°. See text for renormalization procedure and data selection. d) Difference of the experimental data to the corresponding SigmaCalc-2012 values. Note that outliers larger than ±75% are not visible. Thick solid line: Mean value of all experimental data. Grey area: Uncertainty range of the mean value.

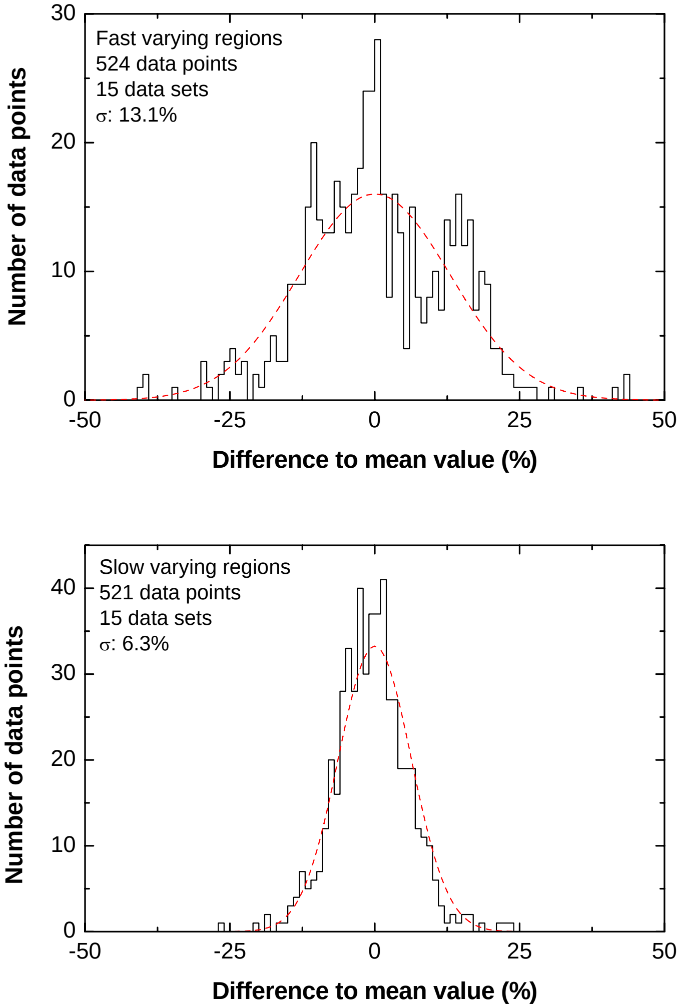

Figure 3: Frequency distribution of the difference of experimental data points to the mean value of all experimental data points at that energy. Resonances excluded. Top: Regions with fast variation of the cross-section with energy. 15 data sets, 524 data points. Bottom: Regions with slow variation of the cross-section with energy. 15 data sets, 521 data points. Dashed lines: Gaussians with identical area and variance as the frequency distribution.

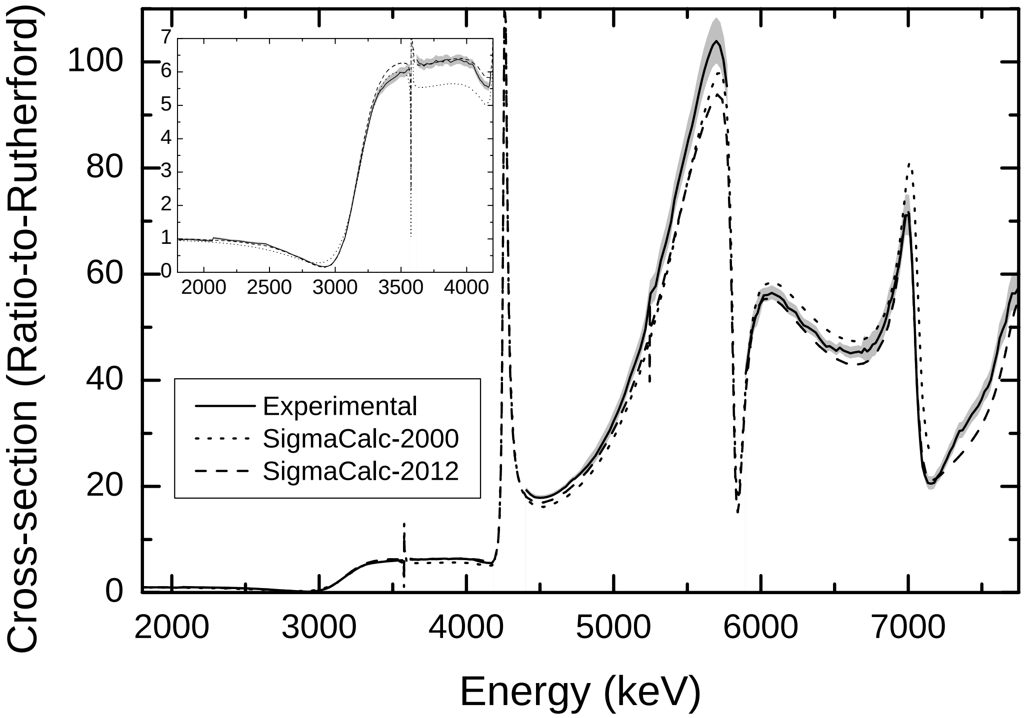

Figure 4: Cross-section at a scattering angle of 165°. Dotted line: SigmaCalc-2000. Dashed line: SigmaCalc-2012. Solid line: Cross-section from the average of all experimental data, i.e. the thick solid line in Fig. 2d). Grey area: Uncertainty of the average ($\pm 1\sigma$ interval). The insert shows a magnification of the energy range 1800–4200 keV.

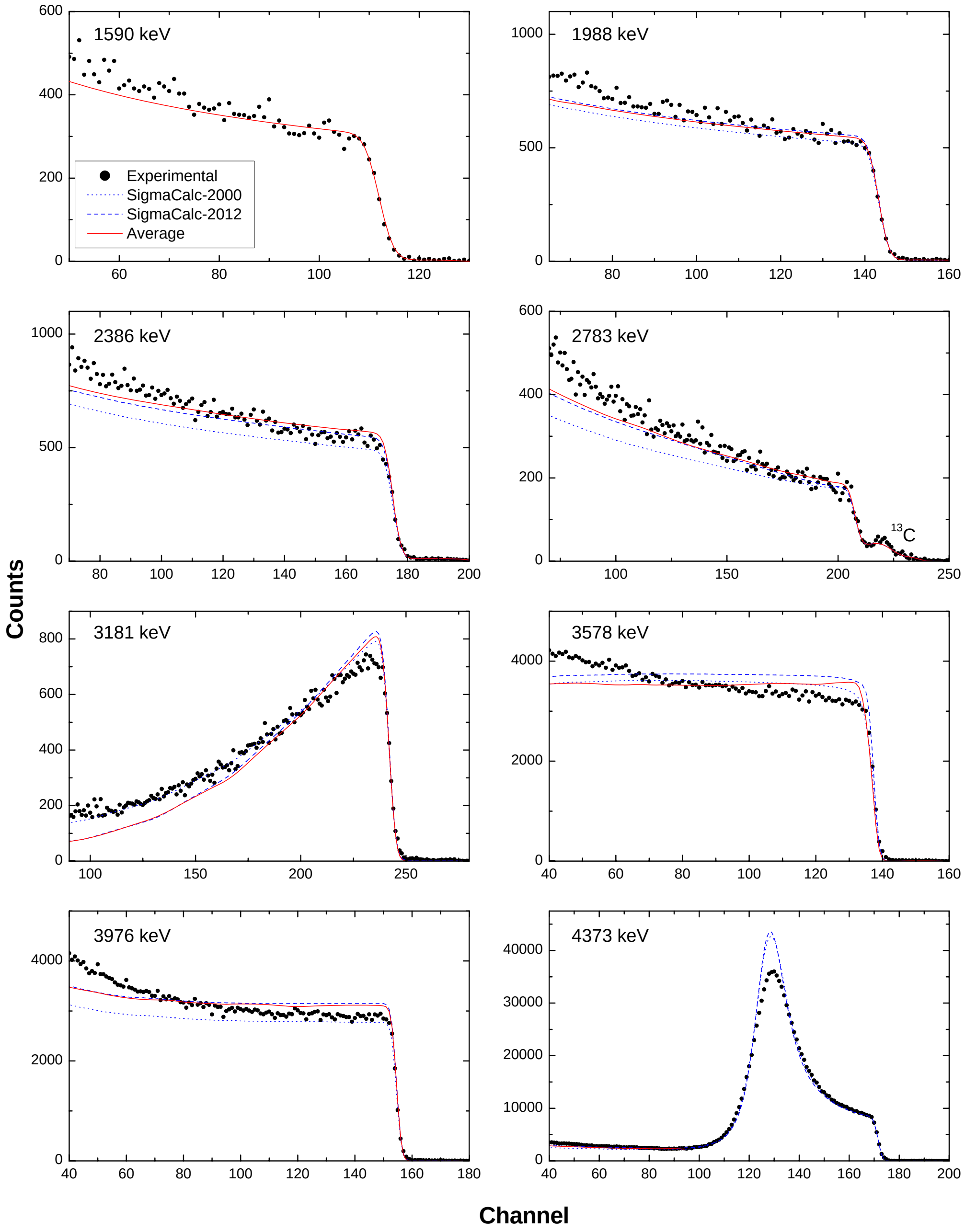

Figure 5: Benchmark measurements at a scattering angle of 165°. Dots: Experimental data; Dotted lines: Simulation calculations using the SigmaCalc-2000 cross-section; Dashed lines: Simulation calculations using the SigmaCalc-2012 cross-section; Solid lines: Simulation calculations using the average cross-section. The average cross-section is undefined in the energy range 4180–4380 keV.

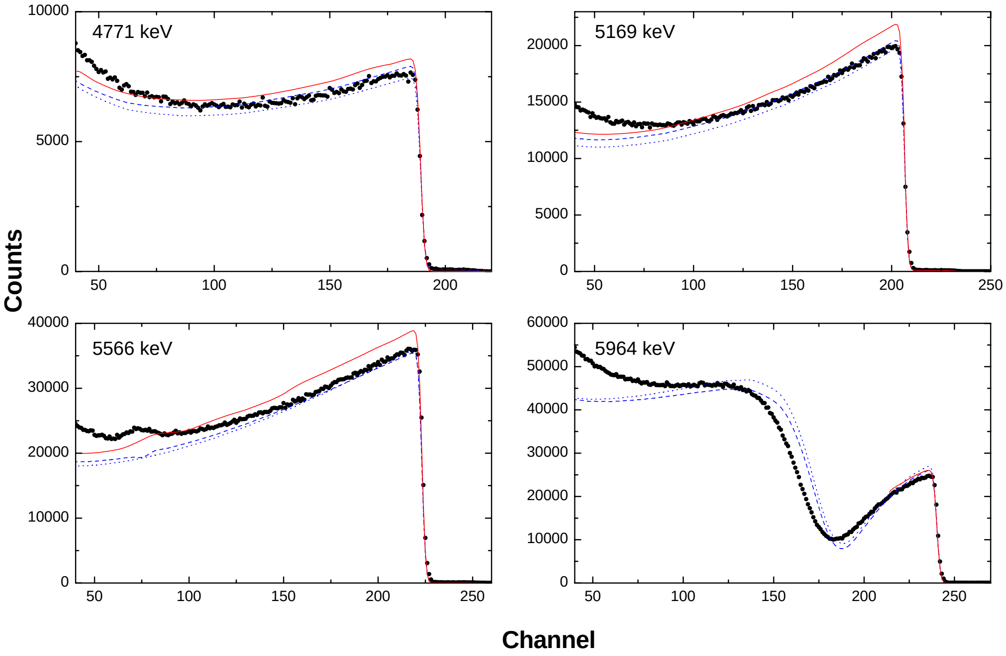

Figure 6: Same as Fig. 5, but at higher energies. The average cross-section is undefined in the energy range 5770–5880 keV.