The A2016 atomic mass evaluation

(I). Evaluation of input data; and adjustment procedures

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Abstract This paper is the first of two articles (Part I and Part II) that presents the results of the new atomic mass evaluation, AMe2016. It includes complete information on the experimental input data (also including unused and rejected ones), as well as details on the evaluation procedures used to derive the tables of recommended values given in the second part. This article describes the evaluation philosophy and procedures that were implemented in the selection of specific nuclear reaction, decay and mass-spectrometric results. These input values were entered in the least-squares adjustment for determining the best values for the atomic masses and their uncertainties. Details of the calculation and particularities of the AMe are then described. All accepted and rejected data, including outweighted ones, are presented in a tabular format and compared with the adjusted values obtained using the least-squares fit analysis. Differences with the previous AMe2012 evaluation are discussed and specific information is presented for several cases that may be of interest to AMe users. The second AMe2016 article gives a table with the recommended values of atomic mass, as well as tables and graphs of derived quantities, along with the list of references used in both the AMe2016 and the NUBASE2016 evaluations (the first paper in this issue).

Amdc: http://amdc.impcas.ac.cn/

Keywords: AMe, trends from the mass surface (TMS), atomic-mass tables, least-squares adjustment


1 Introduction

The mass of an atom equals the sum of the masses of its constituents (protons, neutrons and electrons) minus the binding energy, which includes both the atomic and nuclear binding energies. In general, the binding energy of the electrons outside the nucleus is well known. Therefore, the atomic mass reflects the net consequence of all interactions that hold the nucleons together in the nucleus. Since the strong, weak and electromagnetic interactions act among the nucleons, which on the one hand makes the theoretical description of nuclei very complex, on the other hand it gives us natural laboratories to study these fundamental interactions.

As a fundamental property of nuclei, atomic masses are widely used in many domains of science and engineering. A reliable atomic mass table derived from the experimental data, where the atomic masses and the relevant experimental information can be found conveniently, is in high demand by the research community. To meet the demands, the Atomic Mass Evaluation (AME) was created in 1950’s and now serves the research community by providing the most reliable and comprehensive information related to the atomic masses [1].

The last complete evaluation of experimental atomic mass data AMe2012 [2, 3] was published in 2012. Since then the experimental knowledge of atomic masses has continuously expanded and a large amount of data relevant to atomic masses has been published in the scientific literature. In this article, general aspects of the development of AMe2016 are presented and discussed. In doing this, several local analyses will be given as illustrative examples.

The main AMe2016 evaluation table (Table I) is presented in Part I. All accepted and rejected experimental data are given and compared with the adjusted values deduced using a least-squares fit analysis.

As in the previous AMe versions, all uncertainties are
one-standard deviation ($1\sigma$).

There is no strict literature cut-off date for the data used in the present AME2016 evaluation: all data, available to the authors until the end of October 2016 were included. Results which were not included for particular reasons, such as the need for a heavy revision of the evaluation at too late a stage, were added in remarks to the relevant data. The final mass-adjustment calculations were performed on February 28, 2017.

The present publication includes updated information presented in the previous AME including the data that were not used in the final adjustment due to specific reasons, e.g. data that have too large uncertainties.

Remark: in the following text, several data of general interest will be discussed. Mention of references that can be found in Table I will be avoided. When it is necessary to provide a specific reference, those will be given using the Nsr key-numbers [4], listed at the end of Part II, under “References used in the AME2016 and the NUBASE2016 evaluations” (p. 030003-5) (e.g. [2016De15]).

1.1 Isomers in the AME and the emergence of NUBASE

In the early AME work, a computer data file (called Mfile) that contained the approximate mass values for nuclides in their ground and selected excited isomeric states was maintained. It was used as an approximate input to the adjustment program, which essentially uses the differences between the input and these approximate values in order to improve the precision of the calculations. The other reason for the existence of this file was for isomers, where one has to be careful to identify which state is involved in the reported experimental data, including decay/reaction energies or mass-spectrometric results. Therefore, it was judged necessary to make the Mfile as complete as possible. Thus, the NUBASE evaluation was developed to contain values of the main nuclear properties, such as masses, excitation energies of isomers, half-lives, spin and parities, and decay modes and their intensities, for all known nuclides in their ground and excited isomeric states. The NUBASE evaluation was published independently from AME for the first time in 1997 [5], and was greeted with interest from many colleagues working in the areas of nuclear structure physics, nuclear astrophysics and applied nuclear physics. In 2003 and 2012, the NUBASE and AME were published jointly, which is the case again with the present NUBASE2016 evaluation published in the first part of this issue (41-030001).

Isomers may be involved in mass-measurement experiments. This became even more important for new mass-spectrometric methods that were developed to measure masses of exotic nuclides far from the valley of $\beta$-stability, which have, in general, relatively short lifetimes. The resolving power of mass spectrometers has been improved significantly in recent years and many isomers can be clearly separated. But quite often only an isomeric mixture could be measured and an average mass value for a particular isomeric pair can be obtained. Since the mass of the ground state is the primary aim of the present evaluation, it can be derived only in cases where information on the excitation energies and production rates of the isomers is available. When the excitation energy of a particular isomer is not experimentally known, it is estimated from smooth trends in neighboring nuclides (TNN), as explained in NUBASE2016 (p. 030001-4). Two examples are given in Section 6.2.9 (p. 030002-27) and Section 6.8 (p. 030002-32).

1.2 Highlights

The backbone Nowadays, the highest precision values measured for the atomic masses are obtained by two different experimental techniques: direct mass-spectrometric measurements using Penning traps, and $\gamma$-ray energy measurements following neutron capture reactions.

In the present work, results obtained by both methods are combined consistently (with very few exceptions) to improve considerably the precision of the atomic masses for nuclides along the line of stability in a diagram of the atomic number $Z$ versus neutron number $N$ [6], thus resulting in a reliable ‘backbone’.

The highest relative mass precision $\delta m/m$ of $7 \times 10^{-12}$ has been achieved by a Penning trap spectrometer [2004Ra33]. The masses of some stable alkali-metal nuclides and noble-gas nuclides [2010Mo30] have been determined with relative precision of 10$^{-10}$ or even better, providing reliable reference standards for other mass measurements. While most stable nuclides, and some long-lived ones, could have their mass accuracy improved using Penning traps, the priority has been given by experimentalists to cases where there is a strong motivation from the physics point of view. For example, the $Q_{\beta\beta}$ values for nuclides relevant to neutrino properties have been determined with very high precision [2011Go23], strengthening at the same time the backbone.

Meanwhile, ($n,\gamma$) reactions ([2006De21], [1984Ke15] and [1998Wh01]) determined the binding energies with a relative uncertainty of 10$^{-7}$, providing mass determination with precisions at the level of 10$^{-10}$.

Exotic species The domain of nuclides with experimentally known masses has extended impressively over the last few years, thanks to the developments of radioactive nuclear beam facilities and novel mass spectrometers. In the past, masses of short-lived nuclides were mainly known from $Q_{\beta}$ end-point measurements, while
in the present evaluation, mass spectrometry dominates. Classical time-of-flight mass spectrometry stays at the frontier, exploring the light neutron-rich mass region, albeit with larger uncertainties. Penning traps and storage rings keep on playing an important role in mass measurements for short-lived nuclides. Meanwhile, Multi-Reflection Time-of-Flight spectrometers (Mr-ToF) begin to take the stage. It can be concluded that the shape of the atomic mass surface, and hence understanding of nuclear interactions, has been changed significantly over the last 10-20 years.

Table A. Constants used in this work or resulting from the present evaluation.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
<th>Uncertainty</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 u</td>
<td>$M^{(12)\text{C}}/12$</td>
<td>atomic mass unit</td>
<td>0.020 $\times 10^{-33}$ kg</td>
<td>12 ppb a</td>
</tr>
<tr>
<td>1 u</td>
<td>1 660 539.040</td>
<td>± 0.0057 keV</td>
<td>0.0004 keV</td>
<td>0.45 ppb b</td>
</tr>
<tr>
<td>1 u</td>
<td>931 494.0038</td>
<td>± 0.0004 keV</td>
<td>0.0004 nu</td>
<td>0.45 ppb b</td>
</tr>
<tr>
<td>1 eV$_{90}$</td>
<td>1 000 000.0983</td>
<td>± 0.0061 µeV</td>
<td>0.0004 nu</td>
<td>0.45 ppb b</td>
</tr>
<tr>
<td>1 MeV</td>
<td>1 073 544.1105</td>
<td>± 0.0066 nu</td>
<td>0.0004 nu</td>
<td>0.45 ppb b</td>
</tr>
<tr>
<td>$M_e$</td>
<td>548 579.909070</td>
<td>± 0.00016 nu</td>
<td>0.03 ppb a</td>
<td></td>
</tr>
<tr>
<td>$M_p$</td>
<td>1 007 276 466.93</td>
<td>± 0.09 nu</td>
<td>0.09 ppb c</td>
<td></td>
</tr>
<tr>
<td>$M_n$</td>
<td>4 001 506 179.127</td>
<td>± 0.06 nu</td>
<td>0.015 ppb c</td>
<td></td>
</tr>
<tr>
<td>$M_n - M_H$</td>
<td>839 883.59</td>
<td>± 0.51 nu</td>
<td>610 ppb d</td>
<td></td>
</tr>
<tr>
<td></td>
<td>782 346.52</td>
<td>± 0.48 eV$_{90}$</td>
<td>610 ppb d</td>
<td></td>
</tr>
</tbody>
</table>

a) derived from the work of Mohr and Taylor [7].
b) for the definition of V$_{90}$, see text.
c) derived from this work combined with $M_e$ and total ionization energies for $^1\text{H}$ and $^4\text{He}$ from [7].
d) this work.

2 Units and recalibrations of $\alpha$- and $\gamma$-ray energies

Atomic mass determination for a particular nuclide can be generally performed by establishing an energy relation between the mass we want to deduce and that for a well known nuclide. This energy relation is then expressed in electron-volts (eV). Mass values can also be obtained as an inertial mass from the movement of an ionized atom in an electro-magnetic field. The mass is then derived from a ratio of masses and it is then expressed in ‘unified atomic mass unit’ (u). Those two units are used in the present work.

Since 1960, the mass unit is defined as one twelfth of the mass of one free atom of carbon-12 in its atomic and nuclear ground states, 1 u = $M^{(12)\text{C}}/12$. Before 1960, two mass units were used: the physics one, defined as $^{16}\text{O}/16$, and the chemical one which considered one sixteenth of the average mass of a standard mixture of the three stable oxygen isotopes. This difference was considered as being not at all negligible, when taking into account the commercial value of all concerned chemical substances. Physicists could not convince the chemists to drop their unit. “The change would mean millions of dollars in the sale of all chemical substances”, said the chemists, which was indeed true! Kohman, Mat-tauch and Wapstra [8] then calculated that, if $^{12}\text{C}/12$ was chosen, the change would be ten times smaller for chemists, and in the opposite direction... This led to an unification; ‘u’ stands therefore, officially, for ‘unified mass unit’. It is worth mentioning that the chemical mass-spectrometry community (e.g. bio-chemistry, polymer chemistry) widely use the dalton unit (symbol Da, named after John Dalton [9]). It allows to express the number of nucleons in a molecule, at least as it is presently used in these domains. It is thus not strictly the same as ‘u’.

The unit for energy is the electron-volt. The choice of the volt for the energy unit is not unambiguous. For example, one may use the international volt V, or the volt V$_{90}$ as maintained in national metrology laboratories and defined by adopting an exact value for the
constant \((2e/h)\) in the relation between frequency and voltage from the Josephson effect. Since 1990, by definition \(2e/h = 483597.9\) (exact) \(\text{GHz/V}_{90}\) (see Table B). Already in 1983, an analysis by Cohen and Wapstra \([10]\) showed that all precision measurements of reaction and decay energies were calibrated in such a way that they can be more accurately expressed in \textit{maintained} volts. In fact, the gamma-ray energies determined in wavelength measurements can be expressed in eV without loss in precision, since the conversion coefficient is an exact quantity. Here we take the measurement of the reaction energy for \(^1\text{H}(n,\gamma)^2\text{H}\) as an example. In the experiment, the wavelength of the emitted \(\gamma\) ray is determined by using the Institut Laue-Langevin (ILL) silicon crystal spectrometer. In Ame2003, the recommended value was 2224.5660(4) \(\text{keV}_{90}\), based on the work of Kessler \textit{et al} \([1999\text{Ke05}]\). This result had the highest precision for energy measurement in the input data, with a relative uncertainty of 180 ppb. In the later work from the same group \([2006\text{De21}]\), the value was corrected to be 2224.55610(44) \(\text{keV}\) with new evaluation on the lattice spacing of the crystal. The value of the crystal lattice spacing is used as an adjusted parameter in the CODATA evaluation of Mohr \textit{et al}., but not expressed explicitly. Using the same value of the wave length in \([2006\text{De21}]\), and the length-energy conversion coefficient, we derive 2224.55600(44) \(\text{keV}_{90}\) as an input to our evaluation. During this period, the conversion coefficient with respect to the \textit{international} volt has been changed by \(5.5 \times 10^{-8}\), which is about one third of the measurement uncertainty.

### Table B. Definition of Volt unit, and resulting mass-energy conversion constants.

<table>
<thead>
<tr>
<th>Year</th>
<th>(2e/h)</th>
<th>(u)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1983</td>
<td>483594.21 (1.34) (\text{GHz/V})</td>
<td>931501.2 (2.6) (\text{keV})</td>
</tr>
<tr>
<td>1983</td>
<td>483594 (exact) (\text{GHz/V}_{86})</td>
<td>931501.6 (0.3) (\text{keV}_{86})</td>
</tr>
<tr>
<td>1986</td>
<td>483597.67 (0.14) (\text{GHz/V})</td>
<td>931494.32 (0.28) (\text{keV})</td>
</tr>
<tr>
<td>1990</td>
<td>483597.9 (exact) (\text{GHz/V}_{90})</td>
<td>931493.86 (0.07) (\text{keV}_{90})</td>
</tr>
<tr>
<td>1999</td>
<td>483597.9 (exact) (\text{GHz/V}_{90})</td>
<td>931494.009 (0.007) (\text{keV}_{90})</td>
</tr>
<tr>
<td>2010</td>
<td>483597.9 (exact) (\text{GHz/V}_{90})</td>
<td>931494.0023 (0.0007) (\text{keV}_{90})</td>
</tr>
<tr>
<td>2012</td>
<td>483597.9 (exact) (\text{GHz/V}_{90})</td>
<td>931494.0038 (0.0004) (\text{keV}_{90})</td>
</tr>
</tbody>
</table>

The precision of the conversion factor between mass units and \textit{maintained} volt \((V_{90})\) is higher than that between the former and \textit{international} volt as seen in Table A. Until the end of the last century, the relative precision of \(M - A\) expressed in keV was for several nuclides worse than the same quantity expressed in mass units. Due to the increase of precision of fundamental constants, now the relative precision of \(M - A\) expressed in \(\text{keV}_{90}\) is as good as the same quantity expressed in mass units, whereas the uncertainties expressed in \textit{international} volts are larger than in \(V_{90}\). For example, the mass excess of \(^4\text{He}\) is \(2.603254.130 \pm 0.003 \text{ nu}\) in mass units, \(2.424915.609 \pm 0.059 \text{ eV}_{90}\) in \textit{maintained} volt units and \(2.424915.851 \pm 0.061 \text{ eV}\) in \textit{international} volt units. Therefore, as already adopted in our previous mass evaluations, the \(V_{90}\) (\textit{maintained} volt) unit is used in the present work.

In the most recent CODATA evaluation by Mohr \textit{et al} \([7]\), the relation between \textit{maintained} and \textit{international} volts is given as \(V_{90} = [1+9.83(0.61) \times 10^{-6}]V\), which can be expressed as a difference of 98(6) ppb.

In Table A, the relations between \textit{maintained} and \textit{international} volts, and several constants of interest, obtained from the evaluation of Mohr \textit{et al}. \([7]\) are presented. The ratio of mass units to electronvolts for the two Volt units, and the ratio of the two Volts are also given. In addition, values for the masses of the proton, neutron and \(\alpha\) particle, as derived from the present evaluation, are also given, together with the mass difference between the neutron and the light hydrogen atom.

In the earlier mass tables \((\text{e.g. Ame1993})\), we used to give values for the binding energies, \(ZM_{H} + NM_{\alpha} - M\). The main reason for this was that the uncertainty of this quantity \((\text{in keV}_{90})\) was larger than that of the mass excess, \(M - A\). However, due to the increased precision of the neutron mass, this is no longer important. Similarly to Ame2003 and Ame2012, we now give instead the binding energy per nucleon for educational reasons, connected to the Aston Curve and the maximum stability around the ‘iron-peak’ which is of importance in astrophysics. (See also the note in Part II, Section 2, p. 030003-3)
The defining values and the resulting mass-energy conversion factors are given in Table B. Since 2003, the definition has not been modified. Therefore, no recalibration has been necessary in the present AME2016.

Some more historical points are worth mentioning.

In 1986, Taylor and Cohen [11] showed that the empirical ratio between the two types of volts, which had of course been selected to be nearly equal to 1, had changed by as much as 7 ppm. For this reason, in 1990 a new value was chosen [12] to define the maintained volt $V_{90}$. In their 1998 evaluation, Mohr and Taylor [13] revised the conversion constant to international eV. The result was a slightly higher (and 10 times more precise) value for $V_{90}$.

Since older high-precision, reaction-energy measurements were essentially expressed in keV$_{90}$, we had to take into account the difference in voltage definition that causes a systematic error of 8 ppm. It was therefore necessary, for the AME2003 tables, to adjust the older precise data to the new keV$_{90}$ standard. For $\alpha$-particle energies, Rytz [14] has taken this change into account, when updating his earlier evaluation of $\alpha$-particle energies. We have used his values in the present input data table (Table I) and indicated this by adding in the reference field the symbol “Z”.

A considerable number of $(n, \gamma)$ and $(p, \gamma)$ reactions have precisions not worse than 8 ppm. In 1990, A.H. Wapstra [15] discussed the need for recalibration for several $\gamma$ rays that are often used as calibration standards. This work has been updated in AME2003 (in a special file dedicated to this study, available on the AMDC website [16]) to evaluate the influence of new calibrators, as well as of the new Mohr and Taylor fundamental constants for $\gamma$-ray and particle energies used in $(n, \gamma)$, $(p, \gamma)$ and $(p, n)$ reactions. In doing this, the calibration work of Helmer and van der Leun [17], based on the fundamental constant values at that time, was used. For each of the data concerned, the changes were relatively minor. However, it was necessary to make such recalibrations in AME2003, since otherwise they added up to systematic uncertainties that were non-negligible. The calibration for proton energies has also been undertaken in AME2003. As in the case of Rytz’ recalibrations for $\alpha$-decay energies, such data are marked by “Z” behind the reference key-number. However, there were cases where it was not possible to do so, for example when this position was used to indicate that a remark was added, the same “Z” symbol was added to the uncertainty value mentioned in the remark.

The list of input values (Table I) for our calculations includes many excitation energies derived from $\gamma$-ray measurements that are evaluated and published in Nuclear Data Sheets (NDS) [18]. Only in exceptional cases it made sense to change them to recalibrated results.

3 Input data and their representation - connection diagram

As mentioned above, there are two methods that are used in measurements of atomic masses: the mass-spectrometric one (often called a “direct method”), where the inertial mass is determined from the trajectory of the ion in a magnetic field, or from its time-of-flight; and the so-called “indirect method” where the reaction energy, i.e., the difference between several masses, is determined using a specific nuclear reaction or a decay process. In the present work all available experimental data related to atomic masses (both energy and mass-spectrometric data) are considered. The input data are extracted from the available literature, compiled in an appropriate format and then carefully evaluated.

In the AME data treatment, we try our best to enter the true primary experimental information. In this way, the masses can be recalibrated automatically for any future changes, and the original correlation information can be properly preserved.

One example that illustrates our policy of data treatment is the following. In \cite{1986Ma40}, the $Q$ value of the $^{148}\text{Gd}(p,t)^{146}\text{Gd}$ reaction was measured relative to that of the $^{65}\text{Cu}(p,t)^{63}\text{Cu}$ reference reaction. In AME2003, the corresponding equation was $^{148}\text{Gd}(p,t)^{146}\text{Gd} = -7843 \pm 4$ keV. However, in the present work, it is presented and used as a differential reaction equation: $^{148}\text{Gd}(p,t)^{146}\text{Gd} - ^{65}\text{Cu}(p,t)^{63}\text{Cu} = 1500 \pm 4$ keV. Strictly speaking, those equations are not exact either. What is measured in the experiment is the energy spectra of the ejected particles. Since there are differences between the masses of the measured nuclides and the reference, the response of the ejected particles to the $Q$ values are different for the measured nuclides and the reference, depending also on the angle where the spectra are obtained. While the exact equations are quite complex, we believe that the treatment by differential reaction equation represents the original data more reliably and that most of the primary information is preserved.

Nuclear reaction $A(a,b)B$ and decay $A(b)B$ energy measurements connect the initial ($A$) and final ($B$) nuclides with one or two reaction or decay particles. With the exception of some reactions between very light nuclides, the precision with which the masses of reaction particles $a$ and $b$ are known is much higher than that of the measured reaction and decay energies. Thus, these reactions and decays can each be represented as a link between two nuclides $A$ and $B$. Differential reaction energies $A(a,b)B - C(a,b)D$ are in principle represented by a combination of four masses.

Direct mass-spectrometric measurements, again with exception of a few cases between very light nuclides, can be separated in a class of connections between two or
Figure 1. (a)–(j). Diagram of connections for input data.

For primary data (those checked by other data):

- □ absolute mass-doublet nuclide (i.e. connected to $^{12}$C, $^{35}$Cl or $^{37}$Cl); (or nuclide connected by a unique secondary relative mass-doublet to a remote reference nuclide);
- ○ other primary nuclide;
- \(\bigcirc\) primary nuclide with relevant isomer;
- // mass-spectrometric connection;
- —— other primary reaction connection.

Primary connections are drawn with two different thicknesses. Thicker lines represent the highest precision data in the given mass region

<table>
<thead>
<tr>
<th>Mass Region</th>
<th>Precision</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A &lt; 36)</td>
<td>1 keV</td>
</tr>
<tr>
<td>(36 \leq A \leq 165)</td>
<td>2 keV</td>
</tr>
<tr>
<td>(A &gt; 165)</td>
<td>3 keV</td>
</tr>
</tbody>
</table>

For secondary data (cases where masses are known from one type of data and are therefore not checked by a different connection):

- ■ secondary experimental nuclide determined from mass spectrometry;
- • secondary experimental nuclide determined by a reaction or a decay;
- ○ nuclide for which mass is estimated from trends from the Mass Surface (TMS);
- —— connection to a secondary nuclide. Note that an experimental connection may exist between two estimated TMS nuclides when neither of them is connected to the network of primaries.
three nuclides, and a class that essentially determines the absolute mass value (see Section 5). Penning trap measurements almost always give a ratio of masses between two nuclides (inversely proportional to their cyclotron frequencies in the trap). Sometimes these two nuclides can be very far apart. Thus, those measurements are in most cases best represented as a combination of two masses. Other types of direct experimental methods, such as ‘Smith-type’, ‘Schottky’, ‘Isochronous’, ‘Time-of-flight’ and some ‘Multi-reflection Time-of-flight’ mass spectrometers, are calibrated in a more complex way, and are thus published by their authors as absolute mass values. They are then presented in Table I as a difference: \(^{\text{1}}_{\text{A}}\) El–u.

For completeness, we mention that early mass-spectrometric “triplet” measurements on unstable nuclides (cf. Section 6.2.2, p. 030002-24) can best be represented as linear combinations of masses of three isotopes, with non-integer coefficients [19].

This situation allows us to represent the input data graphically in a diagram of \((N - Z)\) versus \((N + Z)\) as shown in Fig. 1. This is straightforward for absolute mass-doublets and for two-nuclide difference cases; but not for spectrometer triplets and differential reaction energies (see Section 3, p. 030002-5). In general, the differential reactions are more important for one of the two reaction energies. Therefore, we present only the more important one in the graphs. For computational reasons, these data are treated as \(\text{primaries}\) (see below) even though the diagrams show only one connection.

In the present work, all input data are evaluated, i.e. calibrations are checked if necessary, and the data are compared with other results and with the trends from the mass surface (TMS, see next Section) in the region. As a consequence, several input data are corrected or even rejected (see below). All input data, including the rejected ones (not presented in Fig. 1), are given in Table I. As can be seen from Fig. 1, the accepted data may
allow determination of the mass of a particular nuclide using several different routes; such a nuclide is called primary. Their mass values in the table are then derived by least squares methods. In the other cases, the mass of a nuclide can be derived from only one connection to another nuclide; it is called a secondary nuclide. This classification is of importance for our calculation procedure (see Section 5.3, p. 030002-19).

The diagrams in Fig. 1 also show many cases where the relation between two atomic masses is accurately known, but not the actual mass values. Since our policy is to include all available experimental results, we have produced in such cases estimated mass values that are based on TMS in the neighborhood. Also, in this data representation, vacancies occur, which are filled with the estimated values using the same TMS procedure. Estimates of unknown masses are further discussed in the next section.

Some care should be taken in the interpretation of Fig. 1, since excited isomeric states and data relations involving such isomers are not completely represented on these drawings. This is not considered as a serious defect; readers who want to update such values can conveniently consult Table I, where all relevant information is given.

4 Regularity of the mass surface and the use of TMS

When atomic masses are displayed as a function of \( N \) and \( Z \), one obtains a surface in a 3-dimensional space. However, due to the pairing energy, this surface is divided into four sheets. The even-even sheet lies lowest, the odd-odd highest, the other two nearly halfway in-
between, as shown in Fig. 2. The vertical distances from the even-even sheet to the odd-even and even-odd ones are the proton and neutron pairing energies, $\Delta_{pp}$ and $\Delta_{nn}$, respectively, which are nearly equal. The distances of the last two sheets to the odd-odd sheet are equal to $\Delta_{nn} - \Delta_{np}$ and $\Delta_{pp} - \Delta_{np}$, where $\Delta_{np}$ is the proton-neutron pairing energy due to the interaction between the two odd nucleons, which are generally not in the same shell. These energies are represented in Fig. 2, where a hypothetical zero energy represents a nuclide with no pairing among the last nucleons.

Experimentally, it has been observed that the four sheets run nearly parallel in all directions, which means that the quantities $\Delta_{nn}$, $\Delta_{pp}$ and $\Delta_{np}$ vary smoothly and slowly with $N$ and $Z$. In addition, each of the mass sheets also varies smoothly, but rapidly with $N$ and $Z$ [20]. The smoothness is also observed for first-order derivatives (slopes, e.g. the graphs given in Part II, p.030003-4) and all second-order derivatives (curvatures of the mass surface). They are only interrupted in places by cusps or bumps associated with important changes in nuclear structure: shell or sub-shell closures, shape transitions (spherical-deformed, prolate-oblate), and the so-called ‘Wigner’ cusp along the $N = Z$ line.

This observed regularity of the mass sheets in all places, where there is no change in the underlying physics, can be considered as one of the basic properties of the mass surface. Thus, dependable estimates of unknown, poorly known or questionable masses can be obtained by extrapolation from the well-known mass values on the same sheet. In the evaluation of masses the property of regularity and the possibility to make estimates are used for several purposes:
1. Any coherent deviation from the regularity, in a region \((N,Z)\) of some extent, could be considered as an indication that some new physics property is being discovered. However, if only one single mass violates the trends from the mass surface (TMS) defined by the neighboring nuclides, then one may seriously question the correctness of the related datum. In such a case, there might be some undetected systematic \([21]\) contribution to the reported experimental results for this mass. We then re-examine with extra care the available experimental information in the literature for possible errors and often consult with the corresponding authors for additional information. Such a process often leads to corrections.

2. There are cases where several experimental data disagree, but no particular reason can be found for rejecting one, or some of them. In such cases, the measure of agreement with the regularity can be used by the evaluators for selecting which of the conflicting data will be accepted and used in the evaluation, thus following the same policy that was used in our earlier work.

3. There are cases where masses determined from only one experiment (or from the same experiments) deviate severely from the smooth surface. Such cases are carefully examined (Section 4.2).

4. Finally, drawings of the mass surface allow to derive estimates for the still unknown masses, either from interpolations or from short extrapolations (see below, Section 4.3).
4.1 Scrutinizing and manipulating the surface of masses

Direct representation of the mass surface is not convenient, since the binding energy varies very rapidly with \( N \) and \( Z \). Splitting it in four sheets, as mentioned above, complicates even more such a representation. There are two ways that allow to observe the surface of masses with some precision: one of them uses the derivatives of this surface, the other is obtained by subtracting a simple function of \( N \) and \( Z \) from the masses.

The derivatives of the mass surface By derivative of the mass surface we mean a specified difference between the masses of two nearby nuclides. These functions are also smooth and have the advantage of displaying much smaller variations. For a derivative defined in such a way that differences are between nuclides in the same mass sheet, their near parallelism can lead to an (almost) unified surface for the derivative, thus allowing a single display. Therefore, in order to visualize the trends from the mass surface, we found that the derivatives such as \( \alpha \)-decay energies and separation energies of two protons and two neutrons are the best tools to derive such estimates. These three derivatives are plotted against \( N \), or \( Z \) in Part II, Figs. 1–26, p. 030003-74.

However, from the way these derivatives are created, they give information only within one of the four sheets of the mass surface (e-e, e-o, o-e or o-o; e-o standing for even-\( N \) and odd-\( Z \)). When examining the mass surface, an increased or decreased spacing of the sheets cannot be observed. Also, when estimating unknown masses, divergences of the four sheets could be unduly created,
which is unacceptable.

Fortunately, other representations are also possible (e.g. separately for odd and even nuclides: one-neutron separation energies versus $N$, one-proton separation energy versus $Z$, $\beta$-decay energy versus $A$, ...). We have prepared a number of such graphs that can be obtained from the Amdc website [22].

The method of ‘derivatives’ suffers from the involvement of two masses for each point to be drawn, which means that if one point deviates from regularity, it could be due to either the mass of the nuclide it represents or that of the related nuclide, rendering the analysis rather complex. Also, reversely, if one mass is moved, then the two related points are changed in opposite directions, causing confusion in the drawing.

**Subtracting a simple function** Since the mass surface is smooth, one can try to define a function of $N$ and $Z$ as simple as possible and not too far from the real surface of masses. The difference between the mass surface and this function, while displaying reliably the structure of the former, will vary less rapidly, thus improving its observation.

A first and simple approach is the semi-empirical liquid drop formula of Bethe and Weizsäcker [23] with the addition of a pairing term in order to fuse more or less the four sheets of the mass surface. Another possibility, that we prefer [20], is to use the results of one of the modern models. However, we can use only those models that provide masses specifically for the spherical part, forcing the nucleus to be not deformed. The reason is that the models generally describe quite well the shell and sub-
Manipulating the mass surface  In order to make estimates of unknown masses or to test changes on measured ones, an interactive graphical program was developed [20, 24] that allows a simultaneous observation of four graphs, either from the ‘derivatives’ type or from the ‘differences’ type, as a function of any of the variables $N, Z, A, N-Z$ or $N-2Z$, while drawing iso-lines (lines connecting nuclides having same value for a parameter) of any of these quantities. The mass of a nuclide can be modified or created in any view and we can determine how much freedom is left in setting a value for this mass. At the same time, interdependence through secondary connections (Fig. 1) are taken into account. In cases where two tendencies may alternate, following the parity of the proton or the neutron numbers, one of the parities may be deselected.

The replaced values for data yielding the ‘irregular masses’ as well as the ‘estimated unknown masses’ (see below) are thus derived by observing the continuous property in several views of the mass surface, with all the consequences due to connections to masses in the same chain. Comparisons with the predictions of 16 nuclear mass-models are presently available in this program.

With this graphical tool, the results of ‘replacement’ analyses are felt to be most robust; and also the estima-
Figure 1 (i). Diagram of connections for input data — continued.

Figure 1 (j). Diagram of connections for input data — continued.
tion of unknown masses is more reliable.

All mass values dependent on interpolation procedures and indeed all values not derived from experimental data alone have been clearly marked with the sharp ‘#’ symbol in all tables, and elsewhere in the text.

Since publication of Ame1983 [25], estimates are also given for the precision of data derived from TMS. These uncertainties are not based on a formalized procedure, but rather on previous experience with such estimates.

In the case of extrapolation, however, the uncertainty of the estimated mass will increase with the distance of extrapolation. These uncertainties are obtained by considering several graphs of TMS with a guess on how much the estimated mass may change without causing the extrapolated surface to look too distorted. This recipe is unavoidably subjective, but has proven to be efficient through the agreement of these estimates with newly measured masses in a large majority of cases [26].

4.2 Irregular mass values

When a single mass deviates significantly from regularity with no similar pattern for nuclides with same $N$ or with same $Z$ values, then the correctness of the data determining this mass may be questioned.

Our policy, redefined in Ame1995 [27], for those locally irregular masses, and only when they are derived from a unique mass relation (i.e., not confirmed by a different experimental method), is to replace them by values derived from trends from the mass surface (TMS). Table C lists 31 such cases in the present evaluation that were removed, to avoid strongly oscillating plots (to be compared to 27 cases in Ame2012, 27 in Ame2003, 59 in Ame1995 and 67 in Ame1993). Although these numbers reflects a more strict use of this procedure, the user of our tables should not assume that the remaining 31 items are the same ones carried on from generation to generation. The opposite, however, is true: most of the old ones have been replaced by new data, thus showing that we were correct in our choice. Generally, only one experimental result is reported for such unique mass relation. But sometimes there are two measurements (2 cases) or three (in previous evaluations) that we still treat the same way, since use of the same method and the same type of relation may well lead to the same systematic uncertainty (for example a mis-assignment or ignorance of a final level). Taking into account the connecting chains for secondaries (Figs. 1a–1j) has the consequence that several more ground state masses are affected (and twice as many values in each type of plot of derivatives as given in Part II). It should be stressed that only the most striking cases have been treated in this way, those necessary to avoid, as much as possible, confusions in the graphs in Part II. In particular, the plots of $\alpha$-decay energies of light nuclides (Fig. 18 and 19 in Part II, p. 030003-252 and 253) exhibit many overlaps and crossings that obscure the drawings; no attempt was made to locate possible origins of such irregularities.

Replacing these few irregular experimental values by the ones we recommend, in all tables and graphs in Ame2016, means also that, as explained already in Ame1995, we discontinued an older policy that was introduced in Ame1993, where original irregular experimental values were given in all main tables, and ‘recommended’ ones given separately in secondary tables. This policy led to confusion for many users of our tables. Since Ame1995, we only give what we consider the “best recommended values”, using, when we felt necessary and as explained above, ‘values derived from TMS’. Data which are not used following this policy are given in Table C and they can be easily located in Table I, where they are flagged ‘D’ and always accompanied by a comment.

Figure 2. The surface of masses is split into four sheets. This scheme represents the pairing energies responsible for this splitting. The zero energy surface is purely hypothetical with no pairing at all among the outer nucleons.
explaining in which direction the value has been changed and by what amount.

Such data, as well as other local irregularities that can be observed in the figures in Part II, could be considered as incentive for remeasurements, preferably by a different method, in order to remove any doubt and possibly point out true irregularities due to physical properties.

Table C. Experimental data that we recommend replacing by values derived from TMS in AME2016.

<table>
<thead>
<tr>
<th>Item</th>
<th>Reference</th>
<th>Experimental value</th>
<th>Recommended value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{49}$Al−u</td>
<td>2007Ju03</td>
<td>21653</td>
<td>22170# 430#</td>
</tr>
<tr>
<td>$^{42}$Si−u</td>
<td>2007Ju03</td>
<td>16275</td>
<td>17680# 540#</td>
</tr>
<tr>
<td>$^{44}$P−u</td>
<td>2007Ju03</td>
<td>10070</td>
<td>11220# 540#</td>
</tr>
<tr>
<td>$^{47}$Cl−u</td>
<td>2007Ju03</td>
<td>−9576</td>
<td>−10500# 430#</td>
</tr>
<tr>
<td>$^{49}$Ar−u</td>
<td>2015Me01</td>
<td>−19110</td>
<td>−18450# 430#</td>
</tr>
<tr>
<td>$^{67}$Mn−u</td>
<td>2015Me.A</td>
<td>−36600</td>
<td>−35920# 320#</td>
</tr>
<tr>
<td>$^{69}$Fe−u</td>
<td>2015Me.A</td>
<td>−42240</td>
<td>−41900# 430#</td>
</tr>
<tr>
<td>$^{70}$Co−u</td>
<td>2011Es06</td>
<td>−50370</td>
<td>−50060# 320#</td>
</tr>
<tr>
<td>$^{74}$Ni−u</td>
<td>2011Es06</td>
<td>−52830</td>
<td>−52020# 210#</td>
</tr>
<tr>
<td>$^{77}$Cu−u</td>
<td>2006Ha62</td>
<td>−51850</td>
<td>−52200# 160#</td>
</tr>
<tr>
<td>$^{79}$Cu−u</td>
<td>2006Ha62</td>
<td>−46700</td>
<td>−44810# 320#</td>
</tr>
<tr>
<td>$^{80}$Zr−u</td>
<td>1998Is06</td>
<td>−59600</td>
<td>−58360# 320#</td>
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<td>−50242</td>
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<td>17700</td>
<td>20180# 300#</td>
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<td>1992Ba28</td>
<td>11810</td>
<td>12480# 200#</td>
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<td>1977Bo28</td>
<td>12300</td>
<td>13100# 100#</td>
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<tr>
<td>$^{118}$Ru−u</td>
<td>1976Jo.A</td>
<td>12400</td>
<td>13100# 100#</td>
</tr>
<tr>
<td>$^{118}$In− ($^{\beta^-}$) $^{118}$Sn</td>
<td>1978Al18</td>
<td>5340</td>
<td>5420# 50#</td>
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<td>4270</td>
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<td>$^{126}$Ag−u</td>
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<td>−65140# 220#</td>
</tr>
<tr>
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<td>5300</td>
<td>5930# 200#</td>
</tr>
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<td>6390# 50#</td>
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<td>6440# 200#</td>
</tr>
<tr>
<td>$^{143}$I−u</td>
<td>2016Kn03</td>
<td>−53849</td>
<td>−54350# 220#</td>
</tr>
<tr>
<td>$^{150}$Ba−u</td>
<td>2016Kn03</td>
<td>−55309</td>
<td>−53570# 320#</td>
</tr>
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<td>$^{154}$Ce−u</td>
<td>2016Kn03</td>
<td>−56404</td>
<td>−56060# 220#</td>
</tr>
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<td>1987Fa.A</td>
<td>9829</td>
<td>9650# 50#</td>
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<tr>
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<td>2014Kh04</td>
<td>8019</td>
<td>8260# 200#</td>
</tr>
<tr>
<td>$^{281}$Rg− ($^{\alpha}$) $^{277}$Mt</td>
<td>2013Og04</td>
<td>9454</td>
<td>9900# 400#</td>
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</tbody>
</table>

a) References are listed in Part II in this issue, Section 6, p. 030003-5.
The present authors insist that only the most striking irregularities have been replaced by estimates. Here we give the mass of $^{84}$Nb as an example. The $Q_\beta$ value was measured in [1996Sh27] with an uncertainty claimed to be 300 keV. However, trends from mass surface strongly suggested that $^{84}$Nb should be 3200 keV less bound. Therefore the experimental value was labeled with “D” in AME2012 and replaced by an estimate. Recently the mass of $^{84}$Nb was measured by mass spectrometry [2016Xi.A], and the value is very close (200 keV) to our estimate, which was given with a precision of 300 keV.

4.3 Estimates for unknown masses

Estimates for unknown masses also are made with the use of trends from the mass surface, as explained above, by demanding that all graphs should be as smooth as possible, except where they are expected to be affected by shell closures or nuclear deformation effects. Therefore, we warn the user of our tables that the present extrapolations will be wrong if new regions of deformation or (semi-) magic numbers appear.

In addition to the rather severe constraints imposed by the requirement of simultaneous regularity of all graphs, many further constraints result from knowledge of reaction or decay energies in the regions where these estimates are made. These regions and these constraints are shown in Figs. 1a–1j. Two kinds of constraints are present. In some cases the masses of $(Z,A)$ and $(Z,A+4)$ are known but not the mass of $(Z,A+2)$. Then, the values of $S_2n(A+2)$ and $S_2n(A+4)$ cannot both be chosen freely from the graphs; their sum is known. In other cases, the mass differences between several nuclides $(A+4n,Z+2n)$ are known from $\alpha$-decays and also those of $(A-2+4n,Z+2n)$. Then, the differences between several successive $S_{2n}(A+4n,Z+2n)$ are known. Similar situations exist for two or three successive $S_{2p}$ or $Q_{\alpha}$ values.

Knowledge of stability or instability against particle emission, or limits on proton or $\alpha$ emission, yields upper or lower limits on the separation energies.

For proton-rich nuclides with $N < Z$, mass estimates can be obtained from the charge symmetry. This feature gives a relation between masses of isobars around the $N = Z$ line. In several cases, we made a correction by including the Thomas-Ehman effect [28], which makes proton-unstable nuclides more bound than what follows from the above estimate. For very light nuclides, we can use the estimates of this effect as proposed by Comay et al. [29].

Another often good estimate can be obtained from the observation that masses of nuclear states belonging to an isobaric multiplet are represented quite accurately by a quadratic equation of the charge number $Z$ (or of the third components of the isospin, $T_3 = \frac{1}{2}(N-Z)$): the Isobaric Multiplet Mass Equation (IMME) [30]. The use of this relation is attractive, since it uses experimental information such as the excitation energies of the isobaric analog states (IAS). New mass measurements regularly question the validity of the IMME, followed soon by other work showing that another member of the same multiplet needs to be questioned. For example, [2012Zh34] found, by measuring the mass of $^{53}$Ni, a breakdown of the quadratic form of IMME for the $A = 53$ quartet, from which a non-zero coefficient $d$ was derived to be 39(11) keV. In a later experiment, the lowest $T = 3/2$ state in $^{53}$Co was established via the measurement of the $\beta$-delayed $\gamma$ deexcitation of $^{53}$Ni [2016Su10], which questioned the isobaric-analog state (IAS) assignment in a previous $\beta-p$ decay experiment [2007Do17]. The validity of the IMME in the quadratic form was thus restored for $A = 53$.

Up to AME1983, we indeed used the IMME for deriving mass values for nuclides for which no, or little information was available. This policy was questioned with respect to the correctness in stating ‘experimental’ a quantity that was derived by combination with a calculation. Since AME1993, it was decided not to present any IMME-derived mass values in our evaluation, but rather use the IMME as a guideline when estimating masses of unknown nuclides. We continue this policy here, and do not replace experimental values by an estimated one from IMME, even if orders of magnitude more precise. Typical examples are $^{26}$S and $^{40}$Ti, for which IMME predicts masses with precisions of 24 keV and 22 keV, respectively, whereas the experimental masses are known for both from double-charge-exchange reactions with 160 keV precision.

The extension of the IMME to higher energy isobaric analog states has been studied by Wapstra [31]. The validity of the method, however, is made uncertain by possible effects spoiling the relation. In the first place, the strength of some IASs at high excitation energies is known to be distributed over several levels with the same spin and parity. Even in cases where this interference effect has not been observed, it remains a possibility, and as such, introduces an uncertainty in the energy level to be attributed to the IAS. In the second place, as argued by Thomas and Ehman [28], particle-unstable levels must be expected to be shifted somewhat.

It also happens that information on excitation energies of $T_3 = -T + 1$ IASs is available from measurements on proton emission following $\beta$ decays of their $T_3 = -T$ parents. The authors, in some cases, derived a mass value from their results for the parent nuclide, using a formula, derived by Antony et al. [32], from a study of known energy differences between IAS. We observe, however, that one obtains somewhat different mass values by combining Antony differences with the
mass of the mirror nuclide of the mother. Also, earlier considerations did not take into account the difference between proton-pairing and neutron-pairing energies, which A.H. Wapstra noticed have a non-negligible influence on the IMME constants.

Another possibility is to use a relation proposed by Jänecke [33], as done for example by Axelsson et al. [34] in the case of $^{31}$Ar. In several cases we have compared the results of different ways for extrapolating, in order to find a best estimate for the desired mass value.

Enough values have been estimated to ensure that every nuclide for which there is any experimental Q-value is connected to the main group of primary nuclides. In addition, the evaluators want to achieve continuity of the mass surface. Therefore, an estimated value is included for any nuclide if it is between two experimentally studied masses. Thus, $^{31}$Ar. In several cases we have compared the results of different ways for extrapolating, in order to find a best estimate for the desired mass value.

Enough values have been estimated to ensure that every nuclide for which there is any experimental Q-value is connected to the main group of primary nuclides. In addition, the evaluators want to achieve continuity of the mass surface. Therefore, an estimated value is included for any nuclide if it is between two experimentally studied masses on a line defined by either $Z =$ constant (isotones), $N = constant$ (isotopes), $N - Z =$ constant (isodiaspheres), or, in a few cases $N + Z =$ constant (isobars). It would have been desirable to also give estimates for all unknown nuclides that are within reach of the present accelerators and mass separator technologies. Unfortunately, such an ensemble is not easy to define. Instead, we estimate mass values for all nuclides for which at least one piece of experimental information is available (e.g. identification or half-life measurement or proof of instability towards proton or neutron emission). Then, the ensemble of experimental and estimated masses has the same contour as in the NUBASE2016 evaluation.

5 Calculation Procedures

The atomic mass evaluation is unique when compared to the other evaluations of data [20], in a sense that almost all mass determinations are relative measurements, not absolute ones. Even those called ‘absolute mass doublets’ are relative to $^{12}$C, $^{32}$Cl or $^{37}$Cl. Each experimental datum sets a relation in mass or in energy among two (in a few cases three or more) nuclides. It can be therefore represented by one link among these two nuclides. The ensemble of these links generates a highly entangled network. Figs. 1a–1j, in Section 3 above, show a schematic representation of such a network.

The masses of a large number of nuclides are multiply determined, entering the entangled area of the canvas, mainly along the backbone. Correlations do not allow determining their masses in a straightforward manner.

To take into account these correlations we use a least-squares method weighed according to the precision with which each piece of data is known. This method allows to determine a set of adjusted masses.

5.1 Least-squares method

Each piece of data has a value $q_i \pm dq_i$ with the accuracy $dq_i$ (one standard deviation) and makes a relation between two, three or four masses with unknown values $m_\mu$. An overdetermined system of $Q$ data to $M$ masses ($Q > M$) can be represented by a system of $Q$ linear equations with $M$ parameters:

$$
\sum_{\mu=1}^{M} k_{\mu}^i m_\mu = q_i \pm dq_i,
$$

(1)
e.g. for a nuclear reaction $A(a,b)B$ requiring an energy $q_i$ to occur, the energy balance is written:

$$
m_A + m_a - m_b - m_B = q_i \pm dq_i.
$$

(2)
Thus, $k_A^i = +1$, $k_a^i = +1$, $k_b^i = -1$ and $k_B^i = -1$.

In matrix notation, $K$ being the $(Q,M)$ matrix of coefficients, Eq. 1 is written: $|K|m = |q|$. Elements of matrix $K$ are almost all null: e.g. for $A(a,b)B$, Eq. 2 yields a line of $K$ with only four non-zero elements.

We define the diagonal weight matrix $W$ by its elements $w_i^i = 1/(dq_i dq_i)$. The solution of the least-squares method leads to a very simple construction:

$$
|KWK|m = |KWq|.
$$

(3)
The normal matrix $A = |KWK|$ is a square matrix of order $M$, positive-definite, symmetric and regular and hence invertible [35]. Thus the vector $|\overline{m}|$ for the adjusted masses is:

$$
|\overline{m}| = A^{-1} |KWq| \quad \text{or} \quad |\overline{m}| = R|q|.
$$

(4)
The rectangular $(M,Q)$ matrix $R$ is called the response matrix.

The diagonal elements of $A^{-1}$ are the squared errors on the adjusted masses, and the non-diagonal ones $(a^{-1})_{\mu}^i$ are the coefficients for the correlations between masses $m_\mu$ and $m_i$. Values for correlation coefficients for the most precise nuclides are given in Table B of Part II (p. 030003-3). Following the advice of B.N. Taylor, we now give on the website of the AMDC [22] the full list of correlation coefficients, allowing any user to perform exact calculation of any combination of masses.

One of the most powerful tools in the least-squares calculation described above is the flow-of-information matrix, discovered in 1984 by one of us [36]. This matrix allows to trace back the contribution of each individual piece of data to each of the parameters (here the atomic masses). The AME uses this method since 1993.

The flow-of-information matrix $F$ is defined as follows: $K$, the matrix of coefficients, is a rectangular $(Q,M)$ matrix. The transpose of the response matrix $R$ is also a $(Q,M)$ rectangular one. The $(i,\mu)$ element of $F$
is defined as the product of the corresponding elements of $\mathbf{R}$ and of $\mathbf{K}$. In Ref. [36], it is demonstrated that such an element represents the “influence” of datum $i$ on parameter (mass) $m_i$. A column of $\mathbf{F}$ thus represents all the contributions brought by all data to a given mass $m_i$, and a line of $\mathbf{F}$ represents all the influences given by a single piece of data. The sum of influences along a line is the “significance” of that datum. It has also been proven [36] that the influences and significances have all the expected properties, namely that the sum of all the influences on a given mass (along a column) is unity, that the significance of a datum is always less than unity and that it always decreases when new data are added. The significance defined in this way is exactly the quantity obtained by squaring the ratio of the uncertainty on the adjusted value over that of the input one, which was the recipe used before the discovery of the $\mathbf{F}$ matrix to calculate the relative importance of data.

A simple interpretation of influences and significances can be obtained in calculating, from the adjusted masses and Eq. 1, the adjusted data:

$$|q| = \mathbf{KR}|q|.$$  \hspace{1cm} (5)

The $i^{th}$ diagonal element of $\mathbf{KR}$ represents then the contribution of datum $i$ to the determination of $q_i$ (same datum): this quantity is exactly what is called above the significance of datum $i$. This $i^{th}$ diagonal element of $\mathbf{KR}$ is the sum of the products of line $i$ of $\mathbf{K}$ and column $i$ of $\mathbf{R}$. The individual terms in this sum are precisely the influences defined above.

The flow-of-information matrix $\mathbf{F}$, provides thus insight on how the information from datum $i$ flows into each of the masses $m_i$.

The flow-of-information matrix cannot be given in full in a printed table. It can be observed along lines, displaying for each datum, the nuclides influenced by this datum and the values of these influences. It can be observed also along columns to display for each primary mass all contributing data with their influence on that mass.

The first display is partly given in the table of input data (Table I) in column ‘Signf.’ for the significance of primary data and ‘Main infl.’ for the largest influence. Since in the large majority of cases only two nuclides are concerned in each piece of data, the second largest influence could easily be deduced. It is therefore not felt necessary to give a table of all influences for each primary datum.

The second display is given in Part II, Table II (p. 030003-3) for the up to three most important data with their influence in the determination of each primary mass.

5.2 Consistency of data

The system of equations being largely overdetermined ($Q >> M$) offers the evaluator several interesting possibilities to examine and judge the data. One might for example examine all data for which the adjusted values deviate significantly from the input ones. This helps to locate erroneous pieces of information. One could also examine a group of data in one experiment and check if the uncertainties assigned to them in the experimental paper were not underestimated.

If the precisions $dq_i$ assigned to the data $q_i$ were indeed all accurate, the normalized deviations $v_i$ between adjusted $q_i$ (Eq. 5) and input $q_i$ data, $v_i = (q_i - q_i)/dq_i$, would be distributed as a Gaussian function of standard deviation $\sigma = 1$, and would make $\chi^2$:

$$\chi^2 = \sum_{i=1}^{Q} \left( \frac{q_i - q_i}{dq_i} \right)^2 \quad \text{or} \quad \chi^2 = \sum_{i=1}^{Q} v_i^2.$$  \hspace{1cm} (6)

equal to $Q - M$, the number of degrees of freedom, with a standard deviation of $\sqrt{2(Q - M)}$.

One can define as above the normalized chi, $\chi_n$ (or ‘consistency factor’ or ‘Birge ratio’): $\chi_n = \sqrt{\chi^2/(Q - M)}$ for which the expected value is $1 \pm 1/\sqrt{2(Q - M)}$.

Another quantity of interest for the evaluator is the partial consistency factor, $\chi_p^n$, defined for a (homogeneous) group of $p$ data as:

$$\chi_p^n = \sqrt{\frac{Q}{Q - M} \frac{1}{p} \sum_{i=1}^{p} v_i^2}.$$  \hspace{1cm} (7)

Of course the definition is such that $\chi_p^n$ reduces to $\chi_n$ if the sum is taken over all the input data. One can consider for example the two main classes of data: the reaction and decay energy measurements and the mass-spectrometric data (see Section 5.5). One can also consider groups of data related to a given laboratory and with a given method of measurement and examine the $\chi_p^n$ of each of them. There are presently 278 groups of data in Table I (among which 185 have at least one measurement used in determining the masses), identified in column ‘Lab’. A high value of $\chi_p^n$ might be a warning on the validity of the considered group of data within the reported uncertainties. We used such analyses in order to be able to locate questionable groups of data. In bad cases they are treated in such a way that, in the final adjustment, no really serious conflicts occur. Remarks in Table I report where such corrections have been made.

5.3 Separating secondary data

In Section 3, while examining the diagrams of connections (Fig. 1), we noticed that, whereas the masses of secondary nuclides can be determined uniquely from the
chain of secondary connections going down to a primary nuclide, only the latter see the complex entanglement that necessitated the use of the least-squares method.

In terms of equations and parameters, we consider that if, in a collection of equations to be treated with the least-squares method, a parameter occurs in only one equation, removing this equation and this parameter will not affect the result of the fit for all other data. Thus, we can redefine more precisely what was called secondary in Section 3: the parameter above is a secondary parameter (or mass) and its related equation is a secondary equation. After the reduced set has been solved, then the secondary equation can be used to determine the final value and uncertainty for that particular secondary parameter. The equations and parameters remaining after taking out all secondaries are called primary.

Therefore, only the system of primary data is over-determined, and thus will be improved in the adjustment, so that each primary nuclide will benefit from all the available information. Secondary data will remain unchanged; they do not contribute to $\chi^2$.

The diagrams in Fig. 1 show that many secondary data exist. Thus, taking them out simplifies considerably the system. More importantly, if a better value is found for a secondary datum, the mass of the secondary nuclide can easily be improved (one has only to be careful since the replacement can change other secondary masses down the chain, see Fig. 1). The procedure is more complicated for new primary data.

We define degrees for secondary nuclides and secondary data. They reflect their distances along the chains connecting them to the network of primaries. The first secondary nuclide connected to a primary one will be a nuclide of degree 2; and the connecting datum will be a datum of degree 2 as well. Degree 1 is for primary nuclides and data. Degrees for secondary nuclides and data range from 2 to 18. It is the heaviest nuclide $^{299}$Ei that has the highest degree number 18. Its mass is determined through a long $\alpha$ chain, albeit many of them are just estimates. In Table I, the degree of data is indicated in column ‘Dg’. In the table of atomic masses (Part II, Table I, p.030003-6), each secondary nuclide is marked with a label in column ‘Orig.’ indicating from which other nuclide its mass value is determined.

To summarize, separating secondary nuclides and secondary data from primaries allow to significantly reduce the size of the system that will be treated by the least-squares method described above. After treatment of the primary data alone, the adjusted masses for primary nuclides can be easily combined with the secondary data to yield masses of secondary nuclides.

In the next Section we will show methods for reducing further this system, but without loss of any information. Methods that reduce the system of primaries for the benefit of the secondaries not only decrease computational time (which nowadays is not so important), but allows an easier insight into the relations between data and masses, since no correlation is involved.

Remark: the word primary used for these nuclides and for the data connecting them does not mean that they are more important than the others, but only that they are subject to the least-squares treatment above. The labels primary and secondary are not intrinsic properties of data or nuclides. They may change from primary to secondary or vice versa when other information becomes available.

5.4 Compacting the set of data

5.4.1 Pre-averaging

Two or more measurements of the same physical quantities can be replaced without loss of information by their average value and precision, reducing thus the system of equations to be treated. By extending this procedure, we consider parallel data: reaction data occur that give essentially values for the mass-difference between the same two nuclides, except in rare cases where the precision is comparable to that in the masses of the reaction particles. Example: $^{14}$C($^7$Li,$^7$Be)$^{14}$B and $^{14}$C($^{14}$C,$^{14}$N)$^{14}$B; or $^{22}$Ne(t,$^3$He)$^{22}$F and $^{22}$Ne($^7$Li,$^7$Be)$^{22}$F.

Such data are represented together, in the main least-squares fit calculations, by one of them carrying their average value. If the $Q$ data to be pre-averaged are strongly conflicting, i.e. if the consistency factor (or Birge ratio) $\chi_n = \sqrt{\chi^2/(Q-1)}$ resulting in the calculation of the pre-average is greater than 2.5, the (internal) precision $\sigma_i$ in the average is multiplied by the Birge ratio ($\sigma_{av} = \sigma_i \times \chi_n$). There are no cases where $\chi_n > 2.5$, see Table D (there were 2 cases in Ame2012, and 6 in Ame2003). The quantity $\sigma_n$ is often called the ‘external error’. However, this treatment is not used in the rare cases where the precisions of the input values differ too much, since the assigned uncertainties lose any significance. If such a case occurs, considering policies from the Particle Data Group [37] and some statistical-treatment methods reviewed by Rajput and MacMahon [38], we adopt an arithmetic average and the dispersion of values as an uncertainty, which is equivalent to assigning to each of these conflicting data the same uncertainty.

In the present evaluation, we have replaced 2977 data by 1186 averages. As can be seen from Fig. 3, as much as 23% of which have values of $\chi_n$ (Birge ratio) beyond unity, 1.6% beyond two and none beyond 3, giving an overall very satisfactory distribution for our treatment.

As a matter of fact, in a complex system like the one here, many values of $\chi_n$ beyond 1 or 2 are expected to exist, and if the uncertainties were multiplied by $\chi_n$ in all these cases, the $\chi^2$-test on the total adjustment would have been invalidated.
Table D. Worst pre-averagings. $n$ is the number of data in the pre-average.

<table>
<thead>
<tr>
<th>Item</th>
<th>$n$</th>
<th>$\chi_n$</th>
<th>$\sigma_n$</th>
<th>Item</th>
<th>$n$</th>
<th>$\chi_n$</th>
<th>$\sigma_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{186}$W(n,γ)$^{187}$W</td>
<td>2</td>
<td>2.44</td>
<td>0.11</td>
<td>$^{177}$Pt(α)$^{177}$Os</td>
<td>2</td>
<td>2.06</td>
<td>6.06</td>
</tr>
<tr>
<td>$^{144}$Ce(β−)$^{144}$Pr</td>
<td>2</td>
<td>2.44</td>
<td>2.18</td>
<td>$^{204}$Cf(α)$^{204}$Cm</td>
<td>2</td>
<td>2.03</td>
<td>3.97</td>
</tr>
<tr>
<td>$^{220}$Fr(α)$^{216}$At</td>
<td>2</td>
<td>2.34</td>
<td>4.66</td>
<td>$^{15}$N(p,n)$^{15}$O</td>
<td>2</td>
<td>2.03</td>
<td>1.28</td>
</tr>
<tr>
<td>$^{75}$As(n,γ)$^{76}$As</td>
<td>2</td>
<td>2.32</td>
<td>0.17</td>
<td>$^{58}$Fe(t,p)$^{60}$Fe</td>
<td>4</td>
<td>2.03</td>
<td>7.38</td>
</tr>
<tr>
<td>$^{110}$In(β−)$^{110}$Cd</td>
<td>3</td>
<td>2.29</td>
<td>28.4</td>
<td>$^{204}$Tl(β−)$^{204}$Pb</td>
<td>2</td>
<td>2.03</td>
<td>0.39</td>
</tr>
<tr>
<td>$^{146}$Ba(β−)$^{146}$La</td>
<td>2</td>
<td>2.24</td>
<td>107.4</td>
<td>$^{278}$Mt(α)$^{278}$Bh</td>
<td>3</td>
<td>1.98</td>
<td>43.6</td>
</tr>
<tr>
<td>$^{40}$Cl(β−)$^{40}$Ar</td>
<td>2</td>
<td>2.21</td>
<td>76.1</td>
<td>$^{167}$Os(α)$^{167}$W</td>
<td>4</td>
<td>1.98</td>
<td>3.50</td>
</tr>
<tr>
<td>$^{219}$U(α)$^{215}$Th</td>
<td>2</td>
<td>2.18</td>
<td>38.5</td>
<td>$^{106}$Ag(ε)$^{106}$Pd</td>
<td>2</td>
<td>1.98</td>
<td>6.63</td>
</tr>
<tr>
<td>$^{153}$Gd(n,γ)$^{154}$Gd</td>
<td>2</td>
<td>2.16</td>
<td>0.39</td>
<td>$^{78}$Se(n,γ)$^{79}$Se</td>
<td>3</td>
<td>1.96</td>
<td>0.28</td>
</tr>
<tr>
<td>$^{36}$Si(11B,15N)$^{34}$Si</td>
<td>3</td>
<td>2.14</td>
<td>32.4</td>
<td>$^{46}$Ca(n,γ)$^{47}$Ca</td>
<td>2</td>
<td>1.94</td>
<td>0.56</td>
</tr>
<tr>
<td>$^{111}$Cs(p)$^{112}$Xe</td>
<td>3</td>
<td>2.10</td>
<td>5.03</td>
<td>$^{181}$Pt(α)$^{177}$Hg</td>
<td>3</td>
<td>1.93</td>
<td>15.2</td>
</tr>
<tr>
<td>$^{223}$Pa(α)$^{219}$Ac</td>
<td>2</td>
<td>2.09</td>
<td>10.0</td>
<td>$^{145}$Sm(ε)$^{145}$Pm</td>
<td>2</td>
<td>1.92</td>
<td>7.92</td>
</tr>
<tr>
<td>$^{27}$P(2p)$^{25}$Al</td>
<td>2</td>
<td>2.08</td>
<td>74.7</td>
<td>$^{234}$Th(β−)$^{234}$Pa$m$</td>
<td>3</td>
<td>1.90</td>
<td>2.10</td>
</tr>
<tr>
<td>$^{204}$Rn$^{208}$Pb$_{981}$</td>
<td>2</td>
<td>2.06</td>
<td>18.2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

This explains the choice we made here of a rather high threshold ($\chi_n^0 \approx 2.5$), compared e.g. to $\chi_n^0 = 2$ recommended by Woods and Munster [39] or $\chi_n^0 = 1$ used in a different context by the Particle Data Group [37], for departing from the rule of 'internal error' of the weighted average.

Figure 3. Birge Ratios of all the pre-averaged data.

Besides the computer-automated pre-averaging, we found it convenient, in some $\beta^+$-decay cases, to combine results stemming from various capture ratios in an average. These cases are $^{109}$Cd(ε)$^{109}$Ag (average of 3 data), $^{139}$Ce(ε)$^{139}$La (average of 10) and $^{195}$Au(ε)$^{195}$Pt (5 results), and they are detailed in Table I. Four more cases ($^{147}$Tb, $^{152}$Ho, $^{166}$Yb and $^{207}$Bi) occur in our list, but they carry no weight and are labeled with ‘U’ in Table I.

5.4.2 Used policies in treating parallel data

In averaging $\beta^-$ (α-) decay energies derived from branches observed in the same experiment, to or from different levels in the decay of a given nuclide, the uncertainty we use for further evaluation is not the one resulting from the weighted average adjustment, but instead we use the smallest experimental one. In this way, we avoid decreasing artificially the part of the uncertainty that is not due to statistics. In some cases, however, when it is obvious that the uncertainty is dominated by weak statistics, we do not follow the above rule (e.g. $^{20}$Al(p)$^{22}$Mg of [1997Bl04]). Some quantities have been reported more than once by the same group. If the results are obtained by the same method in different experiments and are published in regular refereed journals, only the most recent one is used in the calculation, unless explicitly mentioned otherwise. There are two reasons for this policy. The first is that one might expect that the authors, who believe their two results are of the same quality, would have averaged them in their latest publication. The second is that if we accept and average the two results, we would have no control on the part of the uncertainty that is not due to statistics. Our policy is different if the newer result is published in a secondary reference (not refereed abstract, preprint, private communication, conference, thesis or annual report). In such cases, the older result is used in the calculations, except when the newer one is an update of the previous value. In the latter case, the original reference in our list mentions the unreferred paper.
5.4.3 Replacement procedure

Large contributions to $\chi^2$ have been known to be caused by a nuclide $G$ connected to two other ones $H$ and $K$ by reaction links with large uncertainties compared to those deduced from the mass difference between $H$ and $K$, in cases where the two disagreed. Evidently, contributions to $\chi^2$ of such local discrepancies suggest an unrealistically high value of the overall consistency parameter. This is avoided by a replacement procedure: one of the two links is replaced by an equivalent value for the other. The pre-averaging procedure gives the most reasonable mass value for $G$ and do not cause undesirably large contributions to $\chi^2$.

5.4.4 Insignificant data

Another feature to increase the meaning of the final $\chi^2$ is to not use, in the least-squares procedure, data with weights at least a factor 10 smaller than other data, or combinations of all other data giving the same result. Such data were labeled ‘U’ in the list of input data; comparison with the output values allows to check our judgment. Earlier, data were labeled ‘U’ if their weight was 10 times smaller than that of a simple combination of other data. This concept has been extended, since AME1993, to data that weigh 10 times less than the combination of all other accepted data. Until the AME2003 evaluation, our policy was not to print data labeled ‘U’ if they already appeared in one of our previous tables, reducing thus the size of the table of data to be printed. This policy has been changed since AME2012, and we try as much as possible to give all relevant data, also including insignificant ones. The reason for this is that conflicts might appear amongst recent results, and access to older ones might shed some light on our judgement, when evaluating the new data.

5.5 Used policies – treatment of undependable data

The important interdependence of most data, as illustrated by the connection diagrams (Figs. 1a–1j), allows local and general consistency tests. These can indicate that something may be wrong with the input values. We follow the policy of checking all significant data that differ by more than two (sometimes 1.5) standard deviations from the adjusted values. Fairly often, examination of the experimental results shows that a correction is necessary. Possible reasons could be that a particular decay has been assigned to a wrong final level or that a reported decay energy belongs to an isomer, rather than to a ground state, or even that the mass number assigned to a decay was incorrect. In such cases, the values are corrected and remarks are added below the corresponding $A$-group of data in Table I, in order to explain the reasons for the corrections.

It also happens that a careful examination of a particular paper would lead to serious doubts about the validity of the results within the reported precision, but could not permit making a specific correction. Doubts can also be expressed by the authors themselves. The results are given in Table I and compared with the adjusted values. They are labeled ‘F’, and not used in the final adjustment, but always followed by a comment to explain the reason for this label. The reader may observe that in several cases the difference between the experimental and adjusted values is small compared to the experimental uncertainty: this does not disprove the correctness of the label ‘F’ assignment.

It happens quite often that two (or more) pieces of data are discrepant, leading to important contribution to the $\chi^2$. A detailed examination of the papers may not allow correction or rejection, indicating that at least the results in one of them could not be trusted within the given uncertainties. Then, based on past experience, we use in the calculations the value that seems to be the most reliable, while the other is labeled ‘B’, if published in a regular refereed journal, or ‘C’ otherwise.

Data with labels ‘F’, ‘B’ or ‘C’ are not used in the calculations. We do not assign such labels if, as a result, no experimental value published in a regular refereed journal could be given for one or more resulting masses. When necessary, the policy defined for ‘irregular masses’ with ‘D’-label assignment may apply (see Section 4.2).

In some cases, detailed analysis of strongly conflicting data could not lead to reasons to assume that one of them is more dependable than the others or could not lead to a rejection of a particular data entry. Also, bad agreement with other data is not the only reason to doubt the correctness of the reported data. As in previous AME, and as explained above (see Section 4), we made use of the property of regularity of the surface of masses in making a choice, as well as in further checks on the other data.

We do not accept experimental results if information on other quantities (e.g. half-lives), derived in the same experiment and for the same nuclide, were in strong contradiction with well established values.

5.6 The AME computer program

Our computer program in four phases has to perform the following tasks: i) decode and check the data file; ii) build up a representation of the connections between masses, allowing thus to separate primary masses and data from secondary ones, to pre-average same and parallel data, and thus to reduce drastically the size of the system of equations to be solved (see Section 5.3 and 5.4), without any loss of information; iii) perform the least-squares matrix calculations (see above); and iv) deduce
the atomic masses (Part II, Table I), the nuclear reaction and separation energies (Part II, Table III), the adjusted values for the input data (Table I), the influences of data on the primary nuclides (Table I), the influences received by each primary nuclide (Part II, Table II), and display information on the inversion errors, the correlations coefficients (Part II, Table B), the values of the $\chi^2$'s, the distribution of the $v_i$ (see below), among others.

5.7 Results of the calculation

In this evaluation, we have 13035 experimental data of which 5663 are labeled ‘U’ (see above), 844 are labeled ‘O’ (old result from same group) and 853 are not accepted and labeled ‘B’, ‘C’, ‘D’ or ‘F’ (respectively 502, 157, 33 and 161 items). In the calculation we have thus 5675 valid input data, compressed to 3884 in the pre-averaging procedure. Separating secondary data, leaves a system of 2023 primary data, representing 1094 primary reactions and decays, and 929 primary mass-spectrometric measurements. To these are added 835 data estimated from TMS trends (see Section 4), p.030002-9), some of which are essential for linking unconnected experimental data to the network of experimentally known masses (see Figs. 1a–1j).

In the atomic mass table (Part II, Table I) there is a total of 3923 masses (including $^{12}\text{C}$) of which 3435 are ground state masses (2497 experimental masses and 938 estimated ones), and 488 are excited isomers (369 experimental and 119 estimated). Among the 2497 experimental ground state masses, 11 nuclides have a precision better than 0.1 keV, 378 better than 1 keV and 1477 better than 10 keV (respectively 87, 315 and 1438 in Ame2012). There are 153 nuclides known with uncertainties larger than 100 keV (123 in Ame2012). Separating secondary masses in the ensemble of 3923, leaves 1207 primary masses ($^{12}\text{C}$ not included).

Thus, we have to solve a system of 2023 equations with 1207 parameters. Theoretically, the expectation value for $\chi^2$ should be $816 \pm 20$ (and the theoretical $\chi_n = 1 \pm 0.025$).

The total $\chi^2$ of the adjustment is actually 825 ($\chi_n = 1.005$), thus showing that the ensemble of evaluated data was of excellent quality, and that the adopted criteria of selection and rejection were adequate. In the past this was not always the case and in Ame2003 we could observe that on average the uncertainties in the input values were underestimated by 23%. The distribution of the $v_i$'s (the individual contributions to $\chi^2$, as defined in Eq. 6, and given in Table I) is also acceptable. If we consider all the 11511 data that are used in the adjustment plus the ‘obsolete’ ones (label ‘O’) and the unweighed ones (label ‘U’), the distribution of $v_i$'s yields 20% of the cases beyond unity, 3.3% beyond two, and no items beyond 3.

Considering separately the two main classes of data, the partial consistency factors $\chi^2_n$ are respectively 1.021 and 0.987 for energy measurements and for mass-spectrometric data, showing that both types of selective input data are of excellent quality.

As in our previous works [2, 40, 41], we have estimated the average accuracy for 185 groups of data used in the evaluation that were related to a given laboratory and a specific method of measurement, by calculating their partial consistency factors $\chi^2_n$ (see Section 5.2). As much as 98 groups have $\chi^2_n$ larger than unity, and 2 groups larger than 2.

6 Discussion of the input data

In most cases, values given by authors in the original publication are accepted, but there are also exceptions. One example is the performed recalibration due to change in the definition of volt, as discussed in Section 2. For somewhat less simple cases, a remark is added in Table I at the end of the concerned A-group. A curious example of combinations of data that cannot be accepted without change follows from the measurements of the Edinburgh-Argonne group [1997Da07]. They reported a series of $\alpha$-decay energies, where the ancestors were isomers between which the excitation energy was accurately known from the difference of their proton-decay energies. These authors gave values for the excitation energies between isomeric daughter pairs with considerably smaller uncertainties than those derived from the uncertainties quoted for the measured $\alpha$-decay energies. The reason is that the decay energies of two parallel $\alpha$-decay chains are correlated; this means that the uncertainties in their differences are relatively small. Unfortunately, the presented data do not allow an exact calculation of both the masses and the isomeric excitation energies. This would have required that, in addition to the two $E_\alpha$ values of an isomeric pair, the uncertainty of the $\alpha$-energy difference should also have been given. Instead, entering all their $Q_\alpha$ and $E_1$ (isomeric excitation energies) values in our adjustment would yield outputs with too small uncertainties, while accepting any partial collection makes some uncertainties too large. Therefore, in this case we do enter a selection of the input values, which are slightly changed, but chosen in such a way that our adjusted $Q_\alpha$ and $E_1$ values and corresponding uncertainties differ as little as possible from those given by the authors. A further complication could occur if some of the $Q_\alpha$ values are also measured by other groups. But until now, we found no serious deviations in such cases.

A change in uncertainties, not values, is caused by the fact that, in several cases, we do not necessarily accept the reported $\alpha$-energy values as belonging to transitions between ground states. This also causes uncertainties in
the derived proton-decay energies to deviate from those reported by the authors (e.g. in the α-decay chain of \(^{170}\text{Au}\)), see also Section 7.9.

6.1 Improvements along the backbone

Since AME2012, all new mass-spectrometric data constituting the backbone were obtained from precision measurements of cyclotron frequencies of ions in Penning traps. Like to the classical measurements, where ratios of voltages or resistances were used, we found that the Penning trap results can be converted to a linear combination of masses of electrically neutral atoms (in \(\mu\text{n}\)), without any loss of accuracy. A special mention is needed for the MIT-FSU group [2005Ra34] which reports their original results as linear equations, including corrections for electron and molecular binding energies. Other groups give their results as ratio of cyclotron frequencies (see also next paragraph), which we convert to linear equations as described in Appendix C, (p. 030002-43) and finally we add corrections for electron and molecular binding energies. In such cases, we added a remark to the equation used in the input data table (Table I), to describe the original data and our treatment. Some authors publish their results directly as masses, but this is not a recommended practice for high-precision mass measurements.

6.1.1 Calculation of molecular binding energies for very precise mass measurements

The most precise mass-spectrometric measurements use Penning trap spectrometers, which measure the cyclotron frequency of a reference ion and an ion of interest in a uniform magnetic field \(B\). Not only the electronic binding energy (single or multiple ionization), but also the molecular binding energy (dissociation energy) can be involved in the measured frequency ratios, as described for example in Ref. [1995Di08]. For most molecules used in the experiments, the binding energy represents typically a correction of a few parts in \(10^{10}\) and its uncertainty only limits the accuracy of the neutral atomic mass to a few parts in \(10^{12}\), for example in Ref. [2004Ra33]. For measurements with precisions not better than \(10^{-9}\)(100 eV/100 u), the molecule binding energy could be neglected without loss of accuracy. In cases where the precision is better than \(10^{-10}\)(10 eV/100 u), e.g. at MIT [1995Di08] and FSU [2015My03], it is necessary to take into account the molecular binding energy.

6.2 Mass spectrometry away from \(\beta\)-stability

The reader interested in the history of mass-spectrometric measurements, the resolving powers, resolutions and the discoveries they rendered possible in nuclear physics and cosmology, can refer to the publication by one of us (G.A.) [1].

6.2.1 Penning trap spectrometers

Nowadays, seven Penning traps are being operated at the major accelerator facilities around the world: ISOLTRAP-Cern, CPT-Argonne, JYFLTRAP-Jyväskylä, LEBIT-East-Lansing, SHIPTRAP-Darmstadt, TITAN-Vancouver, and TRIGA-Trap-Mainz. They measure the atomic masses for nuclides farther from the valley of \(\beta\)-stability, using the cyclotron frequencies of charged ions captured in the trap. Such a frequency is always compared to that of a (well) known reference nuclide in order to determine the ratio of two masses, which is converted, without loss of accuracy, to a linear relation between the two masses (see also Section 6.1 above and Appendix C, p. 030002-43). Experimental methods that utilize measurements of cyclotron frequency have an advantage compared to volt or magnetic field measurements in a sense that the observable needed in the former, namely the frequency, is the physical quantity that can be measured with the highest precision. In fact, very high resolving power (\(10^6\)) and accuracies (up to \(10^{-8}\)) are routinely achieved for nuclides located quite far from the line of \(\beta\)-stability. Such high resolving power made it possible in 1991 [42], for the first time in the history of mass spectrometry, to resolve nuclear isomers from their ground state (\(^{82}\text{Rb}\)\(^m\)) and to determine their excitation energies. Another beautiful demonstration of complementarity between mass spectrometry and nuclear spectroscopy was given in [2004Va07] for \(^{70}\text{Cu}\), \(^{70}\text{Cu}\)\(^m\) and \(^{70}\text{Cu}\)\(^n\), where in the same work the masses of the three isomers were determined directly by mass spectrometry, while the excitation energies were measured by \(\beta\gamma\) spectroscopy. Typically, the precision can reach 100 eV or better (60 eV for the difference between \(^6\text{He}\) and \(^7\text{Li}\) at TITAN-Vancouver [2012Br03]). Even the most exotic nuclides, such as \(^{11}\text{Li}\) (8.75 ms) or \(^{74}\text{Rb}\) (64.78 ms), were measured with precisions of 600 eV and 4 keV with the TITAN-Vancouver [2008Sm03] and ISOLTRAP-Cern [2007Ke09] facilities, respectively.

In earlier evaluations, we found it necessary to multiply uncertainties from some groups of mass-spectrometric data [43] with discrete factors \(F = 1.5, 2.5\) or 4.0 following the partial consistency factors \(\chi^2_k\) we found for these groups (see Section 5.2). Such a treatment is not necessary for most of the Penning trap results, which almost all have \(F = 1\).

6.2.2 Double-focussing mass spectrometry

Classical double-focussing mass spectrometry was performed on-line at ISOLDE-CERN to measure masses of nuclides far away from the valley of stability. In these experiments, a relationship between three masses was established. These mass-triplet measurements, in which undetectable systematic effects could build-up in large
deviations when the procedure is iterated [1986Au02], could be recalibrated with the help of the Penning trap measurements. Recalibration was automatically obtained in the evaluation, since each mass-triplet was originally converted to a linear mass relation among the three nuclides, allowing both easy application of least-squares procedures, and automatic recalibration. In the present adjustment of data, most of the 181 original data, performed in the 80’s, are now outweighed, except for the most exotic (and thus the most interesting) ones. There are still five of them that contribute to the present adjustment, essentially for some very exotic nuclides: $^{91}$Rb for 12% of the determination of its mass, $^{95}$Rb (49%), $^{144}$Cs (20%). In Table I, the relevant equations are normalized to make the coefficient of the middle isotope unity, so that they read e.g.

$$\text{97Rb} - (0.490 \times ^{99}\text{Rb} + 0.511 \times ^{95}\text{Rb}) = 350 \pm 60 \text{ keV},$$

$$\text{145Cs} - (0.392 \times ^{148}\text{Cs} + 0.608 \times ^{143}\text{Cs}) = -370 \pm 90 \text{ keV},$$

the $^{148}$Cs symbol represents the mass excess of nuclide $^{148}$Cs in keV. The other two coefficients are three-digit approximations of

$$\frac{A_2}{A_3 - A_1} \times \frac{A_3 - A_1}{A_3} \text{ and } \frac{A_2}{A_3 - A_1} \times \frac{A_3 - A_2}{A_1}.$$  

We took $A$ instead of $M$ in order to arrive at coefficients that do not change if the $M$-values change slightly. The difference is, however, unimportant.

### 6.2.3 Radio-frequency mass spectrometry

The Orsay Smith-type mass-spectrometer MISTRAL, which was also connected to ISOLDE, had performed quite precise measurements of very short-lived light nuclides, before the Penning traps could cover all the possibilities that were offered by a transmission mass spectrometer. There are eight of the measurements performed with MISTRAL that are still used in this evaluation for the determination of the masses of $^{26}$Ne, $^{26,27,28}$Na and $^{29}$Mg.

### 6.2.4 Classical time-of-flight

Mass measurements by the time-of-flight mass-spectrometry technique, firstly at SPEG (GANIL) and TOFI (Los Alamos), later at Michigan State University (MSU), also apply to very short-lived nuclides, due to instant measurements, but the precisions are much lower than those obtained with MISTRAL. Masses of almost undecelerated fragment products, coming from thin targets bombarded with heavy ions [44] or high energy protons [45], are determined from a combination of magnetic deflection and time-of-flight measurements. Nuclides in an extended region in $A/Z$ and $Z$ are analyzed simultaneously. Each individual ion, even if very short-lived (1µs), is identified and has its mass measured. In this way, mass values with precisions of $(3 \times 10^{-6}$ to $5 \times 10^{-5}$) can be obtained for a large number of neutron-rich nuclides of light elements, up to $A = 70$. One difficulty in such experiments is that the obtained value can apply to an isomeric mixture where all isomers with half-lives of the order of, or longer than the time of flight (about 1 µs) may contribute. The limited resolving power, around $10^4$, and cross-contaminations can cause significant shifts in masses. The most critical part in these experiments is the calibration, since it is frequently from an empirically determined function, which, in several cases, had to be extrapolated rather far from the calibrating masses. It is possible that, in the future, a few mass-measurements far from stability may provide better calibration points, thus allowing a re-analysis of the concerned data. Such recalibrations require analysis of the raw data and cannot be done by the evaluators. With new data available from other methods, which allow detailed comparisons to be made, we observed strong discrepancies for these groups, and had to increase the associated partial consistency factor to $F = 1.5$.

### 6.2.5 Cyclotron time-of-flight

Cyclotrons offer very long time-of-flight basis, yielding high resolving power for ions living longer than 50µs. The accelerator radio-frequency is taken as reference to ensure a precise time determination, but this method implies that the number of turns that an ion has to make inside the cyclotron, should be known exactly. This was achieved successfully at SARA-Grenoble in the mass measurement of $^{80}$Y. Experiments performed at GANIL with the CSS2 cyclotron, could not determine the exact number of turns. In the first experiment around $^{108}$Sn [1996Ch32], a careful simulation was done instead. In the second experiment on $^{68}$Se, $^{76}$Sr, $^{86}$Sr and $^{86}$Y [2001La31], a mean value of the number of turns was experimentally determined for the most abundant species only, which mainly involved the calibrants. Penning traps measurements at the CPT-Argonne, JYFLTRAP-Jyväskylä and ISOLTRAP revealed that this method suffered from serious systematic errors. Later, improved measurements at GANIL with the CSS2 cyclotron [2008Go23] were in better agreement with the Penning trap data.

### 6.2.6 Multi-Reflection Time-of-Flight Mass Spectrometer

A new type of instrument, called Multi-Reflection Time-of-Flight mass spectrometer (MR-ToF), has seen the light recently at major nuclear physics facilities. Three MR-ToF’s, operated at ISOLDE-CERN, RIBRIKEN and at the GSI facility, begin to produce interesting results, which are included in the present evaluation.
Several other MR-ToF’s are under construction at other facilities such as TRIUMF, Argonne and SPIRAL2. The MR-ToF mass measurement is based on time-of-flight. Like storage rings, it aims at extending the flight path by reflecting ions back and forth in a static electric field. With this method, a relative mass precision of $10^{-7}$ is routinely achieved in typically 10 milliseconds. Remarkable results have been achieved recently at ISOLTRAP using the MR-ToF: it was possible to reach the most exotic nuclei in the light mass region, $^{52,53,54}$Ca [2013Wi06] and $^{52,53}$K [2015Ro10], as well as in the heavy mass region, $^{131}$Cd [2015At03]. A precision of 10 keV has been obtained for the less exotic nuclide ($^{52}$Ca), and a precision of 110 keV for the most exotic one ($^{53}$K) with half-life of 30 ms.

For mass determination with MR-ToF, the general relation between mass-to-charge ratio ($m/q$) and time-of-flight $t$ is [2013Wi06]:

$$t = \alpha \sqrt{m/q} + \beta,$$  

where $\alpha$ and $\beta$ are constants related to the experimental set-up and are the same for the ion of interest and for the reference ions.

At RIKEN and Gsi, the $\beta$ parameter can be determined independently, thus only one reference nuclide is needed for mass calibration. In this way, the ratio of time-of-flight between the ion of interest and the reference ion is used to extract the linear equation, as it is the case for Penning trap measurement (see Appendix C p. 030002-43). Results from RIKEN ([2013It01], [2016Se.A]) and Gsi ([2015Di03]) are presented in this way in the present evaluation.

However, at ISOLDE-CERN, two reference masses are used to determine the mass of interest, and the so-called $C_{tof}$ method is used. When using this method, we express the linear equation in term of absolute mass.

At first, the two constants ($\alpha$, $\beta$) are extracted from the two reference equations:

$$t_1 = \alpha \sqrt{(m/q)_1} + \beta,$$
$$t_2 = \alpha \sqrt{(m/q)_2} + \beta,$$

where $(m/q)_1$ and $(m/q)_2$ are the mass-to-charge ratios of reference 1 and reference 2, while $t_1$ and $t_2$ are their time-of-flights. We thus obtain:

$$\alpha = \frac{t_1 - t_2}{\sqrt{(m/q)_1} - \sqrt{(m/q)_2}},$$
$$\beta = t_1 - \sqrt{(m/q)_1} \frac{t_1 - t_2}{\sqrt{(m/q)_1} - \sqrt{(m/q)_2}}.$$

To extract the mass of interest, $\alpha$ and $\beta$ are replaced in Eq. (8) and the mass can be written:

$$m/q = C_{tof} \Delta_{ref} + \frac{1}{2} \Sigma_{ref},$$

where $C_{tof}$, $\Delta_{ref}$ and $\Sigma_{ref}$ are defined by:

$$C_{tof} = \frac{t_1 - t_2}{\sqrt{(m/q)_1} - \sqrt{(m/q)_2}},$$
$$\Delta_{ref} = \sqrt{(m/q)_1} - \sqrt{(m/q)_2},$$
$$\Sigma_{ref} = \sqrt{(m/q)_1} + \sqrt{(m/q)_2}.$$

The mass uncertainty is calculated from the uncertainty $\sigma$, of coefficient $C_{tof}$ and the reference mass uncertainties $\sigma_1$ and $\sigma_2$:

$$\sigma^2 = \left(\frac{m}{q}\right)^2 \left(\frac{1}{2} \sigma_1^2 \left(\frac{m}{q}\right)_1 + \sigma_2^2 \left(\frac{m}{q}\right)_2 + 4\left(\sqrt{(m/q)_1} - \sqrt{(m/q)_2}\right)^2 \sigma_1^2\right).$$

6.2.7 Storage-ring time of flight

Similarly, a long flight path can be obtained in a storage ring, which is operated in the mode of isochronous mass spectrometry (IMS). The first set-up of this type was operated at Gsi-Esr at Darmstadt. The precision of the measurements could be as good as 90 keV even for nuclides quite far from stability. Recently, [2016Kn03] reanalyzed some data from two earlier experiments and reported some new masses at Gsi-Esr. For some of the newly reported nuclides, only two events were recorded. The results show the potential of the IMS method. However the systematic uncertainty is rather large and eight results from that work appear in Table C. The Cooler Storage Ring for experiment (CSRe) at the IMP-LANZHOU is the second spectrometer for IMS mass measurements. Precision better than 10 keV has been achieved. The isomer of $^{52}$Co has been resolved from the ground state, demonstrating the excellent resolving power [2016Xu10].

6.2.8 Cooled beam cyclotron frequency

Storage rings could also be used with cooled beams to measure the cyclotron frequency as has been demonstrated since 1997 at the Gsi-Esr storage ring, with precisions sometimes as good as 12 keV. Many of the measured nuclides belong to known $\alpha$-decay chains. Thus, the available information on masses for proton-rich nuclides is considerably extended.

It must be mentioned that in the first group of mass values as given by Gsi authors [2000Ra23], several data could not be accepted without changes. The reason was that in the determination of the mass values they had to combine $\alpha$-decay energies between two or more of the occurring nuclides. Evidently, these energies could not be included without corrections in our calculations, where they would be again combined with these $Q_{\alpha}$ values. Remarks are added to the data in Table I in order to warn for such cases. Fortunately, this group of data is only of historical interest since they were superseded by more recent high-precision results [2005Li24] using the same method.
instruments. A wealth of high-quality data were published recently using this technique, see e.g. [2012Ch19] and references therein.

6.2.9 Isomeric mixtures

As stated above, many mass-spectrometric results yield an average mass value $M_{av}$ for a mixture of isomers. Here, we use a special treatment for the possible mixture of isomers (see Appendix B p. 030002-39) and information about these changes are duly explicit in remarks accompanying these data.

The mass $M_0$ of ground state can be calculated if both the excitation energy $E_1$ of the upper isomer and the relative production rates of the isomers are known. But often this is not the case. If $E_1$ is known but not the production ratio, one must assume equal probabilities for all possible relative intensities. In the case of one excited isomer, the estimated mass for $M_0$ becomes $M_{av} - E_1/2$, and the part of the error due to this uncertainty is $0.29E_1$ (see Appendix B, Section B.4, p. 030002-42). This policy was defined and tested first for the Gsi-Esr cooled beam cyclotron frequency data and was discussed with the authors of the measurements. In 15 cases, more than two excited isomers contribute to the measured line.

A further complication arises if $E_1$ is not known. In such a case, we have to make the best possible estimate for $E_1$. As always this estimated value is flagged with ‘#’. This, in addition to questions related to $\alpha$-decay chains involving isomers, was a reason for us to consider the matter of isomers with even more attention. Part of the results of our estimates are incorporated in the NUBASE evaluation. In estimating the $E_1$ values, we first look at experimental data possibly giving lower limits: e.g. if it is known that one of two isomers decays to the other; or if $\gamma$ rays of known energy occur in such decays. If not, we try to interpolate between $E_1$ values for neighboring nuclides that can be expected to have the same spin and configuration assignments (for odd $A$: isotones if $Z$ is even, or isotopes if $Z$ is odd). If such a comparison does not yield useful results, indications from theory were sometimes accepted, including upper limits for transition energies following from the measured half-lives. Values estimated this way were provided with somewhat generous errors, dutifully taken into account in deriving final results.

In several of these measurements, an isomer can only contribute if its lifetime is relatively long (hundreds of milliseconds or longer). However, half-life values given in NUBASE are those for neutral atoms. For bare nuclides, where all electrons are fully stripped from the atom, the lifetimes of such isomers can be considerably longer, since the decay by conversion electrons is switched off. The reported mass measurements [2005Li24] of the 580 ms $^{151}$Er$^m$ isomer at $E_1=2586.0$ keV excitation energy and the 103 ms $^{117}$Te$^m$ isomer at $E_1=296.1$ keV are two examples.

Considering the isomeric mixtures and combining experimental data from decay spectroscopy and from mass spectrometry can provide valuable information for the atomic masses. This can be demonstrated in the following example. Masses of the nuclides along the $\alpha$-decay chain $^{206}$Ac-$^{202}$Fr-$^{198}$At-$^{194}$Bi-$^{190}$Tl were deemed unknown in Ame2012, while they were considered to be known in Ame2003. For these nuclides, two long-lived states exist with high and low spin, respectively, and two $\alpha$-decay chains are established in parallel. The excitation energies of the isomeric states are unknown. In Ame2003, their masses were determined by storage ring mass spectrometry [2003Li.A], [2005Li24], where the mixture of two states were assumed and the corrections implemented. Later the mass of $^{190}$Tl in its high-spin state was measured with unambiguous assignment of the state from decay spectroscopy. The result was included in Ame2012 as private communication [2012Bo.A] (published later as [2014Bo26]). This state was assumed to be the excited isomer, but the excitation energy was unknown. The excitation energy of $^{190}$Tl was estimated from TNN to be 90#(50#) keV in Ame2012, and then the masses of these five nuclides in their ground state were deemed unknown. By using resonance ionization laser ion source technique, a specific state can be selected, and it can be identified through decay spectroscopy. In this way, the ground state mass of $^{198}$At was unambiguously measured by ISOLTRAP [2013St25]. The excitation energy of $^{190}$Tl$^m$ was determined to be 89(12) keV for the first time, which agrees with the estimated value. In Ame2016, the masses of all five nuclides connected via $\alpha$ decays are now being experimentally known.

6.3 Masses of unbound nuclides

Presently, many nuclides beyond the driplines can be accessed in the light mass region. They can decay via direct proton or neutron emission. The half-lives of these unbound nuclides are too short for them to acquire their outer electrons (which takes around $10^{-14}$ s), and to form atoms. However, we still convert their masses to “atomic masses” so we can treat them consistently with other nuclides. It is experimentally challenging to study these unbound nuclides far from stability: only very few events can be observed. Frequently, theoretical calculations are required to extract their properties from the experimental data.

On the proton rich side, resonant states could be formed due to the Coulomb barrier. There are different approaches to study these states: transfer reaction with missing mass spectrum, proton scattering, and complete kinematic measurement with invariance mass spec-
trum. For a broad resonant state, the definition of the resonance energy and width is not unique. For example, $^{15}\text{F}$ was studied in resonant elastic scattering using a thick CH$_4$ gas target in inverse kinematics with a $^{14}\text{O}$ beam [204HG015]. The proton-decay energy of $^{15}\text{F}$ was obtained to be $1.29^{+0.08}_{-0.06}$ MeV from the energy at which the magnitude of the internal wave function is a maximum, or $1.45^{+0.16}_{-0.10}$ MeV where the elastic scattering cross section is maximum, corresponding to a phase shift of $\delta = \pi/2$. Since the latter value is consistent with those obtained in transfer reaction studies, it is adopted in our evaluation.

Some single-proton resonant states can be accessed and studied in two-proton decay experiments. For example, the 1p-decay energies of 1560(130) and 2850(40) keV for the ground and first excited states in $^{15}\text{F}$ [204LA12] are well reproduced in the angular-correlation studies of two-proton decays of $^{16}\text{Ne}$ [2008Mu13].

On the neutron-rich side of the nuclear chart, the mass of unbound nuclides can be determined by means of the missing-mass method using transfer reactions (e.g. [2015Ma54]), or with the invariant-mass method using radioactive-ion beams (e.g. [2012Ko43]). Recently, various such beams and improved detection techniques have been impressively developed, which allows new masses of unbound nuclides to be determined.

In the case of neutron-induced reaction, only the centrifugal barrier plays a role in the formation of a given resonant state. Since no barrier exists at all for a s-wave neutron, the observation of asymmetric peak near the threshold is a general feature of spectra obtained in invariant-mass experiments (e.g. [2010Jo06]). This state is usually referred to as a virtual state, which has no definite lifetime and thus differs significantly from a real resonance state. The virtual state can be characterized by the s-wave neutron-nucleus scattering length; its eigen energy is approximately $\hbar^2/2\mu a_s^2$, where $\mu$ is the reduced mass and $a_s$ is the scattering length.

### 6.4 Isobaric Analog states (IAS)

The concept of isospin was introduced by Heisenberg [46] and developed by Wigner [47] to describe the charge independence of nuclear forces. This concept is widely used in particle and nuclear physics. Within the isospin formalism, a nucleus composed of $Z$ protons and $N$ neutrons has a fixed isospin projection of $T_z = (N - Z)/2$, while all states in the nucleus can have different total isospins $T \geq |T_z|$. In other words, states of a given $T$ can occur in a set of isobaric nuclei with $T_z = T, T-1, ..., -T$. These states with the same $T$ and $J^+$ are called Isobaric Analog States (IAS). A set of IAS with fixed $A$ and $T$ are believed to have very similar nuclear structure properties and to be energetically degenerate in the framework of isospin symmetry. Their relative masses can be used to explore the charge symmetry and charge independence of the nuclear interaction via the Isobaric Mass Multiplet Equation (IMME) [48], and with calculations of the Coulomb Displacement Energy (CDE) (see for example [32], and references therein).

As in AME2012, IASs that are determined via external relations were evaluated. In some cases, one IAS can be involved in a local network thus influencing other masses. Such an IAS was included in the present evaluation, although its excitation energy may be determined mainly through an internal relation. An example is $^{49}\text{Mn}$, which is connected to $^{47}\text{Cr}$ through proton decay, thus building a loop when its internal transition is included.

#### 6.5 Proton and $\alpha$ decays

In some cases, proton-decay energies can be estimated from proton-decay half-lives. Estimates for the following nuclides can thus be obtained as:

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>$T_{1/2}$ (s)</th>
<th>$S_p$ (keV)</th>
<th>Adopted $S_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{64}\text{As}$</td>
<td>40±30 ns</td>
<td>$&gt; -100$</td>
<td>$-100# \pm 200#$</td>
</tr>
<tr>
<td>$^{68}\text{Br}$</td>
<td>&lt;1.5 µs</td>
<td>$&lt; -500$</td>
<td>$-500# \pm 250#$</td>
</tr>
<tr>
<td>$^{73}\text{Rb}$</td>
<td>&lt;30 ns</td>
<td>$&lt; -500$</td>
<td>$-500# \pm 200#$</td>
</tr>
<tr>
<td>$^{81}\text{Nb}$</td>
<td>&lt;44 ns</td>
<td>$&lt; -600$</td>
<td>$-700# \pm 500#$</td>
</tr>
</tbody>
</table>

These limits were used as a guide to obtain estimates for the masses of those nuclides.

These results are important for two main reasons. Firstly, knowledge of proton separation energies just beyond the proton drip line is quite valuable in estimating the mass values for nuclides for which no experimental data are available. Secondly, there are several cases where proton-decay energies from both members of an isomeric pair were measured, so one can determine the excitation energy of a particular isomer. In addition, the lifetime of a proton-emitting nuclide is sensitive to the orbital angular momentum value $l$ carried by the proton and this can be used in turn to obtain reliable information about the spins and parities of the parent and daughter states. This feature is even more valuable, when $\alpha$ decays of both members are observed. Combination of long $\alpha$-decay chains with proton decays offers a view of extended regions of the chart in the neighborhood of the proton drip-line. These studies showed that several decays that were earlier assigned to ground states actually belong to excited isomers. Also, these measurements are found to yield good values for the excitation energies of the isomers among the descendants. We usually followed the judgment of the authors, including their recommendations about the final levels fed in those $\alpha$ decays.

Often in $\alpha$-decay studies of odd-$N(Z)$ and odd-odd nuclides, the level fed directly by the $\alpha$ particle is not known. A comprehensive investigation that we per-
formed some time ago suggested that, in most cases, when the decay does not go directly to the ground state, the final level is relatively close to the ground state. In such cases, we adopted the policy of accepting the measured $E_\alpha$ as feeding the ground state, but assigning a special label to indicate that a close-lying excited level may also be fed. This label, which is not given in Table I, will indicate to our computer program that the uncertainty, after possible pre-averaging of data of the same kind (also given in Table I), is to be increased to 50 keV.

The existence of proton-decay branches, as mentioned above, provided sufficient arguments to omit the mentioned label in several cases. One has also to be careful with the use of this label if mass-spectrometric results with a precision of about 50 keV or better are known for the parent and daughter nuclides. Comparison with theoretical models may also suggest dropping the mentioned above label; or conversely to not accept a reported $\alpha$-decay energy.

In some cases, TMS estimates and theoretical predictions of $\alpha$-decay energies indicate that the excitation energy $E_1$ of the final level may be much higher. Then, an estimate for the excited level energy (provided with a generous error) is added as an input value.

In regions where the Nilsson model for deformed nuclides applies, it is expected that the most intense $\alpha$ transition connects parent and daughter levels that have the same quantum numbers and configurations. In such a case, adding an estimate for $E_1$ is attractive. Frequently, the energy difference between the excited and ground states can be estimated by comparisons with the energy differences between the corresponding Nilsson levels in nearby nuclides.

For nuclei with A > 190, as well as for proton-rich nuclei far from the line of stability, $\alpha$ decay is the main decay mode providing information about atomic masses. Most measurements involve position-sensitive silicon detectors, which require careful energy calibration. Such calibrations usually use the recommended $E_{\alpha}$ values evaluated by Rytz [1991Ry01]. The recent development in mass spectrometry allowed independent mass measurements in this region of the nuclear chart using Penning Traps. Such measurements have already been carried out for several No and Lr nuclides [2010Mi.A] and their results were already included in AlE2012.

### 6.5.1 Particle energy vs. decay energy

Unfortunately, some authors misuse the meaning of particle and decay energies. Energy values are referred to by some authors as the particle energy $E$, while others quote it as decay energy $Q$. Actually, the decay energy is the sum of kinetic energies of the emitted particle and the recoiling daughter nuclide. In general, the $\alpha$ particle carries about 97-98% of its $Q$ value and the recoiling nuclide accounts for about 2-3%. In the literature one can find too many cases of confusion, especially in proton-decay experiments where $Q_\alpha$ and $E_\alpha$ are numerically closer to each other. Sometimes, the confusion could be resolved through a meticulous inspection of the paper and a discussion with the authors. However, ambiguities still remain in many cases.

### 6.5.2 Recalibration of alpha- and proton-decay energies in implantation experiments

In experiments where the $\alpha$-emitting nuclei are implanted in a silicon detector, both the $\alpha$ particle and the recoiling daughter nuclide deposit energies in the detector. Often authors make the simple assumption that only the $\alpha$-particle energy is measured in the detector. While in similar cases of proton decays, it is often considered that both the proton and the heavy recoil are detected at the same time. Neither of these statements is correct: $\alpha$ particles and protons with energies of a few MeV have almost 100% detection efficiency, which is not the case for the heavy recoiling nuclides, where only part of the recoiling energy contributes to the signal.

This effect has been discussed in Ref. [2012Ho12], where approximately 28% of the recoil energy contributes to the signal. In that experiment, the recoil energy of the 11.65 MeV $\alpha$-particle line of $^{212}$Po$^m$, which was used for calibration, is 224 keV, whereas the recoil energy of a superheavy nucleus with mass number 292 is only 162 keV for the same $\alpha$ energy. Thus the difference of the recoil energies which contribute to the signals is 17 keV, which is larger than the 10 keV energy uncertainty. For this reason, the partial recoil energy of the daughter nuclide has been taken into account in the energy calibration [2012Ho12].

However, not all the experimentalists notice this effect and we need to make our own corrections of the published results. We have developed a procedure [49] to calculate the detection efficiency for heavy nuclides in Si detectors based on Lindhard’s integral theory [50], which has been experimentally proven to be reliable [51, 52].

The correction has been done for some of the experimental results included in the present tables. After discussions with the authors of the original publication, the $\alpha$-decay energy of $^{255}$Lr$^m$ Ref. [2008Ha31] has been corrected and the difference turns out to be 7(10) keV. The corrected value is used in the current evaluation with a remark given to the relevant data in Table I. Another example is from Ref. [2014De41], where the proton-decay of $^{69}$Br was measured by using $\beta$-delayed protons from $^{20}$Mg and $^{23}$Si for the energy calibration. The authors assumed (erroneously) that the recoil energy would be fully recorded at the same time. From our calculations the detection efficiency for the recoil nuclide ($^{68}$Se) is
about 30% and its neighboring nuclides show similar behavior. Applying the correction, the β-delayed proton-decay energy of $^{69}$Kr changed from 2939 keV to 2916 keV. The difference is 23 keV, comparable with the 22 keV uncertainty. The same correction procedure was also applied to the ground-state proton-decay energy of $^{69}$Br in the same work [2014De41], which changed its proton-decay energy from 641 keV to 631 keV, with uncertainty of 42 keV.

The correction should, in principle, be applied to all implantation α- and proton-decay experiments of some precision if the recoil effect was not taken into account. This work is not yet complete in the present version of the AME.

Some authors derive a value which they call $Q_\alpha$ from the measured α-particle energy by not only correcting for the recoil energy, but also for screening by atomic electrons (see Appendix A p. 030002-38). In our calculations, the latter corrections have been removed.

Finally, some measured α-particle energies are affected by the coincidence summing between the α particle that feeds an excited level of the daughter nuclide and the conversion electrons that follow the decay of this level. This is sometimes apparent from the reported α spectra, since the width of the observed line is larger than that of other ones. In some cases, spurious α peaks can be observed. When deriving the corresponding $Q_\alpha$ values, appropriate (small) corrections are made for the escaping X-rays. Those are mentioned in a remark added to such a case.

### 6.6 Decay energies from capture ratios and relative positron feedings

For allowed transitions, the ratio of electron capture in different shells is proportional to the ratio of the squares of the energies of the emitted neutrinos, with a proportionality constant being dependent on $Z$ [53]. For (non-unique) first forbidden transitions, the ratio is similar, but with a few exceptions. The neutrino energy is determined as the difference of the transition energy $Q$ and the electron binding energy in the pertinent shell. Especially if the transition energy is not too much larger than the binding energy in, say, the K shell, it can then be determined rather well from a measurement of the ratio of capture in the K and L shells.

The non-linear character of the relation between $Q$ and the capture ratio introduces two problems. In the first place, a symmetrical error for the ratio is generally transformed in an asymmetrical one for the transition energy. Since our least-squares fit program cannot handle them, we have symmetrized the probability distribution by considering the first and second moments of the real probability distribution (see NUBASE2016, Appendix A, p. 030001-16). The other problem is related to averaging of several values that are reported for the same ratio. Since AME1993, our policy is to average the capture ratios, and calculate the decay energy from that average. An example is $^{139}$Ce($\varepsilon$)$^{139}$La (see p. 030002-211), where 10 results were averaged and the individual values given in the associated remarks. In this procedure we used the best values [53] of the proportionality constant. We also recalculated the older decay energies using the new value for this constant.

The ratio of positron emission and electron capture in the transition to the same final level also depends on the transition energy. It is well known for allowed and not much delayed first forbidden transitions. Thus, the transition energy can be derived from the measured positron intensity to a given level, rather than from the positron spectrum end-point (e.g. $^{109}$Cd($\varepsilon$)$^{109}$Ag, p. 030002-170). In the case of positron decay, one must remember that it can only occur when the transition energy exceeds $2m_e c^2 = 1022$ keV. However, in many cases the level fed by positrons is also fed by γ-rays coming from higher levels that are fed by electron capture. Determination of the intensity of this side feeding is often difficult. Cases exist where such feeding occurs by a large number of weak γ-rays that can be easily overlooked (the pandemonium effect [54]). Then, the reported decay energy may be much lower than the real value. In judging the validity of experimental data, we kept this possibility under consideration.

Total Absorption Spectrometry (TAS) has been applied to overcome the pandemonium effect [54]. In some cases the ratio of positron emission and electron capture is measured using TAS, e.g. $^{108}$Sn [2005Ka34]. For this case we adopted the value reported by the authors.

### 6.7 $Q_\beta$ far from β-stability

Presently, the mass surface for nuclides far away from the valley of β-stability is observed to be located much higher than was previously believed. This is largely due to the underestimation of the $Q_\beta$ decay energies, which were measured in the past using the end-point energy method. See the discussion in AME2012, p. 1317.

The deduced higher values of atomic masses for exotic nuclides in the present work will have important consequences for nuclear astrophysics and nuclear energy applications, as discussed in Ref. [55].

To conclude, for nuclei very far from the valley of stability, $Q_\beta$ results from end-point measurements should be treated with caution. In such cases, data available from Penning traps and/or storage rings facilities should always be given priority.

### 6.8 Superheavy nuclides

The search for superheavy elements (SHE) and elucidation of their properties is one of the prominent areas
of modern nuclear physics research. In the last several years, the nuclear chart was extended impressively in the heaviest mass region up to the element with atomic number $Z = 118$. However, the mass surface built with the available data is still rough (see Part II, Fig. 9 and also Fig. 26, p. 030003-243 and 030003-260).

Names and symbols At the completion of AME2016, SHE up to $Z = 118$ were officially named by the Commission on Nomenclature of Inorganic Chemistry of the International Union of Pure and Applied Chemistry (IUPAC) [56]:

- 113 Nihonium (Nh),
- 115 Moscovium (Mc),
- 117 Tennessine (Ts), and
- 118 Oganesson (Og).

We were not able to include the new names in AME and NUBASE, but instead we used the provisional symbols Ed, Ef, Eh, and Ei for elements 113, 115, 117, and 118, respectively.

Experimental methods Since $\alpha$ decay is the dominant decay mode in the region of superheavy nuclides, knowledge of masses of SHE is most often obtained from the measured $\alpha$-decay energies within a chain that reaches a nuclide with known mass. Position and time-correlated $\alpha$-decay and Spontaneous Fission (SF) spectroscopy measurements of SHE continue to provide precious information about their properties. However, it often happens that $\alpha$ chains end up with a nuclide decaying only by spontaneous fission, offering no link to known masses. For example, the SF decay of $^{266}$Sg does not allow to determine the mass of the doubly magic nuclide $^{270}$Hs. In order to support the discovery of new elements, an indirect method can be applied, where different nuclear reactions are used to produce the daughter nuclide. This was the case in the discovery of the new elements $^{293}$Eh(Ts) and $^{299}$Ef(Mc), see Ref. [57] and references therein. However, the new analysis of all available data in Ref. [2016Fo16] provided evidence against the proposed cross-reaction link [57] between the $\alpha$-decay chains associated with those two nuclides. New studies would be needed to resolve the discrepancies.

A very important development in this mass region was the first direct mass measurements [2010Dw01] of several isotopes of No ($Z = 102$) and Lr ($Z = 103$) by the SHIPTRAP facility at GSI. Those results provided anchor points for atomic masses in this remote region of the nuclear chart. In general, the newly measured masses agree reasonably well with those deduced from known $Q_\alpha$ values of long $\alpha$ chains, thus giving confidence not only about the reliability of masses for SHE reported in [2010Dw01], but also the treatment and policies used in our work. In AME2016 we included new results from such direct mass measurements for the lighter $^{241,243}$Am, $^{244}$Pu and $^{245}$Cf nuclides [2014Ei01]. However, we have to mention here the disagreement in the $^{240}$Cf – $^{241}$Am mass difference between the Penning trap data and the value deduced using the decay $Q_\alpha$ values, as discussed in Section 7.10 (p. 030002-36).

Alpha decay of superheavy nuclides For even-even nuclides, the strongest (favored) decays connect the parent and daughter ground states. They are directly related to the $Q_\alpha$ values. As a result, masses determined this way are quite reliable. Unfortunately, some of the nuclides are prone to spontaneous fission decay, thus limiting the number of reliable cases.

For many odd-A nuclides, especially for odd-odd ones, the assignments are frequently complicated. In the region of deformed nuclides, $\alpha$ decays preferentially connect levels with the same $J^\pi$ and configurations, and as a consequence the daughter nuclei are often produced in excited states with unknown excitation energies $E_1$. Thus, in order to find the corresponding mass difference, we have to estimate these $E_1$ values. For somewhat lighter nuclides, one may estimate them from known differences in excitation energies for levels with the same Nilsson assignments in neighboring nuclides. But such information is lacking in the SHE region under consideration. Instead, one might consider using values obtained theoretically [58]. We have not done so. However, we have used such theoretical values as a guide, choosing values in such a way that diagrams of $\alpha$ energies and the mass surface looked smooth. Helpful for this purpose were the experimental $\alpha$-decay energies for $Z = 112$, 114 and 116, especially for the even-even nuclides among them. This is especially true near sub-shell closures, since the favored alpha decay occurs between states that have the same quantum numbers and configurations.

The presence of excited, long-lived isomers can also lead to severe complications. While many dedicated $\alpha$–$\gamma$ coincidence studies have been performed for nuclides in the light actinide region, such spectroscopy needs to be extended to the heavier nuclides. In the last several years new results were published in the $Z = 102 – 104$ region, which resolved some of the ambiguities. However, high quality data are still in demand and such studies would be very beneficial to future mass determination of SHE.

A weak $\alpha$-decay branch was observed in the decay of $^{262}$Sg [2010Ac.A], which allowed experimental determination of the mass of $^{262}$Ds, the heaviest nuclide that has an experimental mass value in AME2016. The new data allowed to establish unambiguously the existence of a significantly deformed sub-shell gap at $N = 162$ and $Z = 108$. This gap appears to be much larger than the
one at $N = 152$ and $Z = 100$.

Our policy in this high-$A$ region, where the $\alpha$-decay energies often spread too much, is to adopt the highest $\alpha$-decay group as gs-gs transition. The reason is that, even if this group is formed due to $\alpha$-electron summing, it is still the closest one to the real gs-gs $Q$ value.

An interesting case is the determination of the mass of $^{266}\text{Sg}$. This mass was considered as experimentally known in the Ame2003 mass table (and was then the heaviest nuclide with known mass), derived from the highest $\alpha$-decay group $E_\alpha = 8940 \pm 30$ keV of [1998Tu01] and adopted as gs-gs transition. With more events [2012Ha05], the status of $^{265}\text{Sg}$ has been changed and the former $\alpha$-decay group assigned to the neighboring isotope $^{266}\text{Sg}$ was reassigned to the $^{265}\text{Sg}^{\text{m}}$ state. In the present evaluation we use the strongest group, which may be the unhindered transition, assuming this transition goes to one excited state in the daughter nuclide $^{261}\text{Rf}$ with unknown energy. This energy is estimated from the trends in the neighboring nuclides (TNN). So, the mass of $^{265}\text{Sg}$ is now estimated rather than experimentally as in Ame2003, although the mass value doesn’t change much.

With exception of the nuclide $^{277}\text{Ed}(\text{Nh})$, nuclides with atomic number from 113 to 118 are produced by the “hot fusion” method, decaying by $\alpha$ emission to fissionable nuclides whose masses are unknown experimentally, thus forming a floating island with none of the nuclides having known mass.

7 Special cases

Special cases have been discussed in the Ame series to highlight the issues raised in the evaluation and to call for more efforts to solve them. Some of the special cases discussed in Ame2012 have been solved so we removed them from the current list. Meanwhile some new cases have been added.

7.1 $^3\text{H}^{–3}\text{He}$ atomic mass difference

The $\beta$-decay energy of $^3\text{H}(\beta^-)^3\text{He}$, which can be deduced from the difference between the $^3\text{H}$ and $^3\text{He}$ atomic masses, is very important for neutrino-mass experiments that analyze the shape of the tritium $\beta$-decay spectrum near its end-point energy. Because of the significance in the determination of the neutrino mass, the $Q_\beta$ of $^3\text{H}$ has been measured by many groups using different methods. About thirty years ago, one of us (G.A.) and colleagues evaluated all of the significant experimental results available at that time on the $^3\text{H}–^3\text{He}$ mass difference [1985Au07]. In that evaluation, the methods fell into three categories: mass doublet measurements, tritium $\beta$-decay measurements in magnetic spectrometers and in implanted detectors. It was found that the data within each group are consistent with each other, but there were notable discrepancies among the groups.

In the last three decades, Penning trap mass spectrometers have been developed intensively and now dominate mass measurements with the highest precision. Before Ame2012, the $\beta$-decay measurements always played the most important role in determining the $Q_\beta$ of $^3\text{H}$. In Ame2012, the Penning trap results contributed almost as much as the $\beta$-decay measurements in this case, thanks to the high-precision results from the SMILETRAP group [2006Na49]. These results were in strong conflict with earlier results from the UW (University of Washington) Penning trap (Seattle group) [1993Va04]. The latter reported that the masses of $^3\text{He}$ and $^3\text{H}$ were determined with uncertainties of 1 nu and 1.5 nu, respectively. Thus the $Q_\beta$ of $^3\text{H}$ was deduced with a precision of 1.7 eV by this method. The results from [1993Va04] were used in the Ame1993 with the originally published values. Later, some serious systematic errors in this measurements were discovered. After discussion with the authors, the result for $^3\text{H}$ was temporarily discarded. The value for $^3\text{He}$ was corrected by 3 nu, i.e. 3 sigma away from the original value, and used in Ame2003 and Ame2012. The results from [2006Na49] supports the correction.

Recently, the $^3\text{H}$ and $^3\text{He}$ atomic masses were measured by the Florida State University (FSU) group with precisions of 0.19 nu, as reported in [2015My03]. Because the identical procedures and the same reference ion were used in the mass measurements for these two nuclides, it was concluded that all of the important systematic uncertainties should be cancel. The resulting uncertainty of 0.07 eV is thus much smaller than that for the individual masses.

However, the Seattle group analyzed the results collected in earlier experiments and published the $^3\text{He}$ mass with an uncertainty of 0.043 nu [2015Za13]. This result still disagrees by 3.3 times the sum of their final uncertainty with the FSU result [2015My03]. In the Seattle experiment, carbon ions were used as reference, whose mass is quite different from the measured nuclide. Thus, their result might be vulnerable to undiscovered systematic errors so is provisionally not used in the present evaluation. In the FSU measurement, the HD$^+$ ion was used as the reference, which has similar mass with the measured nuclide. The $^3\text{H}–^3\text{He}$ mass difference is usually more robust than the absolute mass values, since both nuclides are exposed to the same experimental conditions. This robustness was proven in the work [1993Va04], where although the absolute mass value for $^3\text{He}$ has been corrected by 3 nu, the mass difference in the original value agrees with the adopted values in series of Ame evaluations.

In Ame2016, the results from [2015My03] are used...
to determine the masses of $^5$H and $^3$He. Due to the high precision, all of the other results lost their significance. The recommended values for the $Q_β$ decay energy of $^3$H from Ame1983 to Ame2016 are:

<table>
<thead>
<tr>
<th>AME evaluation</th>
<th>$Q_β$ (eV)</th>
<th>Uncertainty (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ame1983</td>
<td>18594</td>
<td>8</td>
</tr>
<tr>
<td>Ame1993</td>
<td>18591</td>
<td>1</td>
</tr>
<tr>
<td>Ame2003</td>
<td>18591.3</td>
<td>1.1</td>
</tr>
<tr>
<td>Ame2012</td>
<td>18590.6</td>
<td>0.8</td>
</tr>
<tr>
<td>Ame2016</td>
<td>18592.01</td>
<td>0.07</td>
</tr>
</tbody>
</table>

It should be noted that in Ame1983, the definition of the maintained Volt differed from later evaluations, as explained in Section 2. But its impact on the $Q$-value is just 0.15 eV, much smaller than the quoted uncertainty. Because of its importance, the precise determination of the $^3$H–$^5$He mass difference will continue to attract interest. The former Seattle trap is now operational at the Max-Planck Institute in Heidelberg and will be dedicated to such measurements in the future [2016Ho.A].

7.2 $^9$He and $^{10}$He

The knockout reaction on $^{11}$Be has been used to produce $^9$He [2001Ch31] and its lowest state has been assigned $l = 0$. An upper limit of the s-wave scattering length $a_s = −10 \text{ fm}$ has been obtained, corresponding to an energy for the virtual state below 0.2 MeV. In [2007Go24], the spectrum of $^9$He was studied by means of the $^2$H($^3$He,p)$^3$He reaction. The lowest resonant state of $^9$He was found at $2.9 ± 0.2 \text{ MeV}$ with a width of 2 MeV and has been identified as a 1/2$^−$ state. For the virtual 1/2$^+$ state, a lower limit $a_s > −20 \text{ fm}$ has been obtained, which is consistent with the result in [2001Ch31]. This assignment has been questioned in [2010Jo06], where $^9$He was studied by using knockout reaction from $^{11}$Li. The $^8$He+n relative-energy spectrum is dominated by a strong peak-like structure at low energy, which may be interpreted within the effective-range approximation as the result of an s-wave interaction with a neutron scattering length $a_s = −3.17 ± 0.66 \text{ fm}$, thus conflicting with [2001Ch31]. It is argued that the s-state may not be the g.s. of $^9$He.

This argument is supported by the structure of $^{10}$He, which should be similar to the structure of $^9$He. If a virtual state in $^9$He[2001Ch31] really existed, a narrow near-threshold 0$^+$ state in $^{10}$He with a [s1/2]$^2$ structure would exist in addition to the [p1/2]$^2$ state [59, 60], in contradiction to the available experimental data on $^{10}$He.

Based on these experimental results, we adopt the 1/2$^−$ as the ground state of $^9$He. In earlier work [1987Se05], [1988Bo20], and [1991Bo.B], transfer reactions were used, yielding values of $E_\gamma$ (resonance energy) of this state around 1.1 MeV. More recently, [1999Bo26] and [2010Jo06] determined $E_\gamma$ $≈$ 1.3 MeV. In [2007Go24], the 1/2$^−$ state of $^9$He was found at $E_\gamma = 2.0 ± 0.2 \text{ MeV}$ with a width $≈ 2 \text{ MeV}$ in this work, significantly higher than in the other reports. The energy resolution in this experiment was 0.8 MeV (FWHM), which is quite large compared to the energy difference of $≈ 1.1 \text{ MeV}$ between the 1/2$^−$ and 3/2$^−$ states [1988Bo20], [1999Bo26], [2010Jo06]. Therefore, we suspect this state to be a mixture due to the poor energy resolution in this experiment.

The case related to $^{10}$He was discussed in Ame2012. At that time four experimental results were known concerning the mass of $^{10}$He, and two new results were published since. The six experimental results are:

<table>
<thead>
<tr>
<th>Reference</th>
<th>$Q_α$ (in keV)</th>
<th>Method of production</th>
</tr>
</thead>
<tbody>
<tr>
<td>1994Os04</td>
<td>1070 $±$ 70</td>
<td>$^{10}$Be($^{14}$C,$^{14}$O)$^{10}$He</td>
</tr>
<tr>
<td>1994Ko16</td>
<td>1200 $±$ 300</td>
<td>C($^{14}$Li,$^{14}$He)</td>
</tr>
<tr>
<td>2010Jo06</td>
<td>1420 $±$ 100</td>
<td>$^4$H($^{11}$Li,$^{10}$He)</td>
</tr>
<tr>
<td>2012Si07</td>
<td>2100 $±$ 200</td>
<td>$^3$H($^5$He,p)$^{10}$He</td>
</tr>
<tr>
<td>2012Ko43</td>
<td>1600 $±$ 250</td>
<td>C($^{14}$Be,$^{10}$He)</td>
</tr>
<tr>
<td>2015Ma54</td>
<td>1400 $±$ 300</td>
<td>$^{11}$Li($^3$He,$^3$He)$^{10}$He</td>
</tr>
</tbody>
</table>

The mass of $^{10}$He from [1994Os04] is significantly lower than the others, with poor statistic compared to the high background. The values obtained in previous invariant-mass measurements [1994Ko16, 2010Jo06] agree with each other, both using $^{11}$Li to produce $^{10}$He. In [2012Si07] the value is higher than the others, while the authors stated that “the results reported in Refs. [1994Ko16] and [2010Jo06] do not contradict the g.s. energy of $^{10}$He obtained in the present work”, based on the calculations of Ref. [60]. They argued that due to the large initial state effect, the observable g.s. peak position in [1994Ko16] and [2010Jo06] is shifted towards lower energy because of the abnormal size of $^{11}$Li, which exhibits one of the most extended known neutron halos. Based on the $^9$He spectrum from [2007Go24], the $^{10}$He g.s. with structure [p1/2]$^2$ is predicted to have a 2.0–2.3 MeV two-neutron separation energy. However, the result of $^9$He from [2007Go24] is not adopted, as discussed earlier. The model has problems in interpreting all of the experimental data, indicating the states may have a more complex structure. In the Ame2012 evaluation, we adopted the result from [2010Jo06] provisionally and called for more experiments to clarify this case.

Two experimental results were published after Ame2012. In [2012Ko43], a group from Msu has studied $^{10}$He using the fragmentation of $^{14}$Be. In [2015Ma54], the missing mass spectrum of $^{10}$He was measured at RIKEN using the $^{11}$Li($^3$He,$^3$He) reaction at 50.4 MeV. Their results support the choice in Ame2012. The discrepancy with
the result in [2012Si07] could not be explained simply by the exotic structure of $^{11}\text{Li}$, which was the argument used in [2012Si07], since in the later experiments different reaction channels are explored.

The discrepancy among the results for the mass of $^{10}\text{He}$ has attracted wide attention. To reconcile this case it has been proposed recently that all the experiments were measuring two overlapping $0^+$ states that were populated with different ratios in different experiments. Thus the lowest state reported up to now was adopted as the ground state in [61]. However, there are too many assumptions in this argument. Four experimental results published up to now are consistent with each other. We use the two most precise ones among them ([2010Jo06] and [2012Ko43]) to determine the mass of $^{10}\text{He}$. Meanwhile, we call for more experiments to further clarify this case.

7.3 The mass of $^{32}\text{Si}$

In AME2012, we discussed in details the difficulties we met in the determination of the mass of $^{32}\text{Si}$. We then decided not to use the $(n,\gamma)$ data. No new experimental result relevant to this case appeared since then. In the PTB (Physikalisch-Technische Bundesanstalt) experiment [2001Pa52], the nuclide $^{32}\text{Si}$ is produced by neutron capture on $^{31}\text{Si}$, which is radioactive and it is also produced in neutron capture reaction. It seems reasonable to question whether the measurement of the $\gamma$ rays from $^{32}\text{Si}$ could involve a substantial background. In the present evaluation, we keep using the Penning trap values, as we did in AME2012.

7.4 The $Q$-value for $^{99}\text{Rh}(\beta^+)^{99}\text{Ru}$

The $Q$-value for $^{99}\text{Rh}(\beta^+)^{99}\text{Ru}$ was adjusted to be 2043(7) and 2044(7) keV in AME2003 and AME2012, respectively. In both evaluations, $Q_{\beta^+}$ was mainly determined from the two $\beta$-decay results in Ref. [1952Sc11] and [1959To25]. A higher $Q$-value of 2170(30) keV was reported in the later work [1974An23], but was not used in AME due to its large uncertainty. However, it was found that the $Q$-value should be larger than 2059.34 keV because this state was populated in beta-decay experiments. In [1959To25], the authors reported that the highest end-point energy of the $\beta^+$ spectrum was 1030 keV and no $\gamma$ ray was observed in coincidence. While [1974An23] reported that the highest energy component of the $\beta^+$ spectrum was largely connected with the transition to the 89.76 keV level, and the authors suggested that in [1959To25] the $\beta^+$ spectrum should also be associated with that $\gamma$ transition. If we accept this explanation, then the deduced $Q_{\beta^+}$ would be in strong conflict with the result from [1952Sc11], where the $\beta^+$ spectrum was measured from the excited isomer, whose excitation energy has been well established from the $\gamma$-ray spectroscopy.

Both $^{99}\text{Rh}$ and $^{99}\text{Ru}$ are primary nuclides (cf. Section 5.3) in our evaluation. The mass of $^{99}\text{Ru}$ is mainly determined by $(n,\gamma)$ reaction to $^{100}\text{Ru}$, which in turn is determined from Penning trap measurement. The uncertainty of the adjusted $^{99}\text{Rh}$ mass is 6.7 keV. The mass of $^{99}\text{Rh}$ can also be determined through the $Q_{\beta^+}$ value of $^{99}\text{Pd}$, which in turn is measured with a Penning trap with an uncertainty of 5.4 keV. Consequently, even if we don’t use any of the experimental results from the beta-spectrum measurements of $^{99}\text{Rh}$, we can still determine the $Q$-value of $^{99}\text{Rh}(\beta^+)^{99}\text{Ru}$ to be 2032(21) keV. If we increase the $Q$-value of $^{99}\text{Rh}(\beta^+)^{99}\text{Ru}$, then strong tension will be built around this region.

Confronting all of the difficulties, in this evaluation we follow the same treatment used in AME2012. Meanwhile, direct mass measurements of $^{99}\text{Rh}$ with high accuracy are needed, in order to solve this issue.

7.5 The mass of $^{100}\text{Sn}$

The determination of the mass of $^{100}\text{Sn}$ was the subject of a detailed discussion in AME2003 and again in AME2012. This result is particularly interesting due to the doubly magic character of $^{100}\text{Sn}$ which is, moreover, the heaviest known nuclide with $N = Z$. No new results have been reported since then for $^{100}\text{Sn}$. We therefore still recommend using the $Q_{\beta^+}$ value from Gsi [2012Hi07], which is also the most precise, for the determination of its mass, and are in demand of more experimental results.

7.6 The $^{102}\text{Pd}$ double-electron capture energy

In the AME2012 evaluation, we described the discrepancies we found between data coming from combinations of the very precise $(n,\gamma)$ reactions with $\beta^+$, $\beta^-$ and $\varepsilon$ decay energies versus direct Penning trap data [2011Go23]. Having found no reason to distrust any of the measurements involved then, and having on one side one result obtained with a very reliable method, on the other side derived from a combination of several quite trustworthy measurements, we finally decided at that time to provisionally not use the new Penning trap result and called for more measurements in order to clarify this issue.

Recently, we were aware of the experimental results for $^{102}\text{Pd}$ and $^{103}\text{Pd}$ from the Esr mass measurements through a private communication [2014Ya.A]. Their results support the SHIPTRAP datum, although with relatively large uncertainties. We therefore decided to discard two pieces of data: $^{102}\text{Rh}(\beta^-)^{102}\text{Pd}$ and $^{103}\text{Pd}(\varepsilon)^{103}\text{Rh}$, and to use the SHIPTRAP result. The local consistency is then restored.
7.7 The mass of $^{105}$Sb

The matter of the determination of the mass of $^{105}$Sb was discussed at length in Ame2012. No new data were published since then. Therefore, the $Q_{\alpha}$ measurement in [2007Ma35] is again provisionally adopted in the present evaluation, and determines the mass of $^{105}$Sb. We still appeal for direct proton-decay studies of $^{105}$Sb in order to clarify this case.

7.8 The $^{163}$Ta($\alpha$) $^{159}$Lu($\alpha$) $^{155}$Tm decay chain

This $\alpha$-decay chain was discussed in the previous Ame2003 and Ame2012 publications.

To summarize, by combining all available information, and by discarding only one piece of data, we were able to build up a scenario for the double (ground states and excited isomers) $^{147}$Tb–$^{179}$Tl decay chain. However, most of the adopted values for excitation energies, and also for the $^{167}$Re ground state are still labeled with the ‘#’ flag, due to the estimated excitation energy of $^{179}$Tl$^\text{m}$. Experimental determination of any of the excitation energy in $^{159}$Lu, $^{163}$Ta, $^{167}$Re, $^{171}$Ir, $^{175}$Au, or $^{179}$Tl will allow to access all other ones. Future measurements would be beneficial not only in order to firmly establish these excitation energies, but even more importantly, to provide also useful parent-daughter correlations on $\alpha$ decays that feed the $^{159}$Lu ground state and decays out of the excited isomer.

7.9 The $^{170}$Au($\alpha$) and $^{169}$Pt($\alpha$) decay chains

It has been previously mentioned that some proton-rich nuclides can decay by both $\alpha$ and proton emission. In some cases, a loop of interconnected nuclides can be formed. Two long $\alpha$-decay chains illustrate this case:

$^{170}$Au $\to$ $^{166}$Ir $\to$ $^{162}$Re $\to$ $^{154}$Ta $\to$ $^{154}$Lu and
$^{169}$Pt $\to$ $^{165}$Os $\to$ $^{161}$W $\to$ $^{157}$Hf $\to$ $^{153}$Yb.

These two chains are connected by $^{170}$Au($p$)$^{169}$Pt and $^{166}$Ir($p$)$^{165}$Os, thus forming a loop as shown in Fig. 4.

However, all the masses shown in Fig. 4 are unknown. If the mass of at least one nuclide is measured in the future, then all of the masses along the above two decay chains will be determined. The specific difficulty here, is that if all of the experimental information is used in the evaluation, then a closed loop would be formed, and all nuclides involved would become primaries. The consequence is that two estimated (non-experimental) data would then automatically become primary data (the ones with the “#” flag in Fig. 5).

To avoid this undesirable side-effect, the $^{170}$Au($\alpha$)$^{166}$Ir value is not used in the mass adjustment, despite its good precision. A local evaluation is carried out in this region, involving all the corresponding nuclides, using least-squares method. The input and adjusted values are listed in Table E, as well as the adjusted values listed in Table I.
7.10 A mass difference between $^{249}\text{Cf}$ and $^{241}\text{Am}$

Recent results from TRIGA-TRAP for $^{241}\text{Am}$, $^{243}\text{Am}$, $^{244}\text{Pu}$ and $^{249}\text{Cf}$ [2014Ei01] yield a mass difference between $^{249}\text{Cf}$ and $^{241}\text{Am}$: $\Delta_T=M(^{249}\text{Cf})-M(^{241}\text{Am})=16781.2(2.2)$ keV. This difference can also be independently obtained from combining the $Q_\alpha$ values of $^{249}\text{Cf}$ and $^{241}\text{Cm}$, with the $Q_\beta$ value of $^{241}\text{Am}$: $\Delta_Q=Q_\alpha(^{249}\text{Cf})+Q_\alpha(^{241}\text{Cm})+Q_\beta(^{241}\text{Pu})+2\times M(^4\text{He})$, where $M(^4\text{He})$ is the mass of $^4\text{He}$ atom. Using the recommended $Q_\alpha$ values in AME2012, one obtains $\Delta_{2012}=16789.7(1.2)$ keV, which is $8.5(2.5)$ keV larger (more than $3\sigma$) than the value deduced from the TRIGA-TRAP data [2014Ei01] alone. It should be pointed out that the $Q_\alpha(^{249}\text{Cf})$ and $Q_\alpha(^{241}\text{Cm})$ values in AME2012 were heavily weighed by the results of Baranov et al. [1971Bb10], [1975Ba65]. Both $^{249}\text{Cf}$ and $^{241}\text{Cm}$ are odd-mass nuclei and their $\alpha$ spectra are complex, involving a number of strong $\alpha$ lines to excited states in the daughter $^{245}\text{Cm}$ and $^{244}\text{Pu}$ nuclei. We note also a number of inconsistencies in the $\alpha$-decay energies reported in Refs. [1971Bb10] and [1975Ba65]. For example, in the case of the $^{245}\text{Cm}$ $\alpha$ decay we obtain $Q_\alpha(^{245}\text{Cm})=5621.2(0.5)$ keV from the ground-state to ground-state $\alpha$-decay energy $E_\alpha=5529.2(0.5)$ keV [1975Ba65], while from the favored $\alpha$-decay energy of $E_\alpha=5362.0(1.2)$ keV [1975Ba65] to the excited 175.04 keV level, one gets $Q_\alpha(^{245}\text{Cm})=5626.2(1.2)$ keV, differing by as much as 5.0 keV.

Recently, precise $\alpha$-decay energy measurements were carried out at ANL for $^{249}\text{Cf}$ [2015Ah03] and $^{245}\text{Cm}$ [2016Ko.A] using mass-separated sources that were calibrated using the absolute measured $E_\alpha$ values of $^{244}\text{Cm}$, $^{246}\text{Cm}$ and $^{250}\text{Cf}$, as recommended by Rytz [1991Ry01]. As a result, the AME2016 adjusted $Q_\alpha(^{249}\text{Cf})=6293.3(0.5)$ keV and $Q_\alpha(^{245}\text{Cm})=5624.5(0.5)$ keV yield $\Delta_{2016}=16788.4(0.7)$ keV, which is still $7.2(2.3)$ keV larger than the mass-difference from the TRIGA-TRAP data [2014Ei01]. Nonetheless, all of the relevant data are used in the mass adjustment in AME2016, while strong tensions have been built in this region, especially for $^{249}\text{Cf}$. Future precise mass measurements in this region are necessary in order to understand the discrepancy observed between Penning Trap and $\alpha$-decay spectroscopy data.

7.11 Comparison with the $Q_{\text{EC}}$ evaluation of J.C. Hardy and I.S. Towner

Studies of $0^+ \rightarrow 0^+$ super-allowed $\beta$-decay transitions between isospin analog states can be used to test the validity of the conserved vector current hypothesis that postulates the existence of a universal $F_t$ value for all such decays. This universal value can be used to determine the $V_{ud}$ element of the Cabibbo-Kobayashi-Maskawa (CKM) matrix, which can in turn be used to test its unitarity.

![Figure 5. $Q_{\text{EC}}$ difference between the two evaluations. The error bars represent the uncertainties from Ref. [62], while the shaded areas display the uncertainties from AME2016.](image-url)
The evaluation of super-allowed $\beta$-decay properties, such as their transition energies, $Q_{EC}$, and half-lives, $T_{1/2}$, has been carried out since a long time by Hardy and Towner and regularly updated. Recently, experimental data for 20 super-allowed $\beta$-decay transitions have been evaluated and published [62]. Their evaluation is independent of AME. Although they aim at different goals and use slightly different criteria of evaluation, both are deemed valid and reliable, as can be seen from the comparison of their results for $Q_{EC}$ and for half-lives.

In the first paper of this volume, we presented a comparison (cf. 41-030001-8) between the $T_{1/2}$ values recommended in NUBASE2016 and those given by Hardy and Towner [62]. Below, we report on such a comparison for the $Q_{EC}$ values.

The $Q_{EC}$ values for all ground-state to ground-state transitions are listed in the atomic mass table (Part II, Table I, p. 030003-6 of this issue). The values for transitions involving excited isomeric states are not included in that table, but they can be easily determined with the information provided in NUBASE2016 and AME2016. When calculating the $Q_{EC}$ values from the AME mass tables, the covariances of the mother-daughter mass values must be considered, in order to obtain the correct uncertainties. The importance of the correlation is proven by the examples of the $Q_{EC}$ values of $^{42}$Ti and $^{26}$Al, where the uncertainties of their $Q_{EC}$ are smaller than the individual masses. Figure 5 shows the differences between the $Q_{EC}$ values determined in AME2016 and Ref. [62] for 19 super-allowed $\beta$-decay transitions (the one that is missing in the figure is $^{70}$Br, and it will be discussed below). Most of the $Q_{EC}$ data are consistent and the absolute differences are in most cases below 0.1 keV. In general, the observed differences can be attributed to two main sources, namely the selection of different input data and the implementation of distinct evaluation policies in AME2016 and in Ref. [62].

As mentioned in Section 5.4.4 (Insignificant data, p. 030002-22), data with weights that are a factor of 10 smaller than the other results will not be used in AME and these are labeled with the letter ‘U’ in the AME2016 evaluation. There is no such a threshold defined in the Hardy and Towner’s evaluation [62] and, as a consequence, all experimental data are used, unless rejected for other reasons. For example, the discrepancy for $^{19}$Ne is due to the different masses used in the two evaluations for the daughter $^{19}$F nuclide. There are five experimental results concerning this mass, as reported in [1964Bo13, 1964Ho28, 1967Pr04, 1973Se03] and [1975Ro05], with uncertainties of 0.73, 2.2, 2.8, 3.0 and 0.60 keV, respectively. All of them were used in the Hardy and Towner’s evaluation, while only the two most precise ones were used in AME2016.

The policies for data averaging used in the two evaluations are similar to the one employed by the Particle Data Group [37], where a parameter $\chi_n$ is used to check for the consistency of data. If $\chi_n$ is larger than a threshold value of $\chi_n^0$, all uncertainties in this data set will be multiplied with a scale factor, assuming that all experimental errors were underestimated by the same factor. In AME, $\chi_n^0$ is set to be 2.5, as explained in Section 5.4.1 (Pre-averaging, p. 030002-20) while a value of $\chi_n^0 = 1$ has been adopted by Hardy and Towner [62].

The masses of the long-lived isomer $^{70}_{\text{Br}}$ and its $\beta$-decay daughter $^{70}_{\text{Se}}$ were measured using Penning-trap spectrometry [2009Sa12]. By adopting the evaluated excitation energy from ENDF, the $Q_{EC}$ value of $^{70}_{\text{Br}}$ can be determined. However, this value was found to deviate significantly from the systematic behavior of the $Q_{EC}$ values in the region and it was rejected in Ref. [62]. Furthermore, Hardy and Towner concluded that “It is likely in this case that the trap actually measured an isomeric state in $^{70}_{\text{Br}}$ rather its ground state.” In AME2016, the result of Ref. [2009Sa12] was used following the interpretation in the original paper as in AME2012. Additional experimental data are needed to shed more light on this case.

Differences in the selection of the input data also contribute to the observed deviations between the $Q_{EC}$ values recommended in the AME2016 and the Hardy and Towner [62] evaluations. For example, some of the experimental results that were used in AME2016 were published after the work of Ref. [62] was completed and therefore they were not included in the latter. One example is the recent result for $^{14}$O from Ref. [2015Va08]. Another one is the case of $^{30}$S, where the level energy of the daughter nuclide that was used in Ref. [62] is outdated, while we implemented an updated value from ENDF that is listed in the NUBASE2016 table (p. 030001-27 of this issue).

In AME, all experimental information related to atomic masses are collected. Fig. 6 displays connections related to the $^{42}_{\text{Ti}} \rightarrow ^{42}_{\text{Sc}}$ and $^{42}_{\text{Sc}} \rightarrow ^{42}_{\text{Ca}}$ super-allowed transitions. In Ref. [62], only results from Penning-trap mass measurements [2009Ku19] were considered and, as a consequence, the excitation energy of $^{42}_{\text{Sc}}$ was determined as 617.12±0.39 keV. In AME2016, we have used the more precise value of 616.28±0.06 keV that was obtained from $\gamma$-ray spectroscopy measurements [1989Ki11] and recommended in the latest ENDF evaluation. Thus, the adoption of different internal transition energies for $^{42}_{\text{Sc}}$ can explain the variance in the $Q_{EC}$ values of the $^{42}_{\text{Ti}} \rightarrow ^{42}_{\text{Sc}}$ and $^{42}_{\text{Sc}} \rightarrow ^{42}_{\text{Ca}}$ super-allowed $\beta$ decay transitions in the two evaluations. The same situation occurs in the $^{26}_{\text{Si}} \rightarrow ^{26}_{\text{Al}}^0 - ^{26}_{\text{Al}} - ^{26}_{\text{Mg}}$ connections.

Another peculiar case involves the $^{74}_{\text{Rb}}$ nuclide. In AME2016, one input datum is the $Q_{EC}$ value of $^{75}_{\text{Rb}}$
from [2003Pi08]. However, only the intensities of the decay branches were directly measured in this work. The \( Q_{EC} \) value was deduced from the measured half-life, branching ratios and the average \( \mathcal{F}t \) value obtained from the analysis of other super-allowed transitions. Therefore, the recommended \( Q_{EC} \) value is based on the assumption that \( \mathcal{F}t \) is universal and constant for all super-allowed \( \beta \) decays. This result was used in AME since AME2003 and the original values reported in Ref. [2003Pi08] would be recalculated when new experimental results for the input data were available. We believe, however, that while the deduced \( Q_{EC} \) value in this way is valuable for mass determination, it should not be considered in Ref. [62], where the primary aim is to recommend a single \( \mathcal{F}t \) value.

![Figure 6. Schematic diagram of connections involving two super-allowed transitions \( 42^{\text{Ti}} \rightarrow 42^{\text{Sc}} \) and \( 42^{\text{Sc}} \rightarrow 42^{\text{Ca}} \). The double-headed arrows represent connections from Penning-Trap mass measurements while the single-headed arrow for the \( \gamma \) transition measurement.](image)

8 General information and acknowledgments

The full content of the present issue is accessible on-line at the AMDC website [22]. In addition, several graphs representing the mass surface, beyond the main ones given in Part II, are available on the AMDC website.

Tables of masses (Part II, Table I) and nuclear reaction and separation energies (Part II, Table III) are available in ASCII format to simplify their input to computer programs by the end users. The headers of these files give information on the formats. The first file, named mass.mas16, contains the table of masses. The next two files correspond to the table of reaction and separation energies, in two parts of 6 entries each, as in Part II, Table III: rct1.mas16 for \( S_{2n}, S_{2p}, Q_{\alpha}, Q_{2\beta}, Q_{\gamma p} \) and \( Q_{\beta n} \) (odd pages in this issue); and rct2.mas16 for \( S_{n}, S_{p}, Q_{2\beta}, Q_{d,\alpha}, Q_{p,\alpha} \) and \( Q_{\beta n,\alpha} \) (facing even pages). As explained in Section 4.2, p. 030002-15, since AME1995, we no longer produce special tables.

We wish to thank our many colleagues who provided answers to our questions regarding specific experimental data, as well as those who sent us preprints of their work prior to publication. Continuing interest, discussions, suggestions and encouragements from D. Lunney, A. Lopez-Martens, Yuhu Zhang and Furong Xu are highly appreciated.

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Appendix A The meaning of decay energies

Conventionally, the \( \alpha \)-decay energy, \( Q_\alpha \), is defined as the difference in the atomic masses of the mother and daughter nuclides:

\[
Q_\alpha = M_{\text{mother}} - M_{\text{daughter}} - M_{4^{\text{He}}}. \tag{10}
\]

This value equals the sum of the observed energy of the \( \alpha \) particle and that of the recoiling nuclide (with only a minor correction for the fact that the cortege of atomic electrons in the latter may be in an excited state). Unfortunately, some authors in the literature quote \( Q_\alpha \) as a value ‘corrected for screening’, which essentially means that they take for the values \( M \) in the above equation the masses of bare nuclides.

A similar bad habit has been observed for some published proton-decay energies. We very strongly object to this custom; at the very least, the symbol \( Q \) should not be used for the difference in nuclear masses.

**High precision \( \alpha \)-decay energies**

The most precise \( \alpha \)-decay energies are those measured absolutely using magnetic spectrographs, as summarized in Ref. [1991Ry01] and references therein. All \( \alpha \)-energy standards are determined using this method. The relation between the \( \alpha \)-particle energy \( E_\alpha \) and the decay energy, \( Q_\alpha \), is:

\[
Q_\alpha = (M - m_\alpha) - \sqrt{(M - m_\alpha)^2 - 2 \times M \times E_\alpha} + 78.6 \text{ eV}. \tag{11}
\]

where \( M \) is the mass of the parent nuclide, \( m_\alpha \) is the mass of the doubly ionized \( \alpha \) particle and 78.6 eV is the bind-
ing energy energy of two electrons in helium. This formula had been discussed in AME1977 and has been used since then. Unfortunately, the electron binding energy of helium was not taken into account up to now in AME, which caused a significant deviation for the most precise $\alpha$-energy values that have uncertainty of tens of eV. This error is corrected in the present mass table.

Appendix B Mixtures of isomers or of isobars in mass spectrometry

In cases where two or more unresolved lines may combine into a single one in an observed spectrum, while one cannot decide which ones are present and in which proportion, a special procedure has to be used.

The first goal is to determine what is the most probable value $M_{\text{exp}}$ that will be observed in the measurement, and what is the uncertainty $\sigma$ of this prediction. We assume that all the lines may contribute and that all contributions have equal probabilities. The measured mass reflects the mixing. We call $M_0$ the mass of the lowest line, and $M_1, M_2, M_3, \ldots$ the masses of the other lines. For a given composition of the mixture, the resulting mass $m$ is given by

$$m = (1 - \sum_{i=1}^{n} x_i) M_0 + \sum_{i=1}^{n} x_i M_i,$$

with

$$0 \leq x_i \leq 1, \quad \sum_{i=1}^{n} x_i \leq 1$$

in which the relative unknown contributions $x_1, x_2, x_3, \ldots$ have each a uniform distribution of probability within the allowed range.

If $P(m)$ is the normalized probability of measuring the value $m$, then:

$$\overline{M} = \int P(m) m \, dm$$

and

$$\sigma^2 = \int P(m) (m - \overline{M})^2 \, dm.$$

It is thus assumed that the experimentally measured mass will be $M_{\text{exp}} = \overline{M}$, and that $\sigma$, which reflects the uncertainty on the composition of the mixture, will have to be quadratically added to the experimental uncertainties.

The difficult point is to derive the function $P(m)$.

B.1 Case of 2 spectral lines

In the case of two lines, one simply gets

$$m = (1 - x_1) M_0 + x_1 M_1 \quad \text{with} \quad 0 \leq x_1 \leq 1.$$  \hspace{1cm} (15)

The relation between $m$ and $x_1$ is biunivocal so that

$$P(m) = \begin{cases} 
\frac{1}{M_1-M_0} & \text{if } M_0 \leq m \leq M_1, \\
0 & \text{elsewhere} \end{cases}$$

i.e. a rectangular distribution (see Fig. 7a), and one obtains:

$$M_{\text{exp}} = \frac{1}{2} (M_0 + M_1),$$

$$\sigma = \frac{\sqrt{3}}{6} (M_1 - M_0) = 0.290 \ (M_1 - M_0).$$

\hspace{1cm} (17)

Figure 7. Examples of probabilities to measure $m$ according to an exact calculation in cases of the mixture of two (a) and three (b) spectral lines.
Figure 8. Graphic representation of relations 18 and 19. The length of the segments (full thick lines) inside the triangle are proportional to the probability $P(m)$. Three cases are shown corresponding respectively to $m < \tilde{M}_1$, $m = \tilde{M}_1$, and to $m > \tilde{M}_1$. The maximum of probability is obtained when $m = \tilde{M}_1$.

**B.2 Case of 3 spectral lines**

In the case of three spectral lines, we derive from Eq. 12:

\[ m = (1 - x_1 - x_2)M_0 + x_1M_1 + x_2M_2, \quad (18) \]

with \[
\begin{align*}
0 & \leq x_1 \leq 1 \\
0 & \leq x_2 \leq 1 \\
0 & \leq x_1 + x_2 \leq 1.
\end{align*}
\] (19)

The relations (18) and (19) may be represented on a $x_2$ vs $x_1$ plot (Fig. 8). The conditions (19) define a triangular authorized domain in which the density of probability is uniform. The relation (18) is represented by a straight line. The part of this line contained inside the triangle defines a segment which represents the values of $x_1$ and $x_2$ satisfying all relations (19). Since the density of probability is constant along this segment, the probability $P(m)$ is proportional to its length. After normalization, one gets (Fig. 7b):

\[ P(m) = \frac{2k}{M_2 - M_0}, \quad (20) \]

with \[
\begin{align*}
 k = (m - M_0)/(M_1 - M_0) & \quad \text{if} \quad M_0 \leq m \leq M_1 \\
 k = (M_2 - m)/(M_2 - M_1) & \quad \text{if} \quad M_1 \leq m \leq M_2
\end{align*}
\] (21)

and finally:

\[ M_{exp} = \frac{1}{3}(M_0 + M_1 + M_2), \quad (22) \]

\[ \sigma = \sqrt{\frac{2}{6}} \sqrt{M_0^2 + M_1^2 + M_2^2 - M_0M_1 - M_1M_2 - M_2M_0}. \]

**B.3 Case of more than 3 spectral lines**

For more than 3 lines, one may easily infer $M_{exp} = \sum_{i=0}^{n} M_i/(n+1)$, but the determination of $\sigma$ requires the knowledge of $P(m)$. As the exact calculation of $P(m)$ becomes rather difficult, it is more simple to do simulations.

However, care must be taken that the values of the $x_i$’s are explored with an exact equality of chance to occur. For each set of $x_i$’s, $m$ is calculated, and the histogram $N_j(m_j)$ of its distribution is built (Fig. 9). Calling $nbin$ the number of bins of the histogram, one gets :

\[ P(m_j) = \frac{N_j}{\sum_{j=1}^{nbin} N_j}, \quad (23) \]

\[ M_{exp} = \sum_{j=1}^{nbin} P(m_j)m_j, \]

\[ \sigma^2 = \sum_{j=1}^{nbin} P(m_j)(m_j - M_{exp})^2. \]
Figure 9. Examples of Monte-Carlo simulations of the probabilities to measure \( m \) in cases of two (a), three (b) and four (c) spectral lines.

A first possibility is to explore the \( x_i \)'s step-by-step: \( x_1 \) varies from 0 to 1, and for each \( x_1 \) value, \( x_2 \) varies from 0 to \((1-x_1)\), and for each \( x_2 \) value, \( x_3 \) varies from 0 to \((1-x_1-x_2)\), ..., using the same step value for all.

A second possibility is to choose \( x_1, x_2, x_3 \), ..., randomly in the range \([0,1]\) in an independent way, and to keep only the sets of values which satisfy the relation \( \sum_{i=1}^{n} x_i \leq 1 \). An example of a Fortran program based on the CERN library is given below for the cases of two, three and four lines. The results are presented in Fig. 9.

Both methods give results in excellent agreement with each other, and as well with the exact calculation in the cases of two lines (see Fig. 7a and 9a) and three lines (see Fig. 7b and 9b).

The Fortran program used to produce the histograms in Fig. 9.

```
program isomers
  c-----------------------------------------------------------------
  c- October 15, 2003 C.Thibault
  c- Purpose and Methods : MC simulation for isomers (2-4 levels)
  c- Returned value : mass distribution histograms
  c-----------------------------------------------------------------
  parameter (nwpawc=10000)
```
B.4 Example of application for one, two or three excited isomers

We consider the case of a mixture implying isomeric states. We want to determine the ground state mass $M_0\pm\sigma_0$ from the measured mass $M_{\text{exp}}\pm\sigma_{\text{exp}}$ and the knowledge of the excitation energies $E_1\pm\sigma_1$, $E_2\pm\sigma_2$, ...

With the above notation, we have

$$M_1 = M_0 + E_1,$$
$$M_2 = M_0 + E_2,$$

For a single excited isomer, Eq. 17 can be written:

$$M_0 = M_{\text{exp}} - \frac{1}{2} E_1,$$

$$\sigma^2 = \frac{1}{12} E_1^2 \quad \text{or} \quad \sigma = 0.29 E_1,$$

$$\sigma_0^2 = \sigma_{\text{exp}}^2 + \left(\frac{1}{2} \sigma_1\right)^2 + \sigma^2.$$  

For two excited isomers, Eq. (22) lead to :

$$M_0 = M_{\text{exp}} - \frac{1}{3} (E_1 + E_2),$$

$$\sigma^2 = \frac{1}{18} (E_1^2 + E_2^2 - E_1 E_2) \quad \text{or} \quad \sigma = 0.236 \sqrt{E_1^2 + E_2^2 - E_1 E_2},$$

$$\sigma_0^2 = \sigma_{\text{exp}}^2 + \left(\frac{1}{3} \sigma_1\right)^2 + \left(\frac{1}{3} \sigma_2\right)^2 + \sigma^2.$$
If the levels are regularly spaced, i.e. \(E_2 = 2E_1\),
\[
\sigma = \frac{\sqrt{6}}{12} E_2 = 0.204 E_2,
\]
while for a value of \(E_1\) very near 0 or \(E_2\),
\[
\sigma = \frac{\sqrt{2}}{6} E_2 = 0.236 E_2.
\]

For three excited isomers, the example shown in Fig. 9c leads to:
\[
M_0 = M_{\text{exp}} - \frac{1}{4}(E_1 + E_2 + E_3) = 450,
\]
\[
\sigma = 175,
\]
\[
\sigma^2_0 = \sigma^2 \left( \frac{1}{4} \sigma_1 \right)^2 + \left( \frac{1}{4} \sigma_2 \right)^2 + \left( \frac{1}{4} \sigma_3 \right)^2 + \sigma^2.
\]

**Appendix C Converting frequency ratios to linear equations**

In the following, quantities with the subscript \(r\) describe the characteristics of the reference ion in the Penning Trap. Equivalent quantities, with no subscript, describe characteristics of the ion being measured.

In Ref. [2], linear equations deduced from frequency ratios are only valid for atoms. When molecules are involved, an extra term about the molecular binding energy should be included. In this case, Eq. 21 in Ref. [2] should be rewritten as:
\[
R = \frac{f_r}{f} = \frac{M - D - m_e q + B}{M_r - D_r - m_e q_r + B_r} \frac{q_r}{q},
\]  
(24)

where \(q\) is the charged state of the given ion, \(D\) is the molecular binding energy (dissociation energy), \(B\) is the electron binding energy, \(m_e\) is the mass of the electron and \(M\) the total atomic mass. All masses and energies are in atomic mass units (\(\mu\)) and so, \(u=1\). This expression can be written in terms of the mass excess \(M\) and atomic mass number \(A\):
\[
A + M - D - m_e q + B = R \frac{q_r}{q} (A_r + M_r - D_r - m_e q_r + B_r)
\]  
(25)

or, alternatively:
\[
M - R \frac{q_r}{q} M_r = m_e q (1 - R) + A_r \left( \frac{q_r}{q} - \frac{A}{A_r} \right) + R \frac{q_r}{q} (B_r - D_r) - (B - D).
\]

The general aim is to establish some quantity \(y\) and its associated precision \(dy\). We define \(C\) to be a truncated, three-digit decimal approximation of the ratio \(A\) to \(A_r\), and then we can write:
\[
y = M - C M_r
\]  
(26)

and so
\[
y = y_1 + y_2 + y_3 + y_4,
\]  
(27)

where
\[
y_1 = M_r \left( R \frac{q}{q_r} - C \right),
\]  
(28)
\[
y_2 = m_e \frac{q}{q_r} (1 - R),
\]  
(29)
\[
y_3 = A_r \left( \frac{q}{q_r} R - \frac{A}{A_r} \right),
\]  
(30)
\[
y_4 = R \frac{q}{q_r} (B_r - D_r) - (B - D).
\]  
(31)

To fix relative orders of magnitude, \(M_r\) is generally smaller than 0.1 \(\mu\), \(R - C\) is a few \(10^{-4}\), \((1 - R)\) is usually smaller than unity (and typically 0.2 for a 20% mass change), \(R - \frac{A}{A_r}\) varies from 1 to \(100 \times 10^{-6}\), \(B_r - D_r\) is generally smaller than 0.1 \(\mu\), and \(A_r\) is typically 100 \(\mu\) for atomic mass \(A = 100\). The four terms \(y_1, y_2, y_3,\) and \(y_4\) take values of the order of 10 \(\mu\), 100 \(\mu\), 10 to 10000 \(\mu\), and 0.1 \(\mu\), respectively.

The associated precision \(dy\) is written:
\[
dy = dy_1 + dy_2 + dy_3 + dy_4,
\]  
(32)

where
\[
dy_1 = \frac{q}{q_r} M_r \ dR + \left( R \frac{q}{q_r} - C \right) dM_r \simeq dR \times 10^5 \ \mu, \]
(33)
\[
dy_2 = m_e \frac{q}{q_r} dR \simeq dR \times 10^5 \ \mu, \]
(34)
\[
dy_3 = \frac{q}{q_r} A_r \ dR \simeq dR \times 10^6 \ \mu, \]
(35)

and
\[
dy_4 = \frac{q}{q_r} (B_r - D_r) dR + R \frac{q}{q_r} (dB_r - dD_r)
- (dB - dD) \simeq dR \times 10^{-1} \ \mu. \]
(36)

Consequently, only the 3rd term contributes significantly to the precision of the measurement, and so we write: \(dy = dy_3\).

If the two frequencies are measured with a typical precision of \(10^{-7}\) for ions at \(A = 100\), then the precision on the frequency ratio \(R\) is \(1.4 \times 10^{-7}\) and the precision on the mass is approximately 14 \(\mu\).

Next we will illustrate how to calculate the molecular binding energy for the most precise Penning Trap experiment.
C.1 Bond Dissociation Energy

The bond dissociation energy $D$ is a quantity which signifies the strength of a chemical bond. The bond dissociation energy for a bond $A–B$, which is broken through reaction:

$$AB \rightarrow A + B$$

is defined as the standard enthalpy change at a specified temperature Ref. [63]:

$$D^o(AB) = \Delta H_f^o(A) + \Delta H_f^o(B) - \Delta H_f^o(AB),$$

(37)

where $\Delta H_f^o$ is the standard heat of formation and its value is available for a large number of atoms and compounds on NIST Chemistry Webbook [64]. All $D^o$ values refer to the gaseous state at temperature either $0$ K or $298$ K. When data on the standard heat of formation is absent at $0$ K, $D^o(AB)$ will be converted to $D_{298}(AB)$ by the approximation:

$$D_{298}^o(AB) \approx D^o(AB) + 3.72 \text{ kJ/mol.} \quad (38)$$

Unlike diatomic molecules which involve only one bond, polyatomic molecules have several bonds and their $D^o$'s are the sum of all the single bonds. For example, if one wants to know the dissociation energy of CH$_4$, one needs to calculate the dissociation energy of the four bonds CH–H, CH2–H, CH–H, and C–H, respectively:

$$D^o(CH_3 - H) = \Delta H_f^o(CH_3) + \Delta H_f^o(H) - \Delta H_f^o(CH),$$

$$D^o(CH_2 - H) = \Delta H_f^o(CH_2) + \Delta H_f^o(H) - \Delta H_f^o(CH_2),$$

$$D^o(CH - H) = \Delta H_f^o(CH) + \Delta H_f^o(H) - \Delta H_f^o(CH_3),$$

$$D^o(C - H) = \Delta H_f^o(C) + \Delta H_f^o(H) - \Delta H_f^o(CH). \quad (39)$$

Summing over all four bonds above, we obtain:

$$D^o(CH_4) = D(CH_3 - H) + D(CH_2 - H)$$

$$+ D(CH - H) + D(C - H)$$

$$= \Delta H_f^o(C) + 4 \times \Delta H_f^o(H) - \Delta H_f^o(CH).$$

The dissociation energy can be generalized for a polyatomic molecule which has the form $A_nB_mC_l$:

$$D^o(A_nB_mC_l) = n\Delta H_f^o(A) + k\Delta H_f^o(B) + i\Delta H_f^o(C)$$

$$- \Delta H_f^o(A_nB_mC_l). \quad (40)$$

The ionization energies for molecules are available on NIST Atomic Spectra Database [65]. We now illustrate this treatment through two examples.

C.1.1 $^{13}$C$_2$H$_4^+$ and $^{14}$N$_2^+$ mass doublet

In the work of [2004Ra33], a cyclotron frequency ratio $R = 0.99942146088(7)$ of relative precision $7 \times 10^{-12}$ has been obtained for ions $^{13}$C$_2$H$_4^+$ and $^{14}$N$_2^+$. We first calculate $D^o(C_2H_2)$ by applying Eq. 40:

$$D^o(C_2H_2) = 2 \times \Delta H_f^o(C) + 2 \times \Delta H_f^o(H) - \Delta H_f^o(C_2H_2)$$

$$= 2 \times 716.68 + 2 \times 218.998 - 227.40$$

$$= 1641.956 \text{ kJ/mol}$$

$$= 17.018 \text{ eV}.$$

$D^o(N_2) = 944.9 \text{ kJ/mol} = 9.793 \text{ eV}$ is obtained from Ref. [66], since $\Delta H_f^o(N_2)$ is not on the list of [64]. Combining the ionization energy $B(C_2H_2) = 11.4 \text{ eV}$ and $B(N_2) = 15.6 \text{ eV}$, we obtain the mass difference:

$$^{13}\text{C} + ^{14}\text{H} - ^{14}\text{N} = 8105.862995(98) \text{ } \mu\text{u}.$$  

In the original paper [2004Ra33], this equation is given as:

$$^{13}\text{C} + ^{14}\text{H} - ^{14}\text{N} = 8105.86288(10) \text{ } \mu\text{u},$$

which differs by 12(10) μu from our calculation. The difference is because we used the updated molecular binding energy from Ref. [64, 66]. In this case, the molecular binding energy is 170 times larger than the uncertainty, and even the updates of the molecular energies have significant impact on the deduced values.

C.1.2 Atomic Masses of Tritium and Helium-3

By measuring the cyclotron frequency ratios of $^3\text{He}^+$ and $^3\text{T}^+$ to HD$^+$, using HD$^+$ as a mass reference, atomic masses for $^3\text{He}$ and $^3\text{T}$ were obtained Ref. [2015My03]. The essential part here is to calculate the molecule binding energy $D^o$(HD). Instead of applying Eq. 37 to calculate the molecule binding energy of HD, we used the most recent datum $D^o$(HD) $= 36406.78366 \text{ cm}^{-1} = 4.5137 \text{ eV}$ from [67].

Combining the ionization energies of $B$(HD)$=15.4445$ eV, $B(^3\text{He})=24.5874$ eV and $B(T) = 13.5984$ eV, the mass differences and their uncertainties can be derived:

$$^3\text{He} - H - D = -5897.487710(144) \text{ } \mu\text{u}$$

and

$$T - H - D = -5877.528366(144) \text{ } \mu\text{u}.$$  

The correction of the molecule binding energy $D^o$(HD) $= 4.5 \text{ eV}$ is 30 times larger than the $\sim 0.14 \text{ eV}$ uncertainty. We have created a file called “ionization”, which includes all the information that is needed to calculate the linear equation.

C.2 Program for frequency conversion

Primary data from Penning Trap measurement are typically given in the form of an experimental frequency ratio. An example is given here for a series of nuclides with respect to a various reference nuclides and various charge states. Below is the Fortran frequency conversion program, followed by sample input files and the corresponding output file, all available on the AMDC website [22].

030002-44
The frequency conversion program

conversion of frequency ratios to linear equations including electron and molecular binding energies

```
c real*8 xzero, mel, mref, smref, mrefk, rap, srap, coef
c real*8 prov, membere, sigmem, m118, sm118, meb, e118, y4
integer*4 q118, qref, znum, val, nbion, 1, qel
character txref*4, tx118*4, rev*2, ael*4
character txiref*4, txi118*4
dimension znum(450), ael(450), qel(450), meb(450)
c
mel : electron mass in micro-u
mref, smref, m118, sm118 : Masses and uncert. for reference (ref) and measured (118)
c
filea='ptkl.equat ' ! output file
fileb='ptkl.freq ' ! input file
filec='ionization.data ' ! electron+mol. file
open(unit=1, file=filea, form='formatted', status='new')
open(unit=3, file=fileb, form='formatted', status='old')
open(unit=10, file=filec, form='formatted', status='old')
mel = 568.57990907d0 ! mass of electron in micro-u
xzero = 9.314940038d-1 ! conversion factor micro-u to keV
do i=1,450 ! read electron+mol. file
  read(10, *, iostat=val) znum(i), ael(i), qel(i), meb(i)
  meb(i) = (meb(i) * 1.d-3) / xzero ! in micro-u
  if(val.lt.0) then
    nbion = i - 1 ! nbion: number of lines in elec+mol file
    exit
  end if
end do
close(10)
12 read(3,1001, err=99) iaref, txref, qref, mref, smref ! read ref.name, mass(micro-u) and charge
1001 format(i4, a4, i4, f19.8, a2, f13.8) ! ref. mass in keV
  mrefk = mref * xzero ! ref. mass in micro-u
15 read(3,1001, end=90, err=99) ia118, tx118, q118, rap, srap ! read frequency ratio
   if(tx118.eq.'NEW ') go to 12 ! reset reference
   if(rev.eq. ' ') then ! if reversed freq. ratio: rev=-1
     rap = rap / 1.d+6
     srap = srap / 1.d+6
   else
     rap = 1.d+6 / rap
     srap = rap * srap / 1.d+6
   endif
   coef = 1000. * ia118 / iaref
   coef = anint(coef) / 1000. ! calculate 3-digit coefficient
   prov = (ia118*1.d+0) / iaref - rap * q118 / qref ! start calculating the equation value
   membere = mrefk* (rap * q118 / qref - coef) + m118 * q118 * (1-rap)
   * - iaref * 1.d+6 * prov
   sigmem = srap * iaref * 1.d+6 * q118 / qref ! value (in micro-u) for the equation
   ! its uncertainty
   ef = 0.
   e118 = 0.
do i=1, nbion ! loop over the nbion lines in elec+mol file
    txiref = txref
    if(txiref(3:3).eq.'m' .or. txiref(3:3).eq.'n' .or. txiref(3:3).eq.'x') then
      txiref(3:4) = txiref(4:4) ! isomers m n or x : treated as gs
    endif
```

if(txii18(3:3).eq.'m' .or. txii18(3:3).eq.'n' .or. txii18(3:3).eq.'x') then
    txii18(3:4)=txii18(4:4)//' '
    if(txi118(2:2).eq.'x') txii118(2:3)=txii118(3:3)//' '
endif
if(trim(txi1ref)==trim(ael(i)).and.qref==qel(i)) eref = meb(i)
if(trim(txi118)==trim(ael(i)).and.q118==qel(i)) e118 = meb(i)
end do

if(eref.ne.0. .and. e118.ne.0.) then
    y4 = eref*rap*q118/qref - e118 ! calculate electronic and molecular correction
else
    y4 = 0.
    write (1,*) "WARNING : el.+mol. binding en. not found"
end if
membre = membre + y4
write (1,1020) ia118,tx118,iaref,txref,coef,membre,sigmem
1020 format(5x,i6,a4,'-',i4,a4,'*',f6.3,' =', f15.5,' (',f9.5,')')
ml18 = membre + coef*mref
sm118 = sqrt(sigmem**2 + (coef*smref)**2)
write (1,i1030) ia118,tx118,ml18,sm118
1030 format(13x,i4,a4,' =',f15.6,' +/-',f11.6,' micro-u')
m118 = m118 * xzero
sm118 = sm118 * xzero
write (1,1032) m118,sm118
1032 format(13x,8x,' =',f15.6,' +/-',f11.6,' keV',/)
Corresponding output file

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Energy Difference</th>
<th>Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{4}\text{He} - 6\text{Li}$</td>
<td>$-7483.71665$</td>
<td>0.04620</td>
</tr>
<tr>
<td>$^{4}\text{He}$</td>
<td>2603.247650 +/- 0.050086 micro-u</td>
<td>0.046655 keV</td>
</tr>
<tr>
<td>$^{7}\text{Li} - 6\text{Li}$</td>
<td>$-1644.99050$</td>
<td>0.07860</td>
</tr>
<tr>
<td>$^{7}\text{Li}$</td>
<td>16003.416291 +/- 0.085576 micro-u</td>
<td>0.079714 keV</td>
</tr>
<tr>
<td>$^{8}\text{Li} - 6\text{Li}$</td>
<td>$-2327.42564$</td>
<td>0.10800</td>
</tr>
<tr>
<td>$^{8}\text{Li}$</td>
<td>22486.231245 +/- 0.114710 micro-u</td>
<td>0.106852 keV</td>
</tr>
<tr>
<td>$^{10}\text{Be} - 7\text{Li}$</td>
<td>$-9334.15799$</td>
<td>0.12834</td>
</tr>
<tr>
<td>$^{10}\text{Be}$</td>
<td>13534.737197 +/- 0.128503 micro-u</td>
<td>0.119700 keV</td>
</tr>
<tr>
<td>$^{11}\text{Be} - 7\text{Li}$</td>
<td>$-3479.82956$</td>
<td>0.62193</td>
</tr>
<tr>
<td>$^{11}\text{Be}$</td>
<td>21661.552062 +/- 0.621969 micro-u</td>
<td>0.579360 keV</td>
</tr>
<tr>
<td>$^{44}\text{K} - 39\text{K}$</td>
<td>$2529.42538$</td>
<td>2.20434</td>
</tr>
<tr>
<td>$^{44}\text{K}$</td>
<td>-38409.741096 +/- 2.206428 micro-u</td>
<td>-35778.443518 +/- 2.055275 keV</td>
</tr>
<tr>
<td>$^{74}\text{Rb} - 85\text{Rb}$</td>
<td>$13930.97003$</td>
<td>1.68489</td>
</tr>
<tr>
<td>$^{74}\text{Rb}$</td>
<td>-64929.004193 +/- 1.684896 micro-u</td>
<td>-60480.978079 +/- 1.569470 keV</td>
</tr>
<tr>
<td>$^{99}\text{Sr} - 85\text{Rb}$</td>
<td>$35661.05986$</td>
<td>4.42327</td>
</tr>
<tr>
<td>$^{99}\text{Sr}$</td>
<td>-67103.895368 +/- 4.423274 micro-u</td>
<td>-62506.876167 +/- 4.120253 keV</td>
</tr>
<tr>
<td>$^{3}\text{He} - 3\text{HD}$</td>
<td>$-5897.48771$</td>
<td>0.00014</td>
</tr>
<tr>
<td>$^{3}\text{He}$</td>
<td>16029.322619 +/- 0.000208 micro-u</td>
<td>14931.217905 +/- 0.000194 keV</td>
</tr>
<tr>
<td>$^{3}\text{H} - 3\text{HD}$</td>
<td>$-5877.52837$</td>
<td>0.00014</td>
</tr>
<tr>
<td>$^{3}\text{H}$</td>
<td>16049.281964 +/- 0.000208 micro-u</td>
<td>14949.809914 +/- 0.000194 keV</td>
</tr>
</tbody>
</table>

0Normal End of Freq.Ratios to Equations Conversion
References

References in the text such as [2014Ya.A] or [2016Xu10] are listed under “References used in the AME2016 and the NUBASE2016 evaluations”, p. 030003-261.

9 John Dalton, 1766-1844, who first speculated that elements combine in proportions following simple laws, and was the first to create a table of (very approximate) atomic weights.
12 T.J. Quinn, Metrologia 26: 69 (1989)
21 Systematic errors are those due to instrumental drifts or instrumental fluctuations, that are beyond control and are not accounted for in the error budget. They might show up in the calibration process, or when the measurement is repeated under different experimental conditions. The experimentalist adds then quadratically a systematic error to the statistical and the calibration ones, in such a way as to have consistency of his data. If not completely accounted for or not seen in that experiment, they can still be observed by the mass evaluators when considering the mass adjustment as a whole.
22 The AME2016 files in the electronic distribution and complementary documents can be retrieved from the Atomic Mass Data Center (AMDC) through the Web: http://amdc.impcas.ac.cn/; and mirror site https://www-nds.iaea.org/amdc/
24 H.A. Bethe and R.F. Bacher, Rev. Mod. Phys. 8: 82 (1936)
Each group of mass-spectrometric data is assigned a factor \( F \) according to its partial consistency factor \( \chi^2_{np} \), due to the fact that its statistical uncertainties and its internal systematic error alone do not reflect the real experimental situation. From comparison to all other data and more specially to combination of reaction and decay energy measurements, we have assigned factors \( F = 1.5, 2.5 \) or \( 4.0 \) to the different labs. Only Penning trap data have almost all been assigned a factor \( F = 1.0 \). Example: the group of data H25 has been assigned \( F = 2.5 \), this means that the total uncertainty assigned to \( ^{155}\text{Gd}^{35}\text{Cl} - ^{153}\text{Eu}^{37}\text{Cl} \) is \( 2.4\mu u \times 2.5 \). The weight of this piece of data is then very low, compared to \( 0.79\mu u \) derived from all other data. This is why it is labeled “U”.

46 W. Heisenberg, Z. Phys. 77: 1 (1932)
47 E. P. Wigner, Phys. Rev. 51: 106 (1937)
51 A. Ratkowski, Nuclear Instruments and Methods,