

The AME2003 atomic mass evaluation ^{*}

(I). Evaluation of input data, adjustment procedures

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Abstract

This paper is the first of two parts presenting the result of a new evaluation of atomic masses (AME2003). In this first part we give full information on the used and rejected input data and on the procedures used in deriving the tables in the second part. We first describe the philosophy and procedures used in selecting nuclear-reaction, decay, and mass spectrometric results as input values in a least-squares evaluation of best values for atomic masses. The calculation procedures and particularities of the AME are then described. All accepted data, and rejected ones with a reported precision still of interest, are presented in a table and compared there with the adjusted values. The differences with the earlier evaluation are briefly discussed and information is given of interest for the users of this AME. The second paper for the AME2003, last in this issue, gives a table of atomic masses, tables and graphs of derived quantities, and the list of references used in both this evaluation and the NUBASE2003 table (first paper in this issue).

AMDC: <http://csnwww.in2p3.fr/AMDC/>

1. Introduction

Our last full evaluation of experimental data AME'93 [1]–[4] was published in 1993. Since then an uncommonly large number of quite important new data has become

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available. In fact, as much as 34% of the data used in the present calculation were not used in 1993.

An update AME'95 [5] appeared two years later. Lack of time to evaluate the stream of new quite important data, and also the necessity to create the NUBASE evaluation (see below), prevented the intended further updates of the AME. A certain stabilization, that seems to be reached now, encourages us to publish the present new full evaluation, together with the new version of NUBASE (first paper in this issue).

General aspects of this work will first be discussed. But in doing this, we will mention several local analyses intended, partly, to study points elaborated further below. Other local analyses may be found at the AMDC web site [6].

The main table of the evaluation is given in this Part I. In it (Table I), we present all accepted data, and rejected ones with a reported precision still of interest, and compares them with the adjusted values.

As in our previous evaluations, all the uncertainties in the present tables are one-standard deviation (1σ) errors.

There is no strict cut-off date for the data from literature used in the present AME2003 evaluation: all data available to us until the material is sent (November 19, 2003) to the publisher have been included. Those which could not be included for special reasons, like the need for a heavy revision of the evaluation at a too late stage, are added in remarks to the relevant data. The final calculation was performed on November 18, 2003.

The present publication updates and includes almost all the information given in the two previous AMEs, published in 1983 and 1993.

1.1. The isomers in the AME and the emergence of NUBASE

Already since long, we maintain a file (called *Mfile*) of approximate mass values for atoms in ground-states and in selected isomeric states as input in our computer programs. These programs essentially calculate the differences between input values and these approximate values in order to gain precision in the calculations. One reason was that, where isomers occur, one has to be careful to check which one is involved in reported experimental data, such as α - and β -decay energies. Cases have occurred where authors were not (yet) aware of isomeric complications. For that reason, our *Mfile* contained known data on such isomeric pairs (half-lives; excitation energies; spin-parities). The matter of isomerism became even more important, when mass spectrometric methods were developed to measure masses of exotic atoms far from β -stability and therefore having small half-lives. The resolution in the spectrometers is limited, and often insufficient to separate isomers. Then, one so obtains an average mass for the isomeric pair. A mass of the ground-state, our primary purpose, can then only be derived if one has information on the excitation

energy and on the production rates of the isomers. And in cases where e.g. the excitation energy was not known, it may be estimated, see below. We therefore judged it necessary to make our *Mfile* more complete. This turned out to be a major job. And since it was judged possible, that the result might be useful for others, the resulting NUBASE97 evaluation [7] file was published.

1.2. Highlights

In our earlier work we distinguished a ‘backbone’ of nuclides along the line of stability in a diagram of atomic number A versus charge number Z [8]. For these nuclides the atomic mass values are known with exceptionally high precision. But a difficulty existed here already since 1980 (see ref. [9], especially Fig. 1) with respect to the atomic masses of stable Hg isotopes. As will be discussed below, new data solve this problem.

New precision measurements with Penning traps considerably improve the precision in our knowledge of atomic mass values along the backbone. Only one group at Winnipeg (see e.g. [2003Ba49]) is still making measurements of stable nuclei with a conventional mass spectrometer. The importance and impact of their results will be outlined below, in particular in solving the long-standing Hg-problem. It is somewhat ironical but not unexpected that the new results show that several older data are less good than thought earlier, but the reverse also occurs to be true. Below we will mention the most prominent examples. Strengthening the backbone, a large number of neutron capture γ -ray energies play an essential *rôle*, and determine neutron separation energies with high precision. For comparison the number of couples of nuclides connected by (n,γ) reactions with an accuracy of 0.5 keV or better is now 243 against 199 in AME93, 128 in AME83 and 60 in the 1977 one. The number of cases known to better than 0.1 keV is presently 100 against 66 in AME93 and 33 in AME83. Also, several reaction energies of (p,γ) reactions are known about as precisely (25 and 8 cases with accuracies better than 0.5 keV and 0.1 keV respectively). In fact, the precisions in both cases is so high that one of us [6] has re-examined all calibrations. Several α -particle energies are also known with comparable precision; and here too it was found necessary to harmonize the calibrations. Another feature near the line of stability is the increased number of measurements of reaction energy differences, which can often be measured with a quite higher precision than the absolute reaction energies. Our computer program accepts this kind of inputs which are given as such in the present table of input data (Table I). This might be another incentive for giving *primary* results in publications: in later evaluations the results will be corrected automatically if calibration values change due to new work.

Penning traps, as well as storage rings and the MISTRAL on-line Smith-type spectrometer, are now also used for making mass measurements of many nuclides

further away from the line of stability. As a result, the number of nuclides for which experimental mass values are now known is substantially larger than in our preceding atomic mass tables. These measurements are sometimes made on deeply ionized particles, up to bare nuclei. The results, though, are reduced by their authors to masses of neutral (and un-excited) atoms. They derive the necessary electron binding energies from tables like those of Huang et al. [10] (see also the discussion in Part II, Section 2). These mass-spectrometric measurements are often made with resolutions, that do not allow separation of isomers. A further significant development is presented by the measurements on proton-disintegrations. They allow a very useful extension of the systematics of proton binding energies. But in addition they give in several cases information on excitation energies of isomers. The latter two developments are reasons why we have to give more attention to relative positions of isomers than was necessary in our earlier evaluations. The consequences are discussed below. Especially useful for long chains of α -decays, measured α -decay energies yield often quite precise information about differences in the masses of their members. It is therefore fortunate that new information on α -decay is still regularly reported, mainly by laboratories in Finland, Germany, Japan and the USA. A useful development was also the determination of limits on proton decay energies from measured limits on half-lives (see e.g. [1999Ja02]). The unexpected proton-stability of ^{89}Rh (see also [1995Le14]) forced us to reconsider the systematics of masses in this region.

Remark: in the following text we will mention several data of general interest. We will avoid mention of references when they can be found in Table I. If desirable to still give references, we will give them as key-numbers like [2002Aa15], listed at the end of Part II, under “References used in the AME2003 and the NUBASE2003 evaluations”, p. 579.

2. Units; recalibration of α - and γ -ray energies

Generally a mass measurement can be obtained by establishing an energy relation between the mass we want to determine and a well known nuclidic mass. This energy relation is then expressed in electron-volts (eV). Mass measurements can also be obtained as an inertial mass from its movement characteristics in an electromagnetic field. The mass, thus derived from a ratio of masses, is then expressed in ‘unified atomic mass’ (u). Two units are thus used in the present work.

The mass unit is defined, since 1960, by $1\text{ u} = M(^{12}\text{C})/12$, one twelfth of the mass of one free atom of carbon-12 in its atomic and nuclear ground-states. Before 1960, two mass units were defined: the physical one $^{16}\text{O}/16$, and the chemical one which considered one sixteenth of the average mass of a standard mixture of the three stable isotopes of oxygen. This difference was considered as being not at all

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

1 u	=	$M(^{12}\text{C})/12$	=	atomic mass unit				
1 u	=	1 660 538.73	±	0.13	$\times 10^{-33}$ kg	79	ppb	a
1 u	=	931 494.013	±	0.037	keV	40	ppb	a
1 u	=	931 494.0090	±	0.0071	keV ₉₀	7.6	ppb	b
1 eV ₉₀	=	1 000 000.004	±	0.039	μeV	39	ppb	a
1 MeV	=	1 073 544.206	±	0.043	nu	40	ppb	a
1 MeV ₉₀	=	1 073 544.2100	±	0.0082	nu	7.6	ppb	b
M_e	=	548 579.9110	±	0.0012	nu	2.1	ppb	a
	=	510 998.902	±	0.021	eV	40	ppb	a
	=	510 998.903	±	0.004	eV ₉₀	7.6	ppb	b
M_p	=	1 007 276 466.76	±	0.10	nu	0.10	ppb	c
M_α	=	4 001 506 179.144	±	0.060	nu	0.015	ppb	c
$M_n - M_H$	=	839 883.67	±	0.59	nu	700	ppb	d
	=	782 346.60	±	0.55	eV ₉₀	700	ppb	d

a) derived from the work of Mohr and Taylor [11].

b) for the definition of V₉₀, see text.

c) derived from this work combined with M_e and total ionization energies for ¹H and ⁴He from [11].

d) this work.

negligible when taking into account the commercial value of all concerned chemical substances. Kohman, Mattauch and Wapstra [12] then calculated that, if ¹²C/12 was chosen, the change would be ten times smaller for chemists, and in the opposite direction . . . That led to unification; ‘u’ stands therefore, officially, for ‘unified mass unit’! Let us mention to be complete that the chemical mass spectrometry community (e.g. bio-chemistry, polymer chemistry) widely use the dalton (symbol Da, named after John Dalton [14]), which allows to express the number of nucleons in a molecule. It is thus not strictly the same as ‘u’.

The energy unit is the electronvolt. Until recently, the relative precision of $M - A$ expressed in keV was, for several nuclides, less good than the same quantity expressed in mass units. The choice of the volt for the energy unit (the electronvolt) is not evident. One might expect use of the *international* volt V, but one can also choose the volt V₉₀ as *maintained* in national laboratories for standards and defined by adopting an exact value for the constant ($2e/h$) in the relation between frequency and voltage in the Josephson effect. In the 1999 table of standards [11]: $2e/h = 483597.9$ (exact) GHz/V₉₀ (see Table B). An analysis by Cohen and Wapstra [15] showed that all precision measurements of reaction and decay energies were calibrated in such a way that they can be more accurately expressed in V₉₀. Also, the precision of the conversion factor between mass units and *maintained* volts V₉₀ is more accurate than that between it and *international* volts (see Table A). Thus,

already in our previous mass evaluation we decided to use the V_{90} *maintained* volt.

In the most recent evaluation of Mohr and Taylor [11], the difference has become so small that it is of interest only for very few items in our tables. This can be seen in Table A, where the ratio of mass units to electronvolts is given for the two Volt units, and also the ratio of the two Volts. Only for ^1H , ^2D and ^{16}O , the errors if given in international volts are larger, up to a factor of about 2, than if given in V_{90} . Yet, following the advice of B.N. Taylor we will give our final energy data expressed in eV_{90} .

In Table A we give the relation with the international volt, together with several constants of interest, obtained from the most recent evaluation of Mohr and Taylor [11]. In addition, we give values for the masses of the proton, the neutron and the α particle as derived from the present evaluation. Also a value is given for the mass difference between the neutron and the light hydrogen atom. Interestingly, the new value for $M_n - M_H$ is smaller than the earlier ones by slightly over 3 times the error mentioned then ($2.3 eV_{90}$). The reason is that a new measurement [1999Ke05] of the wavelength of the γ -rays emitted by the capture of neutrons in hydrogen gave a result rather different from the earlier one by the same group.

In earlier tables, we also gave values for the binding energies, $ZM_H + NM_n - M$. A reason for this was, that the error (in keV_{90}) of this quantity used to be larger than in $M - A$. Due to the increased precision in the mass of the neutron, this is no longer important. 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’ of importance in astrophysics.

Let us mention some historical points. It was in 1986 that Taylor and Cohen [16] 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 the new value was chosen [17] to define the *maintained* volt V_{90} . In their most recent evaluation, Mohr and Taylor [11] had to revise the conversion constant to *international* eV. The result is a slightly higher (and 10 times more precise) value for V_{90} . The defining values, and the resulting mass-energy conversion factors are given in Table B.

Since older precision reaction energy measurements were essentially expressed in keV_{86} , we must take into account the difference in voltage definition which causes a systematic error of 8 ppm. We were therefore obliged to adjust the precise data to the new keV_{90} standard. For α -particle energies, Rytz [18] has taken this change into account in updating his earlier evaluation of α -particle energies. We have used his values in our input data table (Table I) and indicated this by adding in the reference-field the symbol “Z”.

Also, a considerable number of (n, γ) and (p, γ) reactions has a precision not much worse than the 8 ppm mentioned. One of us [19] has discussed the necessary

Table B. Definition of used Volt units, and resulting mass-energy conversion constants.

		$2e/h$			u		
1983	483594.21	(1.34)	GHz/V	931501.2	(2.6)	keV	
1983	483594	(exact)	GHz/V ₈₆	931501.6	(0.3)	keV ₈₆	
1986	483597.67	(0.14)	GHz/V	931494.32	(0.28)	keV	
1990	483597.9	(exact)	GHz/V ₉₀	931493.86	(0.07)	keV ₉₀	
1999	483597.9	(exact)	GHz/V ₉₀	931494.009	(0.007)	keV ₉₀	

recalibration for several γ -rays often used for calibration. This work has been updated to evaluate the influence of new calibrators and of the new Mohr and Taylor fundamental constants on γ -ray and particle energies entering in (n, γ), (p, γ) and (p,n) reactions. In doing this, use was made of the calibration work of Helmer and van der Leun [20], based on the new fundamental constants. For each of the data concerned, the changes are relatively minor. We judge it necessary to make them, however, since otherwise they add up to systematic errors that are non-negligible. As an example, we mention that the energy value for the 411 γ -ray in ^{198}Au , often used for calibration, was changed from 411 801.85 (0.15) eV₉₀ [1990Wa22] to 411 802.05 (0.17) eV₉₀. As in the case of Rytz' recalibrations, they are marked by "Z" behind the reference key-number; or, if this was made impossible since this position was used to indicate that a remark was added, by the same symbol added to the error value mentioned in the remark. Our list of inputs (Table I) for our calculations mentions many excitation energies that are derived from γ -ray measurements, and that are generally evaluated in the Nuclear Data Sheets (NDS) [21]. Only in exceptional cases, it made sense to change them to recalibrated results.

For higher γ -ray energies, our previous adjustment used several data recalibrated with results of Penning trap measurements of the masses of initial and final atoms involved in (n, γ) reactions. The use of the new constants, and of more or revised Penning trap results, make it necessary to revise again the recalibrated results [6]. Thus, the energy coming free in the $^{14}\text{N}(n,\gamma)^{15}\text{N}$ reaction, playing a crucial role in these calibrations, was changed from 10 833 301.6 (2.3) eV₉₀ to 10 833 296.2 (0.9) eV₉₀.

Several old neutron binding energies can be improved in unexpected ways. Following case presents an illustration. A value with a somewhat large error (650 eV) was reported for the neutron binding energy in ^{54}Cr . Studying the paper taught that this value was essentially the sum of the energies of two capture γ -rays. For their small energy difference a smaller error was reported. Recent work yields a much improved value for the transition to the ground-state, allowing to derive a considerably improved neutron binding energy. Also, in some cases observed neutron resonance

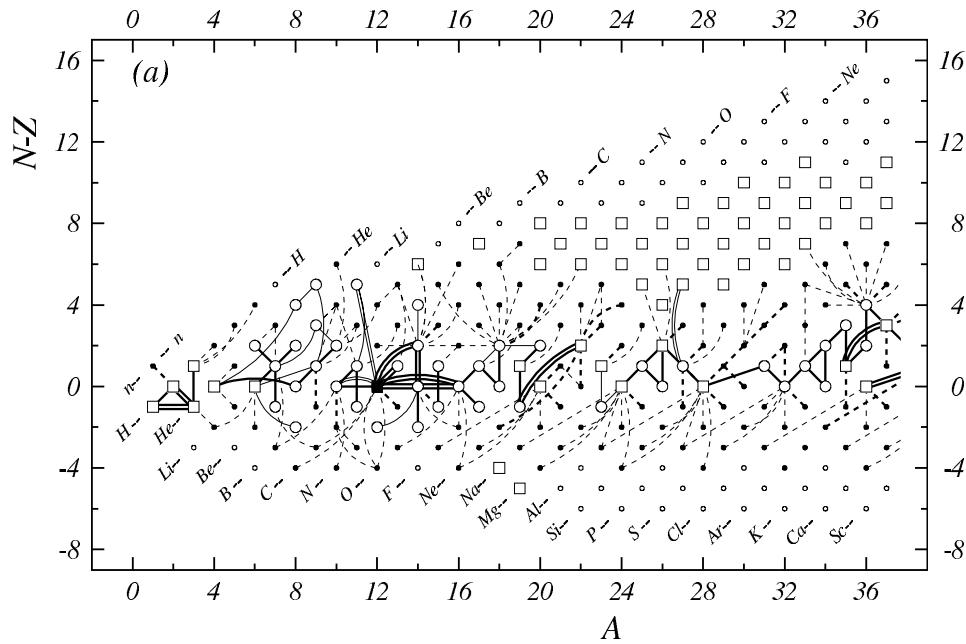


Figure 1: (a)–(i). Diagram of connections for input data.

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;
- ◻ ◉ primary nuclide with relevant isomer;
- // mass-spectrometric connection;
- other primary reaction connection.

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

(limits: 1 keV for $A < 36$,
2 keV for $A = 36$ to 165 and
3 keV for $A > 165$).

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

- secondary nuclide determined from only experimental data;
- nuclide for which mass is estimated from systematical trends;
- connection to a secondary nuclide. Note that an experimental connection may exist between two systematic nuclides when none of them is connected to the network of primaries.

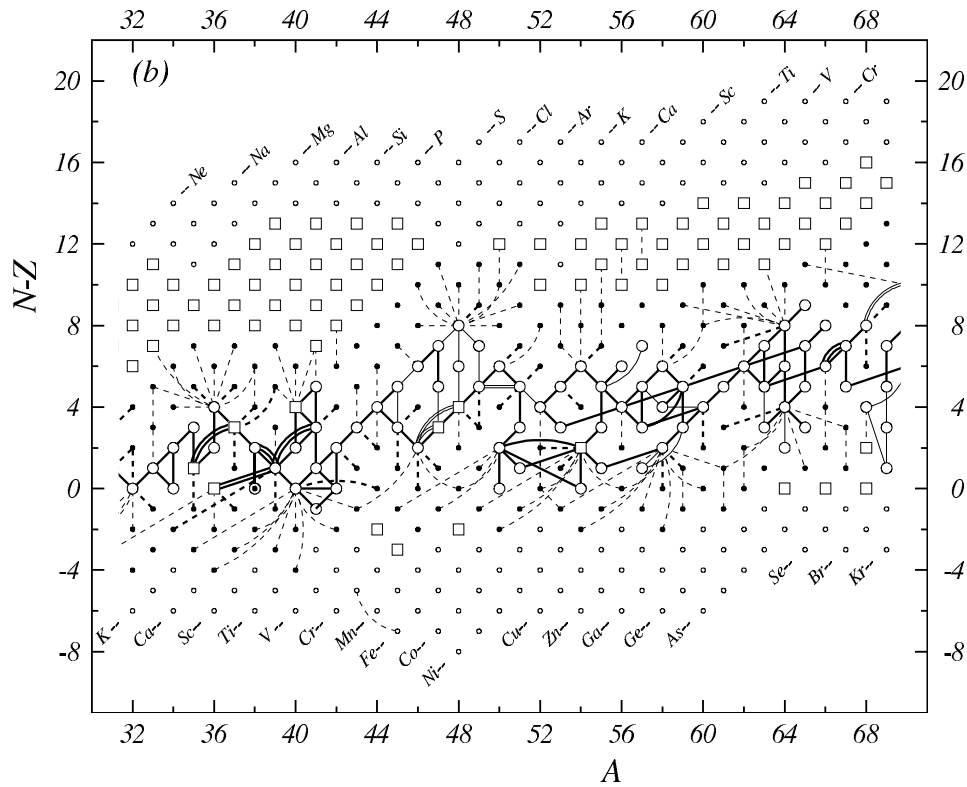


Figure 1 (b). Diagram of connections for input data — continued.

energies can be combined with later measurements of the excitation energies of the resonance states. Discussions can be found at the web site of the AMDC [6].

We also reconsidered the calibration for proton energies, especially those entering in resonance energies and thresholds. An unfortunate development here is that new data [1994Br37] for the 991 keV $^{27}\text{Al}+p$ resonance, (much used for calibration) reportedly more precise than old ones differs rather more than expected. The value most used in earlier work was 991.88 (0.04) keV of Roush *et al.* [22]. In 1990, Endt *et al.* [23] averaged it with a later result by Stoker *et al.* [24] to get a slightly modified value 991.858 (0.025) keV. In doing this, the changes in the values of natural constants used in the derivation of these values was not taken into account. Correcting for this omission, and critically evaluating earlier data, one of us [25] derived in 1993 a value 991.843 (0.033) keV for this standard, and, after revision, 991.830 (0.050) keV. The new measurement of [1994Br37] yields 991.724 (0.021) keV at two standard deviations from the above adopted value.

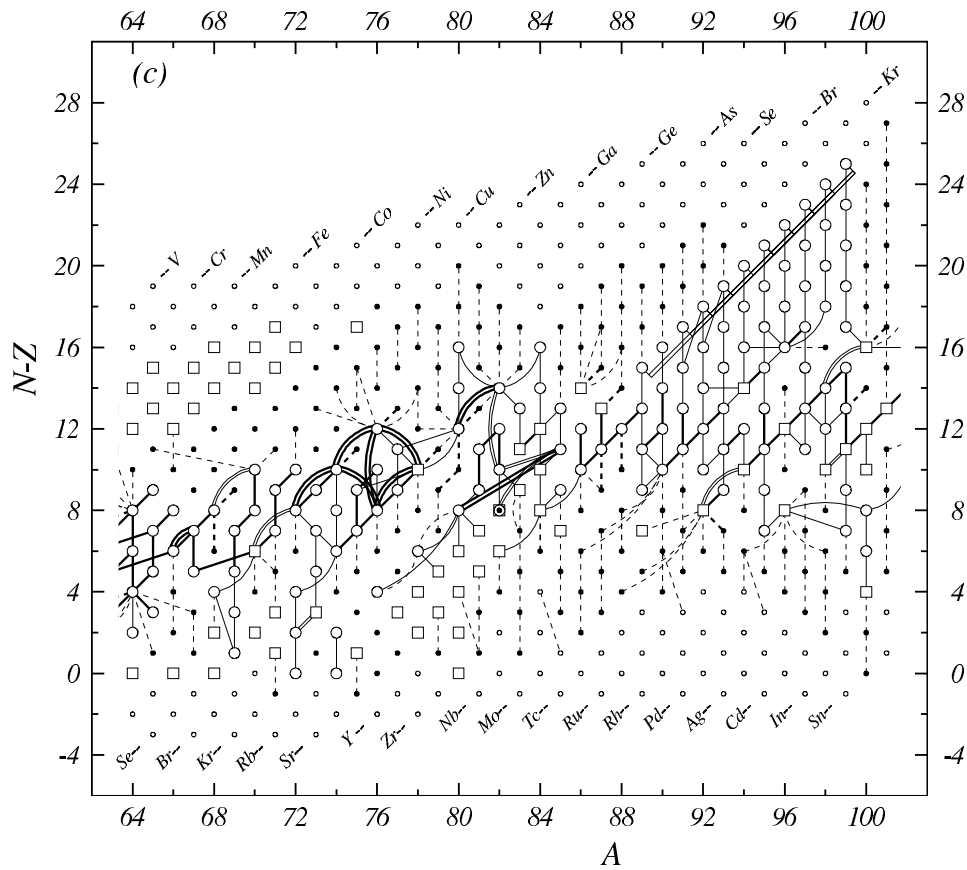


Figure 1 (c). Diagram of connections for input data — continued.

3. Input data, representation in a connections diagram

The input data in this evaluation are results of measurements of mass spectra and of nuclear reaction $A(a,b)B$ and decay $A(b)B$ energies. The last two are concerned with an initial A and a final B nuclide and one or two reaction 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 . Reaction energy differences $A(a,b)B - C(a,b)D$ are in principle represented by a combination of four masses.

Mass spectra, again with exception of a few cases between very light nuclides, can be separated in a class of connections between two or three nuclides, and a class essentially determining an absolute mass value, see Section 5. Penning trap measurements,

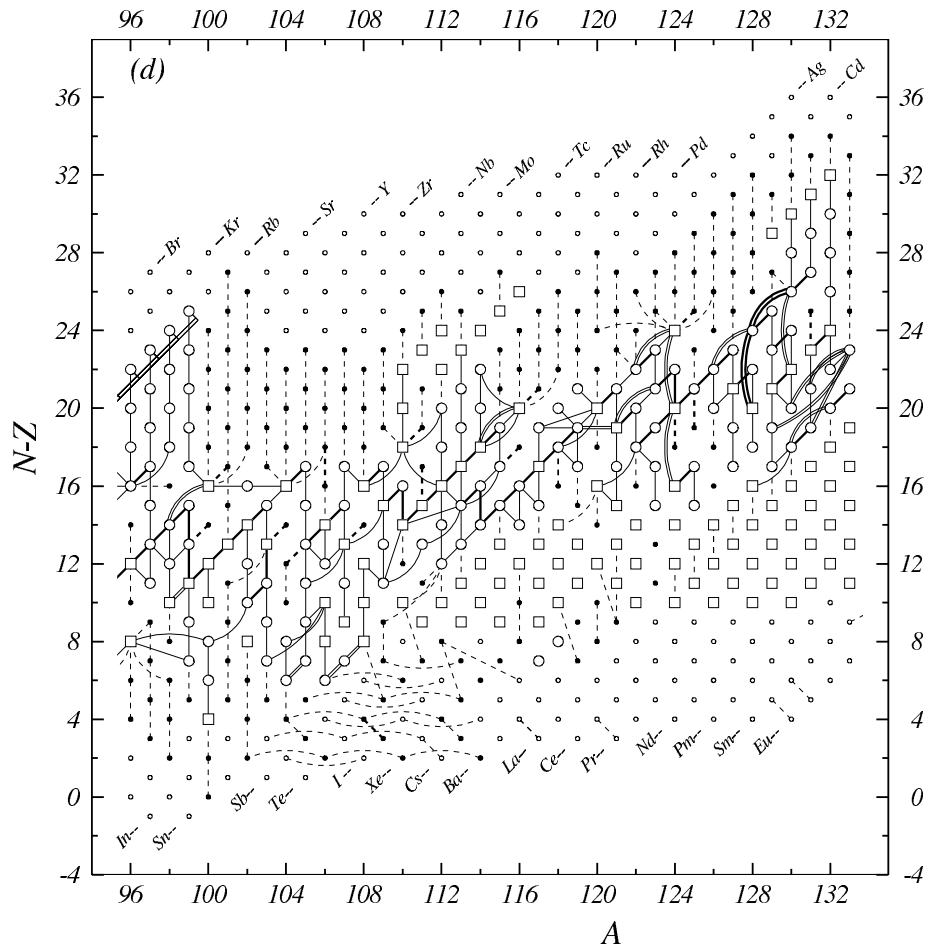


Figure 1 (d). Diagram of connections for input data — continued.

almost always give ratios of masses between two nuclides (inversely proportional to their cyclotron frequencies in the trap). Sometimes these two nuclides can be very far apart. These Penning trap measurements are thus in most cases best represented as combinations of two masses. Other types of experimental set-up, like ‘Smith-type’, ‘Schottky’, ‘Isochronous’ and ‘time-of-flight’ mass-spectrometers, have their calibration determined in a more complex way, and are thus published by their authors as absolute mass doublets. They are then presented in Table I as a difference with ^{12}C .

For completeness we mention that early mass spectrometric measurements on unstable nuclides can best be represented as linear combinations of masses of three isotopes, with non-integer coefficients [26].

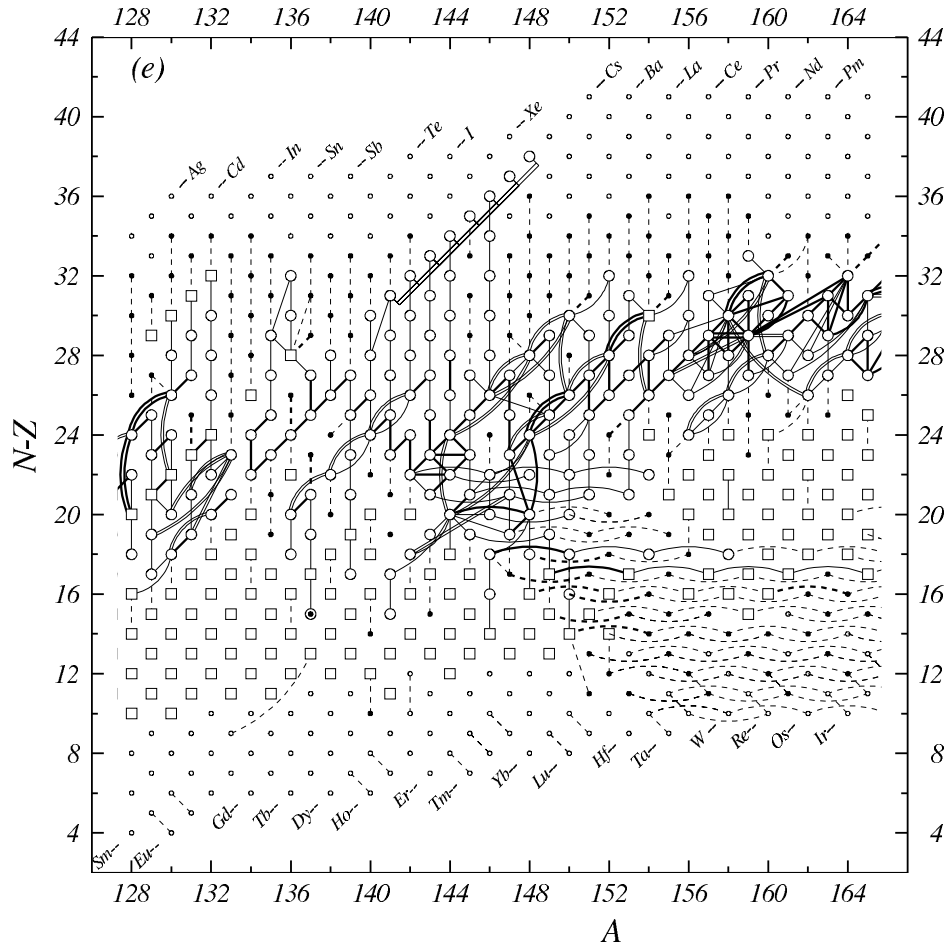


Figure 1 (e). Diagram of connections for input data — continued.

This situation allows us to represent the input data graphically in a diagram of $(N - Z)$ versus $(N + Z)$ as done in Fig. 1. This is straightforward for the absolute mass-doubles and for the difference-for-two-nuclide data; but not for spectrometric triplets and for differences in reaction energies. The latter are in general more important for one of the two reaction energies than for the other one; in the graphs we therefore represent them simply by the former. (For computational reasons, these data are treated as primaries even though the diagrams then show only one connection.)

All input data are evaluated, i.e. calibrations are checked if necessary, and results are compared with other results and with systematics. As a consequence, several input data are changed or, even, rejected. All input data, including the rejected ones,

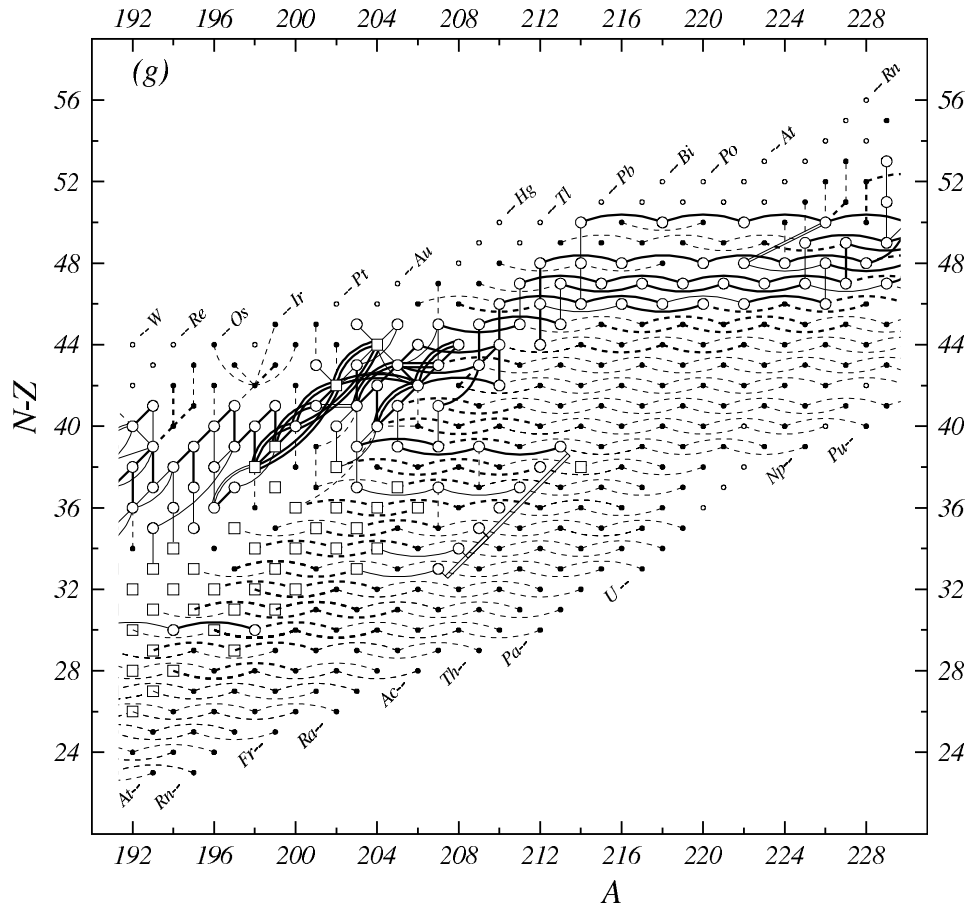


Figure 1 (g). Diagram of connections for input data — continued.

next section.

Some care should be taken in interpreting Fig. 1, since excited isomeric states and data relations involving such isomers are not completely represented on these drawings. This is not considered a serious defect; those readers who want to update such values should, anyhow, consult Table I which gives all the relevant information.

4. Regularity of the mass-surface and use of systematic trends

When nuclear 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 between as represented in Fig. 2. The vertical distances from

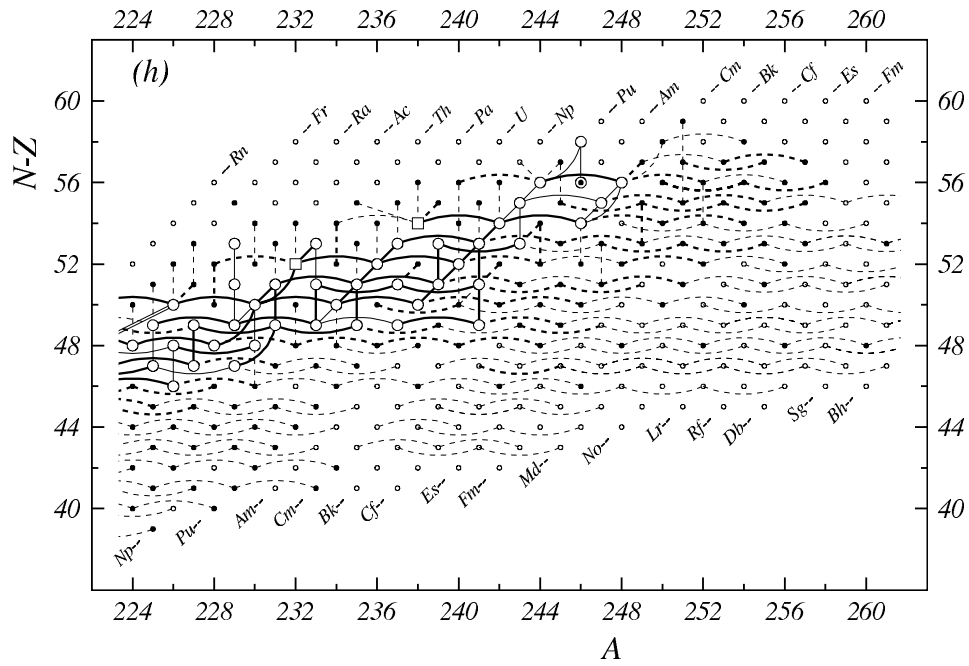


Figure 1 (h). Diagram of connections for input data — continued.

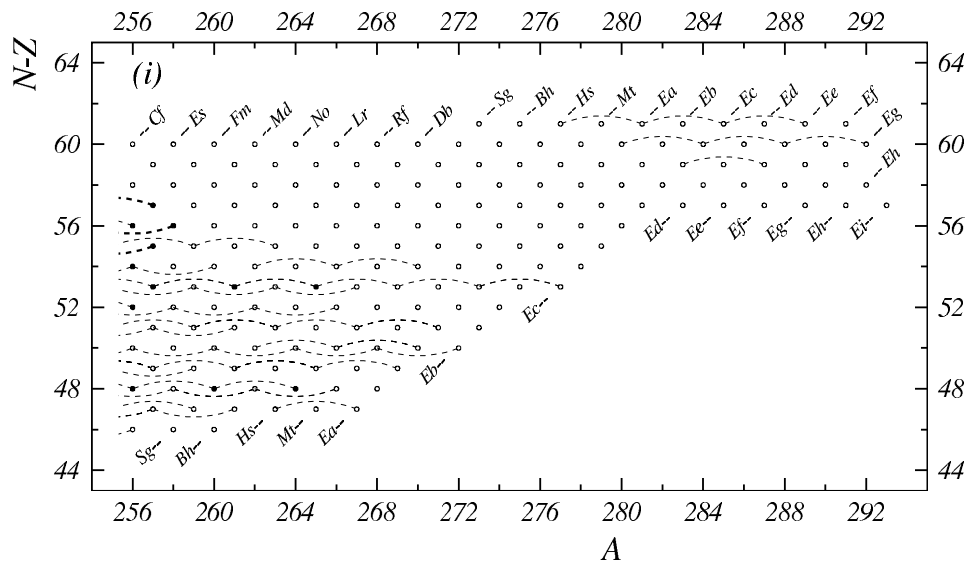


Figure 1 (i). Diagram of connections for input data — continued.

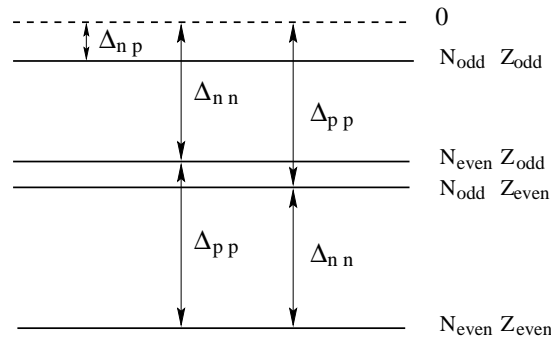


Figure 2: The surface of masses is split into four sheets. This scheme represents the pairing energies responsible for this splitting. The zero energy surface is a purely hypothetical one for no pairing at all among the last nucleons.

the even-even sheet to the odd-even and even-odd ones are the proton and neutron pairing energies Δ_{pp} and Δ_{nn} . They 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 Δ_{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 energy zero 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 Δ_{nn} , Δ_{pp} and Δ_{np} vary smoothly and slowly with N and Z ; and that each of the mass sheets varies smoothly also, but rapidly [13] with N and Z . The smoothness is also observed for first order derivatives (slopes, e.g. the graphs in Part II) 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 no change in the physics of the nucleus are known to exist, 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 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 regularity, in a region (N, Z) of some extent, could be considered as an indication that some new physical property is being discovered. However, if one single mass violates the systematic trends, then

one may seriously question the correctness of the related datum. There might be, for example, some undetected systematic [27] contribution to the reported result of the experiment measuring this mass. We then reread the experimental paper with extra care for possible uncertainties, and often ask the authors for further information. This often leads to corrections.

2. There are cases where some experimental data on the mass of a particular nuclide disagree among each other and no particular reason for rejecting one or some of them could be found from studying the involved papers. In such cases, the measure of agreement with the just mentioned 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 as used in our earlier work.
3. There are cases where masses determined from ONLY ONE experiment (or from same experiments) deviate severely from the smooth surface. Such cases are examined closely and are discussed extensively below (Section 4.1).
4. Finally, drawing the mass surface allows to derive estimates for the still unknown masses, either from interpolations or from short extrapolations (see below, Section 4.2).

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 in four sheets, as mentioned above, complicates even more such a representation. There are two ways to still be able to observe with some precision the surface of masses: 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 nuclei. These functions are also smooth and have the advantage of displaying much smaller variations. For a derivative specified in such a way that differences are between nuclides in the same mass sheet, the near parallelism of these leads to an (almost) unique surface for the derivative, allowing thus a single display. Therefore, in order to illustrate the systematic trends of the masses, we found that such estimates could be obtained best in graphs such as α - and β -decay energies and separation energies of two protons and two neutrons. These four derivatives are plotted against N , Z or A in Part II, Figs. 1–36.

However, from the way these four derivatives are built, they give only information within one of the four sheets of the mass surface (e-e, e-o, o-e or e-e; e-o standing for even N and odd Z). When observing 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 various representations are possible (e.g. separately for odd and even nuclei: one-neutron separation energies versus N , one-proton separation energy versus Z , β -decay energy versus A , . . .). We have prepared such graphs that can be obtained from the AMDC web distribution [6].

The method of ‘derivatives’ suffers from involving two masses for each point to be drawn, which means that if one mass is moved then two points are changed in opposite direction, causing confusion in our drawings.

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 much less rapidly, improving thus its observation.

A first and simple approach is the semi-empirical *liquid drop* formula of Bethe and Weizsäcker [28] 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 [13], is to use the results of the calculation of one of the modern models. However, we can use here only those models that provide masses specifically for the spherical part, forcing the nucleus to be un-deformed. The reason is that the models generally describe quite well the shell and sub-shell closures, and to some extent the pairing energies, but not the locations of deformation. If the theoretical deformations were included and not located at exactly the same position as given by the experimental masses, the mass difference surface would show two dislocations for each shape transition. Interpretation of the resulting surface would then be very difficult. In our work, we currently make use of such differences with models. The plots we have prepared can also be retrieved from the AMDC web site [6].

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 [13, 29] that allows 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 of 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 continuity 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 safer; and also the estimation of unknown masses are felt 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, here and in Part II.

Since 1983 and the AME’83 tables [9], estimates are also given for the precision of such data derived from trends in systematics. These precisions are not based on a formalized procedure, but on previous experience with such estimates.

In the case of extrapolation however, the error in the estimated mass will increase with the distance of extrapolation. These errors are obtained by considering several graphs of systematics with a guess on how much the estimated mass may change without the extrapolated surface looking too much distorted. This recipe is unavoidably subjective, but has proven to be efficient through the agreement of these estimates with newly measured masses in the great majority of cases [30].

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 AME’95 [5], 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 in the systematics. There are only 27 such physical quantities (twice less than in AME1993) that were selected, partly, in order to avoid too strongly oscillating plots. Generally, in such a unique mass relation, only one measurement is reported. But sometimes there are two measurements (8 cases) or three (only once) 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 error (for example a misassignment or ignorance of a final level). Taking into account the connecting chains for secondaries (Figs. 1a–1i) 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 this way, those necessary to avoid, as much as possible, confusions in the graphs in Part II. In particular, as happened previously, the plots of α -decay energies of light nuclei (Fig. 18 and 19 in Part II) 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 ones we recommend, in all tables and graphs in this AME2003, 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 the users of our tables. We now only give what we consider the “*best recommended values*”, using, when we felt necessary and as explained above, ‘*values derived from trends in systematics*’. Data not used, following this policy, can be easily located in Table I where they are flagged ‘D’ and always accompanied by a comment explaining in which direction the value has been changed and by which amount.

Such data, as well as the other local irregularities that can be observed in the figures in Part II could be considered as incentive to remeasure the masses of the involved nuclei, preferably by different methods, in order to remove any doubt and possibly point out true irregularities due to physical properties.

The mass evaluators insist that only the most striking irregularities have been replaced by estimates, those that obscure the graphs in Part II. The reader might convince himself, by checking in Figures 3 and 13, Part II, that the mass of ^{112}Te determined from delayed-proton energy measurement with a precision of 150 keV is evidently 300 keV more bound than indicated by experiment.

4.3. Estimates for unknown masses

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

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–1i. 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 systematics; their sum is known. In other cases, the mass differences

between several nuclides ($A+4n, Z+2n$) are known from α -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} 's or Q_α 's.

Also, knowledge of stability or instability against particle emission, or limits on proton or α emission, yield upper or lower limits on the separation energies.

For proton-rich nuclides with $N < Z$, mass estimates can be obtained from charge symmetry. This feature gives a relation between masses of isobars around the one with $N = Z$. In several cases, we make a correction taking care of the Thomas-Ehrman effect [31], which makes proton-unstable nuclides more bound than follows from the above estimate. For very light nuclides, we can use the estimates for this effect found by Comay *et al.* [32]. But, since analysis of the proton-unstable nuclides (see Section 6.3) shows that this effect is decidedly smaller for $A = 100 - 210$, we use a correction decreasing with increasing mass number.

Another often good estimate can be obtained from the observation that masses of nuclidic 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). Use of this relation is attractive since, otherwise than the relation mentioned above, it uses experimental information (i.e. excitation energies of isobaric analogues). The exactness of the IMME has regularly been a matter of discussion. Recently a measurement [2001He29] of the mass of ^{33}Ar has questioned the validity of the IMME at $A = 33$. The measured mass, with an error of about 4 keV, was 18 keV lower than the value following from IMME, with an error of 3 keV. But, a new measurement [33] showed that one of the other mass values entering in this equation was wrong. With the new value, the difference is only 3 keV, thus within errors.

Up to the AME'83, 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 as 'experimental' a quantity that was derived by combination with a calculation. Since AME'93, 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 ^{28}Si and ^{40}Ti , for which the IMME predicts masses with precisions of respectively 24 keV and 22 keV, whereas the experimental masses are known both with 160 keV precision, from double-charge exchange reactions.

Extension of the IMME to higher energy isobaric analogues has been studied by one of the present authors [34]. The validity of the method, however, is made uncertain by possible effects spoiling the relation. In the first place, the strength of some isobaric analogues at high excitation energies is known to be distributed over

several levels with the same spin and parity. Even in cases where this is not known to happen, the possibility of its occurrence introduces an uncertainty in the level energy to be used for this purpose. In the second place, as argued by Thomas and Ehrman [31], particle-unstable levels must be expected to be shifted somewhat.

Recently, information on excitation energies of $T_3 = -T + 1$ isobaric analogue states has become available from measurements on proton emission following β -decays of their $T_3 = -T$ parents. Their authors, in some cases, derived from their results a mass value for the parent nuclide, using a formula derived by Antony *et al.* [35] from a study of known energy differences between isobaric analogues. 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 one of the present authors noticed to have a not negligible influence on the constants in the IMME.

Another possibility is to use a relation proposed by Jänecke [37], as recently done by Axelsson *et al.* [36] in the case of ^{31}Ar . We have in several cases 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 nucleus for which there is any experimental Q -value is connected to the main group of primary nuclei. In addition, the evaluators want to achieve continuity of the mass surface. Therefore an estimated value is included for any nucleus if it is between two experimentally studied nuclei on a line defined by either $Z = \text{constant}$ (isotopes), $N = \text{constant}$ (isotones), $N - Z = \text{constant}$ (isodiaspheres), or, in a few cases $N + Z = \text{constant}$ (isobars). It would have been desirable to give also estimates for all unknown nuclides that are within reach of the present accelerator and mass separator technologies. Unfortunately, such an ensemble is practically 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 masses and estimated ones has the same contour as in the NUBASE2003 evaluation.

5. Calculation Procedures

The atomic mass evaluation is particular when compared to the other evaluations of data [13], in that almost all mass determinations are relative measurements. Even those called ‘absolute mass doublets’ are relative to ^{12}C , ^{35}Cl or ^{37}Cl . Each experimental datum sets a relation in mass or in energy among two (in a few cases, 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–1i, in

Section 3 above, showed 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 to determine their masses straightforwardly.

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 will allow 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 2, 3 or 4 masses with unknown values m_μ . An overdetermined system of Q data to M masses ($Q > M$) can be represented by a system of Q linear equations with M parameters:

$$\sum_{\mu=1}^M k_i^\mu m_\mu = q_i \pm dq_i \quad (1)$$

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

$$m_A + m_a - m_b - m_B = q_i \pm dq_i \quad (2)$$

thus, $k_i^A = +1$, $k_i^a = +1$, $k_i^B = -1$ and $k_i^b = -1$.

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

We define the diagonal weight matrix \mathbf{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:

$${}^t\mathbf{KWK}|m\rangle = {}^t\mathbf{KW}|q\rangle \quad (3)$$

the NORMAL matrix $\mathbf{A} = {}^t\mathbf{KWK}$ is a square matrix of order M , positive-definite, symmetric and regular and hence invertible [38]. Thus the vector $|\bar{m}\rangle$ for the adjusted masses is:

$$|\bar{m}\rangle = \mathbf{A}^{-1} {}^t\mathbf{KW}|q\rangle \quad \text{or} \quad |\bar{m}\rangle = \mathbf{R}|q\rangle \quad (4)$$

The rectangular (M, Q) matrix \mathbf{R} is called the RESPONSE matrix.

The diagonal elements of \mathbf{A}^{-1} are the squared errors on the adjusted masses, and the non-diagonal ones $(a^{-1})_\mu^\nu$ are the coefficients for the correlations between masses m_μ and m_ν . Values for correlation coefficients for the most precise nuclides are given in Table B of Part II.

One of the most powerful tools in the least-squares calculation described above is the flow-of-information matrix. 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 \mathbf{F} is defined as follows: \mathbf{K} , the matrix of coefficients, is a rectangular (Q, M) matrix, the transpose of the response matrix ${}^t\mathbf{R}$ is also a (Q, M) rectangular one. The (i, μ) element of \mathbf{F} is defined as the product of the corresponding elements of ${}^t\mathbf{R}$ and of \mathbf{K} . In reference [39] it is demonstrated that such an element represents the “*influence*” of datum i on parameter (mass) m_μ . A column of \mathbf{F} thus represents all the contributions brought by all data to a given mass m_μ , 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 [39] 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 on the input one, which is the recipe that was 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:

$$|\bar{q}\rangle = \mathbf{KR}|q\rangle. \quad (5)$$

The i^{th} diagonal element of \mathbf{KR} represents then the contribution of datum i to the determination of \bar{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_μ .

The flow-of-information matrix cannot be given in full in a table. It can be observed along lines, displaying then for each datum which are the nuclei 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 ‘Sig’ for the *significance* of primary data and ‘Main flux’ for the largest *influence*. Since in the large majority of cases only two nuclei 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 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 over-determined ($Q \gg M$) 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 importantly 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 errors 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 \bar{q}_i and input q_i data (cf. Eq. 5), $v_i = (\bar{q}_i - q_i)/dq_i$, would be distributed as a gaussian function of standard deviation $\sigma = 1$, and would make χ^2 :

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

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

One can define as above the NORMALIZED CHI, χ_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, χ_n^p , defined for a (homogeneous) group of p data as:

$$\chi_n^p = \sqrt{\frac{Q}{Q - M} \frac{1}{p} \sum_{i=1}^p v_i^2}. \quad (7)$$

Of course the definition is such that χ_n^p reduces to χ_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 χ_n^p of each of them. There are presently 181 groups of data in Table I, identified in column ‘Lab’. A high value of χ_n^p might be a warning on the validity of the considered group of data within the reported errors. 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 cases 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. We can thus redefine more precisely what was called *secondary* in Section 3: the parameter above is a *secondary* parameter (or mass) and its related equation a *secondary* equation. After solving the reduced set, the *secondary* equation can be used to find value and error for that *secondary* parameter. The equations and parameters remaining after taking out all secondaries are called *primary*.

Therefore, only the system of *primary* data is overdetermined and will thus be improved in the adjustment, each *primary* nuclide getting benefit from all the available information. *Secondary* data will remain unchanged; they do not contribute to χ^2 .

The diagrams in Fig. 1 show, that many *secondary* data exist. Thus, taking them out simplifies considerably the system. More important though, if a better value is found for a *secondary* datum, the mass of the *secondary* nuclide can easily be improved (one has only to watch 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 too. Degree 1 is for primary nuclides and data. Degrees for secondary nuclides and data range from 2 to 14. In Table I, the degree of data is indicated in column ‘Dg’. In the table of atomic masses (Part II, Table I), each *secondary* nuclide is marked with a label in column ‘Orig.’ indicating from which other nuclide its mass value is calculated.

Separating secondary nuclides and data from primaries allow to reduce importantly 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 allowing any loss of 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 special treatment below. The labels *primary* and *secondary* are not intrinsic properties of data or nuclides. They may change from primary to secondary or reversely 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 error, reducing thus the system of equations to be treated. 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 the rare cases where the precision is comparable to the precision in the masses of the reaction particles. Example: ${}^9\text{Be}(\gamma, n){}^8\text{Be}$, ${}^9\text{Be}(p, d){}^8\text{Be}$, ${}^9\text{Be}(d, t){}^8\text{Be}$ and ${}^9\text{Be}({}^3\text{He}, \alpha){}^8\text{Be}$.

Such data are represented together, in the main least-squares calculation, 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, or normalized χ) $\chi_n = \sqrt{\chi^2/(Q-1)}$ resulting in the calculation of the pre-average is greater than 2.5, the (internal) error σ_i in the average is multiplied by the Birge ratio ($\sigma_e = \sigma_i \times \chi_n$). There are 6 cases where $\chi_n > 2.5$, see Table C. The quantity σ_e is often called the ‘external’ error. However, this treatment is not used in the very rare cases where the errors in the values to be averaged differ too much from one another, since the assigned errors lose any significance (only one case, see Table C.) In such cases, considering policies from the Particle Data Group [40] and some possibilities reviewed by Rajput and MacMahon [41], we there adopt an arithmetic average and the dispersion of values as error which is equivalent to assigning to each of these conflicting data the same error.

As much as 25% of the 1224 cases have values of χ_n (Birge ratio) beyond unity, 2.8% beyond two, 0.2% (2 cases) beyond 3, giving an overall very satisfactory distribution for our treatment. With the choice above of a threshold of $\chi_n^0 = 2.5$ for the Birge ratio, only 0.4% of the cases are concerned by the multiplication by χ_n . As a matter of fact, in a complex system like the one here, many values of χ_n beyond 1 or 2 are expected to exist, and if errors were multiplied by χ_n in all these cases, the χ^2 -test on the total adjustment would have been invalidated. This explains the choice we made here of a rather high threshold ($\chi_n^0 = 2.5$), compared e.g. to $\chi_n^0 = 2$ recommended by Woods and Munster [42] or $\chi_n^0 = 1$ used in a different context

Table C. Worst pre-averagings. n is the number of data in the pre-average.

Item	n	χ_n	σ_e	Item	n	χ_n	σ_e	
$^{115}\text{Cd}(\beta^-)^{115}\text{In}$	3	3.61	6.5	$^{146}\text{Ba}(\beta^-)^{146}\text{La}$	2	2.24	107	
$^{149}\text{Pm}(\beta^-)^{149}\text{Sm}$	2	3.54	5.4	$^{154}\text{Eu}(\beta^-)^{154}\text{Gd}$	2	2.22	4.0	
$^{35}\text{S}(\beta^-)^{35}\text{Cl}$	*	9	3.07	0.06	$^{202}\text{Au}(\beta^-)^{202}\text{Hg}$	2	2.22	400
$^{117}\text{La}(\text{p})^{116}\text{Ba}$	2	2.97	12	$^{40}\text{Cl}(\beta^-)^{40}\text{Ar}$	2	2.21	76	
$^{249}\text{Bk}(\alpha)^{245}\text{Am}$	2	2.55	2.4	$^{36}\text{S}(^{14}\text{C}, ^{17}\text{O})^{33}\text{Si}$	3	2.16	37	
$^{76}\text{Ge}(^{14}\text{C}, ^{16}\text{O})^{74}\text{Zn}$	2	2.53	51	$^{153}\text{Gd}(\text{n}, \gamma)^{154}\text{Gd}$	2	2.16	0.39	
$^{186}\text{Re}(\beta^-)^{186}\text{Os}$	4	2.45	2.5	$^{36}\text{S}(^{11}\text{B}, ^{13}\text{N})^{34}\text{Si}$	3	2.13	32	
$^{144}\text{Ce}(\beta^-)^{144}\text{Pr}$	2	2.44	2.2	$^{58}\text{Fe}(\text{t}, \text{p})^{60}\text{Fe}$	4	2.13	7.8	
$^{146}\text{La}(\beta^-)^{146}\text{Ce}$	2	2.42	129	$^{113}\text{Cs}(\text{p})^{112}\text{Xe}$	3	2.11	5.8	
$^{33}\text{S}(\text{p}, \gamma)^{34}\text{Cl}$	3	2.38	0.33	$^{32}\text{S}(\text{n}, \gamma)^{33}\text{S}$	2	2.11	0.065	
$^{220}\text{Fr}(\alpha)^{216}\text{At}$	2	2.34	4.7	$^{223}\text{Pa}(\alpha)^{219}\text{Ac}$	2	2.09	10	
$^{69}\text{Co}-\text{C}_{5.75}$	2	2.33	840	$^{177}\text{Pt}(\alpha)^{173}\text{Os}$	2	2.06	6.1	
$^{136}\text{I}^m(\beta^-)^{136}\text{Xe}$	2	2.33	266	$^{147}\text{La}(\beta^-)^{147}\text{Ce}$	2	2.04	81	
$^{176}\text{Au}(\alpha)^{172}\text{Ir}$	2	2.31	18	$^{244}\text{Cf}(\alpha)^{240}\text{Cm}$	2	2.03	4.0	
$^{131}\text{Sn}(\beta^-)^{131}\text{Sb}$	2	2.29	28	$^{204}\text{Tl}(\beta^-)^{204}\text{Pb}$	2	2.03	0.39	
$^{110}\text{In}(\beta^+)^{110}\text{Cd}$	3	2.29	28	$^{166}\text{Re}^m(\alpha)^{162}\text{Ta}$	2	2.01	17	
$^{178}\text{Pt}(\alpha)^{174}\text{Os}$	2	2.25	6.3	$^{168}\text{Ir}^m(\alpha)^{164}\text{Re}^m$	2	2.00	10	
$^{166}\text{Os}(\alpha)^{162}\text{W}$	2	2.24	10					

*arithmetic average and dispersion of values are being used in the adjustment.

by the Particle Data Group [40], for departing from the rule of internal error of the weighted average.

Used policies in treating parallel data

In averaging β - (or α -) decay energies derived from branches, found in the same experiment, to or from different levels in the decay of a given nuclide, the error we use for the average is not the one resulting from the least-squares, but the smallest occurring one.

Some quantities have been reported more than once by the same group. If the results are obtained by the same method and all published in regular refereed journals, only the most recent one is used in the calculation, unless explicitly mentioned otherwise. The reason is that one is inclined to expect that authors who believe their two results are of the same quality would have averaged them in their latest publication. Our policy is different if the newer result is not published in a regular refereed paper (abstract, preprint, private communication, conference, thesis or annual report), then the older one is used in the calculation, except if the newer is an update of the values in the other. In the latter case the original reference in our list mentions the unrefereed paper.

5.4.2 Replacement procedure

Large contributions to χ^2 have been known to be caused by a nuclide G connected to two other ones H and K by reaction links with errors large compared to the error in the mass difference of H and K , in cases where the two disagreed. Evidently, contributions to χ^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 then takes care both of giving the most reasonable mass value for G , and of not causing undesirably large contributions to χ^2 .

5.4.3 Insignificant data

Another feature to increase the meaning of the final χ^2 is, that data with weights at least a factor 10 less than other data, or than combinations of *all* other data giving the same result, have not been included, generally speaking, in the calculation. They are given in the list of input data (except for most older data of this type that already appeared in our previous tables), but labelled ‘U’; comparison with the output values allows to check our judgment. Earlier, data were labelled ‘U’ if their weight was 10 times less than that of a *simple* combination of other data. This concept has been extended since AME’93 to data that weigh 10 times less than the combination of *all* other accepted data.

5.5. Used policies - treatment of undependable data

The important interdependence of most data, as illustrated by the connection diagrams (Figs. 1a–1i) allows local and general consistency tests. These can indicate that something may be wrong with input values. We follow the policy of checking all significant data differing by more than two (sometimes 1.5) standard deviations from the adjusted values. Fairly often, study of the experimental paper shows that a correction is necessary. Possible reasons are that a transition 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 has been shown to be incorrect. In such cases, the values are corrected and remarks are added below the corresponding data in Table I to explain the reasons for the corrections.

It can also happen, though, that study of the paper leads to serious doubts about the validity of the results within the reported error, but could not permit making a specific correction. In that case, the result is labelled ‘F’ and not used in the adjustment. It is however given in Table I and compared to the adjusted value. The reader might observe that, in several cases, the difference between the experimental value and the adjusted one is small compared to the experimental error: this does not disprove the correctness of the label ‘F’ assignment.

Cases where reading the paper does not lead to correction or rejection, but yet the result is not trusted within the given error, are labelled ‘B’ if published in a regular refereed journal, or ‘C’ otherwise.

Data with labels ‘F’, ‘B’ or ‘C’ are not used in the calculation. 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 thorough analysis of strongly conflicting data could not lead to reasons to think that one of them is more dependable than the others or could not lead to the rejection of a particular piece of data. Also, bad agreement with other data is not the only reason for doubt in the correctness of reported data. As in previous work, and as explained above (see Section 4), we made use of the property of regularity of the surface of masses for helping making a choice and also for making 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 χ^2 s and the distribution of the v_i (see below), . . .

5.7. Results of the calculation

In this evaluation we have 7773 experimental data of which 1230 are labelled U (see above) and 374 are not accepted and labelled B, C, D or F (respectively 207, 58, 37 and 72 items). In the calculation we have thus 6169 valid input data, compressed to 4373 in the pre-averaging procedure. Separating secondary data, leaves a system of 1381 primary data, representing 967 primary reactions and decays, and 414 primary

mass spectrometric measurements. To these are added 887 data estimated from systematic trends, some of which are essential for linking unconnected experimental data to the network of experimentally known masses (see Figs. 1a–1i).

In the atomic mass table (Part II, Table I) there is a total of 3504 masses (including ^{12}C) of which 3179 are ground-state masses (2228 experimental masses and 951 estimated ones), and 325 are excited isomers (201 experimental and 122 estimated). Among the 2228 experimental masses, 192 nuclides have a precision better than 1 keV and 1020 better than 10 keV. There are 231 nuclides known with a precision below 100 keV. Separating secondary masses in the ensemble of 3504, leaves 847 primary masses (^{12}C not included).

We have thus to solve a system of 1381 equations with 847 parameters. Thus, theoretically, the expectation value for χ^2 should be 534 ± 33 (and the theoretical $\chi_n = 1 \pm 0.031$).

The total χ^2 of the adjustment is actually 814; this means that, in the average, the errors in the input values have been underestimated by 23%, a still acceptable result. In other words, the experimentalists measuring masses were, on average, too optimistic by 23%. The distribution of the v_i 's (the individual contributions to χ^2 , as defined in Eq. 6, and given in Table I) is also acceptable, with 15% of the cases beyond unity, 3.2% beyond two, and 8 items (0.007%) beyond 3.

Considering separately the two main classes of data, the partial consistency factors χ_n^p are respectively 1.269 and 1.160 for energy measurements and for mass spectrometry data, showing that both types of input data are responsible for the underestimated error of 23% mentioned above, with a better result for mass spectrometry data.

As in the preceding work [4], we have tried to estimate the average accuracy for 181 groups of data related to a given laboratory and with a given method of measurement, by calculating their partial consistency factors χ_n^p (cf. Section 5.2). On the average the experimental errors appear to be slightly underestimated, with as much as 57% (instead of expected 33%) of the groups of data having χ_n^p larger than unity. Agreeing better with statistics, 5.5% of these groups are beyond $\chi_n^p = 2$. Fortunately though, the impact of the most deviating groups on the final results of our evaluation is reasonably low.

6. Discussion of the input data

Mostly we accept values as given by authors; but in some cases, we must deviate. An example is for recalibration due to change in the definition of the volt, as discussed in Section 2. For somewhat less simple cases, a remark is added.

A curious example of combinations of data that cannot be accepted without change follows from the measurements of the Edinburgh-Argonne group. They report decay energies in α -decay series, where the ancestors are isomers between

which the excitation energy is accurately known from their proton-decay energies. These authors give values for the excitation energies between isomeric daughter pairs with considerably smaller errors than follow from the errors quoted for the measured α -decay energies. The evident reason is, that these decay energies are correlated; this means that the errors in their differences are relatively small. Unfortunately, the presented data do not allow an exact calculation of both masses and isomeric excitation energies. This would have required that, instead of the two E_α values of an isomeric pair, they would have given the error in their difference (and, perhaps, a more exact value for the most accurate E_α of the pair). Instead, entering all their Q_α and E_1 (isomeric excitation energies) values in our input file would yield outputs with too small errors. And accepting any partial collection makes some errors rather drastically too large. We therefore do enter here a selection of input values, but sometimes slightly changed, chosen in such a way that our adjusted Q_α and E_1 values and errors differ as little as possible from those given by the authors. A further complication could occur if some of the Q_α 's are also measured by other groups. But until now, we found no serious troubles in such cases.

Necessary corrections to recent mass spectrometric data are mentioned in Section 6.2.

A change in errors, not values, is caused by the fact explained below that in several cases we do not necessarily accept reported α -energies as belonging to transitions between ground-states. This also causes errors in derived proton decay energies to deviate from those reported by some authors (e.g. in the α -decay chain of ^{166}Ir).

6.1. Improvements along the backbone

Rather few new measurements of stable species with a classical mass spectrometer have become available; all of them of the Winnipeg group.

Most of the new mass spectrometric data were obtained by precision measurements of ratios of cyclotron frequencies of ions in Penning traps. Similarly to the classical measurements of ratios of voltages or resistances, we found that they can be converted to linear combinations in μu of masses of electrically neutral atoms, without any loss of accuracy. In such cases, we added a remark, to the equation used in the table of input data (Table I), to describe the original data. Other groups give their results directly as masses, a not recommended practice for high precision measurements.

The new mass values for ^1H and ^2D have errors about one third of the ones in our previous evaluation, due to new Penning trap measurements. Their values in mass units differ less from the earlier ones [5] than the errors then adopted (in eV_{90} they differ somewhat more). But, for ^4He new evidence showed that measurements used in the previous evaluation were less dependable than thought: the difference in the mass values in mass units is some 4 times the error assigned in 1995 [5]. The new

values are thought more dependable: two new measurements agree. For this reason, we also now replace the old Penning ^3He measurement by one of the two groups mentioned, even though its claimed precision is rather smaller. The new Penning results are tested too by making a separate least square analysis of 30 relations, derived from recent Penning trap results, between H, D, T, ^3He , ^{12}C , ^{13}C , ^{14}N , ^{15}N , ^{16}O , ^{20}Ne and ^{40}Ar . The result was quite satisfactory: the resulting consistency factor is $\chi_n = 1.01$.

In earlier evaluations we found it necessary to multiply errors in values from some groups of mass spectrometric data with discrete factors ($F = 1.5, 2.5$ or 4.0) following the partial consistency factors χ_n^p we found for these groups (see Section 5.2). The just mentioned result was a reason not to do so (that means $F = 1$) for the Penning trap measurements.

The new Penning trap measurements on ^{20}Ne , ^{22}Ne , ^{23}Na and ^{24}Mg agree nicely with earlier precision reaction energies. Their combination with the precision ^{28}Si result, already used in AME95, causes some difficulties, not solved completely by the new Penning ^{26}Mg result, see Section 7.2, Table C.

A somewhat similar problem occurred between ^{35}Cl and ^{40}Ar . It was partly solved by a new Penning trap measurement on ^{36}Ar , see Section 7.4. And a somewhat analogous problem in the connection between lighter Xe isotopes and ^{133}Cs could be solved in a similar way. We note, in connection with the note above on this problem, that the new Penning trap measurements find ^{133}Cs 5 keV less stable than the AME95 value to which a 3 keV error was assigned (see Section 7.5).

Satisfactory new measurements, finally, were made of masses of stable Hg isotopes. As we discuss below (Section 7.1), these data helped to solve the most difficult problem in our evaluations along the backbone since 1983.

6.2. Mass spectrometry away from β -stability

With ISOLTRAP, a Penning trap connected to the CERN on-line mass separator ISOLDE, atomic masses are determined for nuclides further away from β -stability, from the cyclotron frequencies of their ions captured in the trap. Such a frequency is compared to that of a well know calibrator to yield a ratio of the two masses. This ratio is converted, without loss of accuracy, in a linear relation between the two masses. Methods which are relying on cyclotron frequency measurements have the advantage that, roughly speaking, only one parameter has to be measured, namely a frequency, that is the physical quantity that can be measured the best with high accuracy. Very high resolving power ($10^8/A$) and accuracies (recently improved up to 2×10^{-8}) are achieved up till quite far from the line of β -stability. Such high resolving power made it possible, for the first time in the history of mass-spectrometry, to resolve nuclear isomers from their ground-state ($^{84}\text{Rb}^m$) and to determine their excitation energies,

as beautifully just demonstrated [2003Gu.A] for ^{70}Cu , $^{70}\text{Cu}^m$ and $^{70}\text{Cu}^n$. Their measured excitation energies have been confirmed by $\beta\gamma$ spectroscopy [2003Va.2]. Already in the 1993 evaluation ISOLTRAP data were used. The number of such data is now considerably larger and the precision improved by one order of magnitude, due to careful study of the apparatus and calibration obtained with the absolute calibrator ^{12}C from a carbon cluster source allowing to cover the whole atomic mass range. Typically, the precision can reach 1 keV or better (0.3 keV for ^{18}Ne). One of the most exotic nuclides, ^{74}Rb (65 ms), is even reported with a precision of 4 keV.

Far from stability, the 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 ISOLTRAP 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 Table I, the relevant equations are normalized to make the coefficient of the middle isotope unity, so that they read e.g.

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

(the isotope symbol representing the mass excess in keV). The other two coefficients are three-digit approximations of

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

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 unimportant.

Most of the mass-triplet data, performed in the 80's are now outweighed, except for the most exotic (and thus the most interesting) Francium and neutron-rich Rubidium and Cesium isotopes.

The Orsay Smith-type mass spectrometer MISTRAL, also connected to ISOLDE, has performed quite precise measurements of very short-lived light nuclides. In particular, the mass of ^{11}Li (8.75 ms) is already given in our tables with a precision of 28 keV, and a new measurement (under analysis) should reduce this to about 10 keV. Also, the highly accurate results (5×10^{-7}) for ^{30}Na and ^{33}Mg provide important calibration masses for the more exotic nuclides measured by 'time-of-flight' techniques (see discussion below).

Mass measurements by time-of-flight mass spectrometry technique at SPEG (GANIL) and TOFI (Los Alamos), also apply to very short nuclides, but the precision is here lower. Masses of almost undecelerated fragment products, coming from thin targets bombarded with heavy ions [43] or high energy protons [44] are

measured from a combination of magnetic deflection and time of flight determination. Nuclei in an extended region in A/Z and Z are analyzed simultaneously. Each individual ion, even if very short-lived ($1\mu\text{s}$), is identified and has its mass measured at the same time. In this way, mass values with accuracies of (3×10^{-6} to 5×10^{-5}) are obtained for a large number of neutron-rich nuclides of light elements, up to $A = 70$. A difficulty is that the obtained value applies to an isomeric mixture where all isomers with half-lives of the order of, or longer than the time of flight (about $1\mu\text{s}$) may contribute. The resolving power, around 10^4 , and cross-contaminations can cause significant shifts in masses. The most critical part in these experiments is calibration, since obtained 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 and allow a re-analysis of the concerned data, on a firmer basis. Such recalibrations require analysis of the raw data and cannot be done by the evaluators. With new data from other methods allowing now comparison, we observed strong discrepancies for one of the two groups, and had to increase thus the associated partial consistency factor to $F = 1.5$. We noted already earlier that important differences occurred between ensemble of results within this group of data. Using $F = 1.5$ for data labeled ‘TO1-TO6’ in the ‘Lab’ column of Table I, allows to recover consistency.

Longer time-of-flights (50 to 100 μs), thus higher resolving powers, can be obtained with cyclotrons. The accelerating radio-frequency is taken as reference to ensure a precise time determination, but this method implies that the number of turns of the ions inside the cyclotron, should be known exactly. This was achieved successfully at SARA-Grenoble for the mass of ^{80}Y . More recently, measurements performed at GANIL with the CSS2 cyclotron, could not determine the exact number of turns. In a first experiment on ^{100}Sn , a careful simulation was done instead. In a second experiment on ^{68}Se , ^{76}Sr , ^{80}Sr and ^{80}Y , a mean value of the number of turns was experimentally determined for the most abundant species only, thus mainly the calibrants. Recent Penning traps measurements on ^{68}Se (CPT-Argonne) and ^{76}Sr (ISOLTRAP) revealed that this last method suffered serious systematic errors. Also, the measured ^{80}Y mass not only deviates from that of SARA by 10σ , but also contradicts the lower limit set by a recent Q_β measurement at Yale (see [30] for a detailed analysis). For these reasons, results from this second GANIL experiment are not used in our set of data for adjustment.

Atomic masses of nuclides up to rather far removed from stability have recently been determined from their orbital frequency in a storage ring (ESR at GSI), with precisions sometimes as good as a few tens of keV. Many of the measured nuclides belong to known α -decay chains. Thus, the available information on masses of, especially, 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 cannot be accepted without changes. The reason is that, in their derivation, α -decay energies between two, or more, of the occurring nuclides have been used. Evidently, they can therefore not without correction be included in our calculations, where they are again combined with these Q_α 's. Remarks added to the data in Table I warn for this matter where important. This point is added here to show a kind of difficulty we meet more often in this work. Fortunately, for this group of data it is only of historical interest since all their data are outdated by more recent measurements [2003Li.A] with the same instruments and with a much better precision.

As said above, many ESR results in [2003Li.A] yield an average mass value M_{exp} for a mixture of isomers. We here use our new treatment for the possible mixture of isomers (see Appendix B), and take care to mention such changes duly in remarks added to these data.

The mass M_0 of the ground-state can be calculated if both the excitation energy E_1 of the upper isomer, and the relative intensities of the isomers are known. But often this is not the case. If E_1 is known but not the intensity ratio, one must assume equal probabilities for all possible relative intensities. In the case of one excited isomer, see Appendix B.4, the mass estimate for M_0 becomes $M_{exp} - E_1/2$, and the part of the error due to this uncertainty $0.29E_1$ (see Section B.4). This policy was discussed with the authors of the measurements. In eight cases, more than two isomers contribute to the measured line. They are treated as indicated in Appendix B.

A further complication arises if E_1 is not known. This, in addition with some problems connected with α -decay chains involving isomers, was a reason for us to consider the matter of isomers with considerably more care than we did before. Part of the results of our estimates (as always, flagged with '#') are incorporated in the NUBASE evaluation. In estimating values E_1 , we first look at experimental data possibly giving lower limits: e.g. is known that one of two isomers decays to the other; or is even known that γ -rays of known energy occur in such decays. If not, we tried interpolation between values E_1 for neighboring nuclides that can be expected to have the same spin 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. Of course, 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 half-life is at least several seconds. But half-lives as given in tables like NUBASE are those for neutral atoms. For naked nuclei the decay of such an isomer cannot occur by electron conversion; their half-lives may therefore be considerably larger. Examples are the reported mass measurements of the 580 ms ^{151}Er isomer at $E_1=2585.5$ keV;

and even of the 103 ms ^{117}Te isomer at $E_1=296.1$ keV.

An interesting result from the new mass-spectrometric measurements is the following. With ISOLTRAP, masses of several more proton-rich nuclides have been determined with a precision of about 15 keV. In combination with α -decay data, good information is obtained for even- Z nuclei between ^{176}Pt and ^{210}Th . These data, combined with Pb α -energies, allow a check on neutron pairing energies in proton-rich Hg and Pb isotopes. The Jensen-Hansen-Jonson [45] estimate is found decidedly better than the earlier formula $12/\sqrt{A}$ MeV.

In some cases, where in principle corrections for isomerism or contaminations should be made, the mass spectrometric data are insignificant. We found it unnecessary then to make the isomer correction; but as a warning, the reference key number is then provided with a label ‘Z’.

6.3. Proton-decays and α -decays

Limits to proton-decay energies may be estimated from half-lives for this kind of decay. Especially interesting are the limits [1999Ja02] for the series of nuclides with $N = Z - 1$ from ^{69}Br to ^{89}Rh . For them, we gave as inputs values for these decay energies, treated as systematic data (see below) but thought especially dependable.

Our 1995 update [5] used some then recent results of measurements of energies of protons emitted in proton decay. Together with many new data, we now possess results for many proton-rich nuclides, from $^{105}_{51}\text{Sb}$ to $^{185}_{83}\text{Bi}$; among them for all intermediary odd- Z nuclides with the exception of only ^{61}Pm and ^{65}Tb . These data are important for two reasons. In the first place, we apply systematics of some quantities (among them proton separation energies) for estimating mass values for nuclides, for which no experimental mass data are available. For this purpose, knowledge of proton separation energies just beyond the proton drip line is quite valuable.

In the second place, the properties of proton decay allow in several cases to measure proton-decay energies from both members of an isomeric pair. In the many cases that both are observed to decay to the ground-state of the daughter, one so derives the excitation energy of the isomer. And these studies even allow to get a fair estimate of the spin-parities of the separate members.

This feature is the more valuable since often for both members α -decay is observed. In a particular case, even a succession of several such decays was found. Their study showed several decays earlier assigned to ground-states to belong in reality to upper isomers. Also, these measurements are found to yield good values for the excitation energies of the isomers among the descendants. We here follow the judgement of the authors, including their judgement about the final levels fed in those α -decays.

Often, though, knowledge of final levels in observed α -decays is not available. We need to discuss what to do then. A systematic investigation we made long ago suggested, that in most cases the excitation energy of the final level must be small. We therefore adopted the policy of accepting the measured E_α as feeding the ground-state but to provide, in such cases, the resulting decay energy with a label (not given in Table I) that takes care that its error is increased to 50 keV.

Our computer program averages data of the same kind and uses only the average, also given in Table I, in the final calculation. Caution is then necessary with these 50 keV additions: they are applied to the relevant averages.

Yet, systematics of α -decay energies, theory, or preferably both, may in some cases suggest a larger E_1 . In such cases, the estimate for this value (provided with a generous error) has been added as input value.

The mentioned results of proton decay analysis have been a reason to omit the mentioned label in several cases. And we also have 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 mother and daughter. Comparison (preferably in combination with theoretical considerations) may here too suggest to drop the mentioned label; or just reversely not to accept a reported α -energy.

In regions where the Nilsson model for deformed nuclides applies, it is expected that the often most intense α -transition feeds a level in the daughter with the same model assignment as the mother. (It is not rarely the only observed α -ray.) In that case, adding an estimate for the E_1 is attractive. And not rarely the energy difference with the ground-state can be estimated by comparison with the energy differences between the corresponding Nilsson levels in nearby nuclides.

Unfortunately, some authors derive a value they call Q_α from a measured α -particle energy by not only correcting for recoil but also for screening by atomic electrons (see Appendix A). In our calculations, the latter corrections have been removed.

Finally, some measured α particle energies are at least partly due to summing with conversion electrons. This is sometimes clear from the observation, that the width of the observed line is larger than that of other ones. In deriving the desired Q_α , it is then necessary to make a small correction for the escaping X-rays. This is again mentioned in remarks added to the items.

6.4. 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 dependent on Z and quite well known [46]. For (non-unique) first forbidden transitions, the ratio is not notably different; with few exceptions.

The neutrino energy mentioned is the difference of the transition energy Q with 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 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 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 program cannot handle them, we have symmetrized the probability distribution by considering the first and second momenta of the real probability distribution (see NUBASE2003, Appendix A). The other problem is related to averaging of several values that are reported for the same ratio. Our policy, since AME'93, is to average the capture ratios, and calculate the decay energy following from that average. In this procedure we used the best values [46] of the proportionality constant. We also recalculated older reported decay energies originally calculated using now obsolete values 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 in a known way (anyhow for allowed and not much delayed first forbidden transitions). Thus, the transition energy can be derived from a measurement of the relative positron feeding of the level, which is often easier than a measurement of the positron spectrum end-point. For several cases we made here the same kind of combinations and corrections as mentioned for capture ratios. But in this case, a special difficulty must be mentioned. Positron decay can only occur when the transition energy exceeds $2m_e c^2 = 1022$ keV. Thus, quite often, a level fed by positrons is also fed by γ -rays coming from higher levels fed by electron capture. Determination of the intensity of this *side* feeding is often difficult. Cases exist where such feeding occurs by a great number of weak γ -rays easily overlooked (the *pandemonium* effect [47]). Then, the reported decay energy may be much lower than the real value. In judging the validity of experimental data, we kept this possibility in our mind.

6.5. Superheavy nuclides

Unfortunately, the names of four elements beyond $Z=103$ as earlier proposed, and that we accepted in our 1995 evaluation [5], were changed. The Commission on Nomenclature of Inorganic Chemistry of the International Union of Pure and Applied Chemistry IUPAC [48] revised its earlier proposal (see also NUBASE2003, Section 2). As a result, following names and symbols are now definitely accepted (names for $Z = 107$ and 109 are not changed):

104	rutherfordium	Rf	replacing	Db
105	dubnium	Db	”	Jl
106	seaborgium	Sg	”	Rf
108	hassium	Hs	”	Hn

In the 1995 evaluation we already included results assigned to elements 110 and 111; and in 1996 [1996Ho13] the discovery was reported of element 112. The discovery of element 118 and its α -descendants 116 and 114 was announced in Berkeley in 1999 [1999Ni03] but was later withdrawn [2002Ni10]. But authors from Dubna reported observation of isotopes of elements 114 and 116. All these reports have not yet been officially accepted as sufficient evidence for the discovery of these elements, except for element 110. A provisional recommendation of the Inorganic Chemistry Division of the International Union of Pure and Applied Chemistry proposes for it the name darmstadtium, symbol Ds. Until this name and this symbol are officially adopted, we will not use them in our evaluations, to avoid a situation similar to the one described above. No names have been proposed to our knowledge for the heavier elements. We use symbols Ea, . . . Ei for elements 110, . . . 118.

No data are available that allow to give any purely experimental mass value for any isotope of the latter elements, in fact for no nuclide with $A > 265$. One of the reasons is, that α -decays in the present region of deformed nuclides preferentially feed levels with the same Nilsson model assignments as the mother, which in the daughter are most often excited states, with unknown excitation energies E_1 . Thus, in order to find the corresponding mass difference, we have to estimate these E_1 's. For somewhat lighter nuclides, one may estimate them, as said above, from known differences in excitation energies for levels with the same Nilsson assignments in other nuclides. But such information is lacking in the region under consideration. In its place, one might consider to use values obtained theoretically [49]. We have not done so, but used their values as a guide-line. Finally, we choose values in such a way that diagrams of α -systematics and mass systematics looked acceptable. Important for this purpose were the experimental α -decay energies for the heaviest isotopes for $Z = 112, 114$ and 116 , especially for the even- A isotopes among them. The errors we assigned to values thus obtained may be somewhat optimistic; but we expect them not to be ridiculous.

In addition to these uncertainties, it must be mentioned that Armbruster [50] gives reasons to doubt the validity of the Dubna results mentioned. We recognize the seriousness of his criticism, but nevertheless decided to accept the Dubna results for the time being. This has a consequence for our mass estimates from systematics for all nuclides with neutron numbers above the probably semi-magic $N = 162$: they depend strongly on the correctness of the Dubna results.

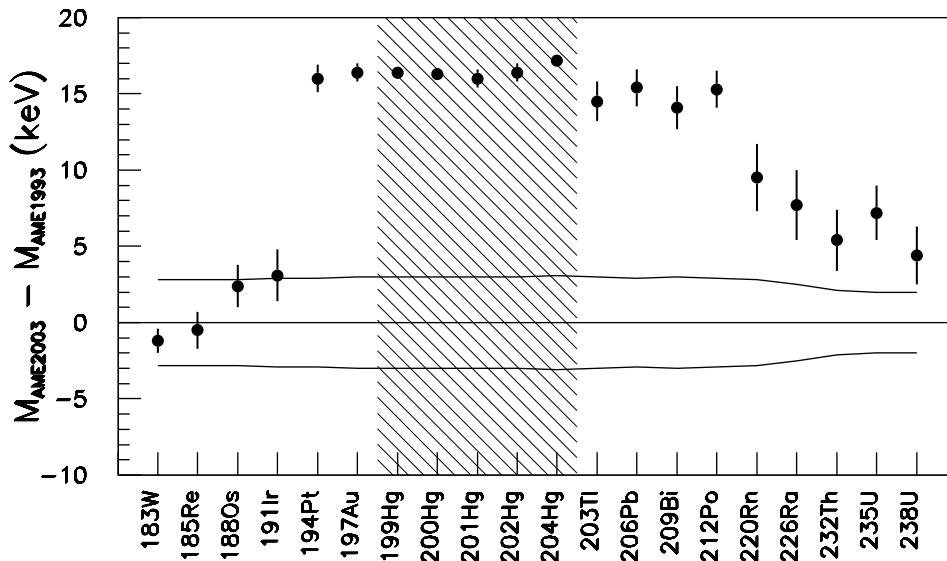


Figure 3: Difference between the mass values obtained in the AME2003 and the AME1993, for nuclides along the line of β -stability around stable Hg's. The errors found in the 1993 evaluation are given by the two lines symmetric around the zero line. Points and error bars refer to the present evaluation.

7. Special cases

7.1. The problem of the stable Hg isotopes

In our earlier evaluations we did not accept the 1980 Winnipeg measurements of the atomic masses of stable Hg isotopes, reported with errors of only about 1 keV. We reconsider the reasons.

In that work [1980Ko25], the mass differences were measured between those Hg isotopes and $^{12}\text{C}_2\text{Cl}_5$ molecules (for $A = 199$ and 201), or $^{12}\text{C}^{13}\text{C}\text{Cl}_5$ ones (for $A = 200, 202$ and 204). The resulting Hg masses values were $22\ \mu\text{u}$ high (odd A) and $17\ \mu\text{u}$ high (even- A), compared with values derived from mass spectrometric results for both lighter and heavier nuclides combined with experimental reaction and decay energies, see Fig. 1 in [9]. The difference suggests an influence on the intensities of the ion beams, since ^{13}C is much less abundant than ^{12}C . Therefore, both sets of results were judged questionable.

Very recently, Winnipeg reported [2003Ba49] a new value for ^{199}Hg , $7\ \mu\text{u}$ lower than their 1980 result. In addition, measurements with the Stockholm SMILETRAP Penning trap spectrometer gave results for ^{198}Hg and ^{204}Hg , essentially agreeing with the 1980 Winnipeg even-mass values. Thus, the latter appear to be reasonable.

We now calculated atomic masses accepting these data, in addition to old and new nuclear reaction and decay results. Fig. 3 shows differences between these results and the values adopted in our previous evaluation AME'95.

The relation with the higher- A mass spectrometric results (Th and U isotopes) is acceptable at present: the new differences nearly equal the old ones but with changed sign. With lower- A , Winnipeg provided further information by new measurements of the mass of ^{183}W and its difference with ^{199}Hg . These essentially confirm the mass values around ^{183}W as given in our earlier evaluations [1, 5]. For completeness, we observe that the new ^{183}W result is $15\ \mu\text{u}$ higher than the 1977 Winnipeg result (error $2.7\ \mu\text{u}$), which was one of the items that helped to suggest the lower Hg masses.

It is therefore significant that Fig. 3 shows a jump between ^{191}Ir and ^{194}Pt . Closer scrutiny, shows that nuclear reaction energies, in the region between these two nuclides, have discrepancies which, as yet, are not resolved. The upshot, though, is that the earlier difficulty in the connection of the Hg's with lower A data appears to be due to errors in the mass spectrometric data then used. We therefore think that the mass values for these Hg isotopes in the present work are definitely more dependable than our earlier ones.

7.2. The masses of ^{26}Al and ^{27}Al

The earlier two results of the $^{25}\text{Mg}(n,\gamma)$ reactions were not in a perfect agreement, neither with one another nor with the combinations of the average of the well agreeing values for $^{25}\text{Mg}(p,\gamma)$ with the two values for $^{26}\text{Mg}(p,n)^{26}\text{Al}$, see Table D. The new Penning trap mass values for ^{24}Mg and ^{26}Mg [2003Be02], combined with the average of the very nicely agreeing values for the $^{24}\text{Mg}(n,\gamma)$ reaction, give a value halfway between the ones just mentioned. This is pleasant but thus it must be concluded that there is an uncertainty in the mass of ^{26}Al . This is unfortunate, especially because of the special interest of the $^{26}\text{Mg}(p,n)^{26}\text{Al}$ reaction for problems connected with the intensity of allowed Fermi β -transitions.

A somewhat similar problem occurs in the connections of ^{27}Al with the nuclides just mentioned and, through the (p,γ) reaction, with ^{28}Si . We found no stringent reasons to trust some of them more than others. Thus the mass value presented here for ^{27}Al is a compromise and its error somewhat optimistic.

7.3. The $^{35}\text{S}(\beta^-)^{35}\text{Cl}$ decay energy

This case has been investigated several times in connection with the report that a neutrino might exist with a mass of 17 keV.

Unfortunately, the reported decay energies are so much different (with a Birge ratio $\chi_n = 3.07$, see Table C, Section 5), that we decided to use all of the nine

Table D. ^{26}Mg neutron binding energies derived in different ways .

Method	S_n	Reference
$^{25}\text{Mg}(n,\gamma)$	11093.10 (0.06)	1990Pr02 Z
$^{25}\text{Mg}(n,\gamma)$	11093.23 (0.05)	1992Wa06 Z
$^{25}\text{Mg}(p,\gamma) - ^{26}\text{Mg}(p,n)$	11092.63 (0.14)	
$^{25}\text{Mg}(p,\gamma) - ^{26}\text{Mg}(p,n)$	11092.36 (0.19)	
$^{24}\text{Mg} - ^{26}\text{Mg} + 2n - ^{24}\text{Mg}(n,\gamma)$	11092.94 (0.05)	2003Be02

available data, irrespective of their claimed precision. Moreover, the most recent, and probably most accurate among the nine $^{35}\text{S}(\beta^-)$ decay-energy values, are all higher than their average. We therefore applied the procedure described in Section 5.4.1 to get an arithmetic average value and error (derived from the dispersion of the 9 data) of 167.222 ± 0.095 keV. In AME'93 we had 7 data with $\chi_n = 3.45$; the situation unfortunately did not improve significantly.

A value $167.19(0.11)$ keV, in good agreement with the above adopted value, can also be derived from the reported reaction energies for the $^{34}\text{S}(n,\gamma)^{35}\text{S}$ and $^{34}\text{S}(p,\gamma)^{35}\text{Cl}$ reactions.

7.4. The masses of $^{35,37}\text{Cl}$ and the new ^{36}Ar mass

The SMILETRAP ^{36}Ar result [2003Fr08] is some 1.2 keV lower than the AME95 value, for which an error of 0.3 keV was claimed. The latter value is, essentially, due to mass spectrometric results for ^{35}Cl and ^{37}Cl , combined with reaction energies for five reactions. These data do agree quite well if combined in a least squares analysis: $\chi_n = 1.13$. Adding the new mass value for ^{36}Ar increases χ_n to 2.00. But this value is reduced to a reasonable 1.35 if, of the two available values for the $^{36}\text{Ar}(n,\gamma)^{37}\text{Ar}$ reaction energy, the oldest not well documented one is no longer used. Also, this removes an earlier hardness in the connection with ^{40}Ar , of which the mass was already known with high precision.

7.5. Consequences of new ^{133}Cs mass

The ^{133}Cs results are important for the determination of masses of many Cs and Ba isotopes: as discussed above. Two new ^{133}Cs mass values have been reported, agreeing well. The resulting ^{133}Cs mass is about 5 keV higher than the AME'95 one, to which an error of 3 keV had been assigned. It was mainly the result of a set of connections, through known Cs β^+ decay energies to Xe nuclides, for which mass

spectrometric mass values were available (see the scheme Fig. 1 in [1]). The nearest ones are those at mass numbers 124, 128, 129, 130 and 132. Analyzing them, we find that the connection with ^{132}Xe would make ^{133}Cs 15(7) keV higher, whereas that with ^{124}Xe , 35(20) keV lower. The first one, thus, is improved by the SMILETRAP result. The other throws some doubt on the reported ^{125}Cs β^+ decay energy. The other connections are not severely affected.

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

What follows is an analysis of α -chains for which also mass-spectrometric mass values are available. It is given as an example; but also because it presents special difficulties.

For ^{159}Lu and ^{163}Ta [2003Li.A] gives mass values with precision 30 keV. The nuclide ^{155}Tm is connected with precision data to nuclides with more accurately known masses. From these mass values one calculates for ^{159}Lu an α -decay energy of 4480(34) keV to the ^{155}Tm ground-state, and 42(5) keV less to its isomer. The experimental value is 4533(7) keV, average of two agreeing measurements, see Table I. The difference suggests that the E_α (two well agreeing measurements) originate in an upper isomer. Let us look critically to the known decay data.

For ^{159}Lu , the half-lives reported for α - and β -decays are not different, not suggesting isomerism.

In order to see a possible consequence of a less stable ^{159}Lu , we examine its α -decay feeding by ^{163}Ta . The mass measurements yield $Q_\alpha = 4652(42)$ keV, to be compared with a rather higher experimental value 4749(6) keV. The difference would even be larger if ^{159}Lu would be less stable!

This quite strongly suggests that the observed ^{163}Ta α 's may originate in a higher isomer. First question: could the half-lives for its α - and β -decays be different? For gamma and X(K) the half-lives is found $T_{1/2} = 11(1)$ s; for α no value. Then, do other $N = 90$ nuclides show isomerism? Yes, but the situations for them seem not comparable. Finally: can we get some information from α ancestors? For $^{179}\text{Tl}(\alpha)^{175}\text{Au}(\alpha)^{171}\text{Ir}(\alpha)^{167}\text{Re}$, [2002Ro17] gives correlations between α branches reported for their isomers. Their analysis suggests that the ^{167}Re isomers must α -decay to different isomers in ^{163}Ta . This induces us to assign the discussed ^{163}Ta α branch to the upper isomer.

This solves part of the problem. For the other part, we label the observed ^{159}Lu Q_α 's with the flag for uncertain assignment (increasing error to 50 keV, see Section 6.3), already because it is unclear which of the two ^{155}Tm isomers is fed. Thus, the main part of the trouble is removed.

7.7. The mass of ^{149}Dy and its α -ancestors

AME95 gives for ^{149}Dy a mass excess of $-67688(11)$ keV. This value was derived with help of [1991Ke11]’s value $Q_{\beta^+} = 3812(10)$ keV for $^{149}\text{Dy}(\beta^+)^{149}\text{Tb}$. But ISOLTRAP finds a 45 keV more bound value, $-67729(18)$ keV [2001Bo59]. And ESR-GSI [2003Fi.A] found mass values for the ^{149}Dy and its α -ancestors ^{157}Yb , ^{161}Hf and ^{165}W that all agreed with the values derived from combining Q_{α} ’s with the ISOLTRAP ^{149}Dy mass. It is not likely that the mentioned Q_{β^+} belongs to an upper ^{149}Dy isomer. And repeated study of the [1991Ke11] paper did not suggest distrust. Therefore we decided just to accept all experimental data mentioned.

7.8. The masses of ^{100}Sn and ^{100}In

The mass of ^{100}In was derived in AME95 from a preliminary result of a GANIL measurement replaced since by a final report, the latter also giving a mass value for ^{100}Sn for which AME95 gave only a value derived from systematics. These results are particularly interesting because of the double magic character of ^{100}Sn which is, moreover, the heaviest known nuclide with $N = Z$. But for both the reported values indicated over 0.5 MeV more stability than in AME’95, and indeed there indicated by systematics. The difference is not really large compared with the claimed precision, yet unpleasant. Therefore it is satisfactory that new measurements of the positron decay energies of these two nuclides indicate indeed higher mass values. The final values are still somewhat low compared with systematics, but no longer seriously so.

8. General informations and acknowledgements

The full content of the present issue is accessible on-line at the web site [6] of the AMDC. In addition, on that site, several local analyses that we conducted but could not give in the printed version, are available. Also, several graphs for representation of the mass surface, beyond the main ones in Part II, can be obtained there.

As before, the table of masses (Part II, Table I) and the table of nuclear reaction and separation energies (Part II, Table III) are made available in plain ASCII format to allow calculations with computer programs using standard languages. The headers of these files give information on the used formats. The first file with name **mass_rmd.mas03** 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_rmd.mas03** for S_{2n} , S_{2p} , Q_{α} , $Q_{2\beta}$, $Q_{\epsilon p}$ and $Q_{\beta n}$ (odd pages in this issue); and **rct2_rmd.mas03** for S_n , S_p , $Q_{4\beta}$, $Q_{d,\alpha}$, $Q_{p,\alpha}$ and $Q_{n,\alpha}$ (facing even pages).

As explained in Section 4.2, we do no more produce special tables in which are included experimental data that we do not recommend to use.

We wish to thank our many colleagues who answered our questions about their experiments and those who sent us preprints of their papers. Special thanks to C. Schwarz and P. Pearson at Elsevier for a particularly good cooperation and reliance in preparing the present publication, resulting in a very short delay between our final calculation and printing. We appreciate the help of C. Gaulard in the preparation of some of the figures of this publication, and of C. Gaulard and D. Lunney for careful reading of the manuscript. One of us (AHW) expresses his gratitude to the NIKHEF-K laboratory for the permission to use their facilities, and especially thanks Mr. K. Huyser for all help with computers.

Appendix A. The meaning of decay energies

Conventionally, the decay energy in an α -decay is defined as the difference in the atomic masses of mother and daughter nuclides:

$$Q_\alpha = M_{\text{mother}} - M_{\text{daughter}} - M_{4\text{He}} \quad (8)$$

This value equals the sum of the observed energy of the α particle and the easily calculated energy 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). Very unfortunately, some authors quote as resulting Q_α a value ‘corrected for screening’, which essentially means that they take for the values M in the above equation the masses of the bare nuclei (the difference is essentially that between the total binding energies of all electrons in the corresponding neutral atoms).

This bad custom is a cause of confusion; even so much that in a certain paper this “correction” was made for some nuclides but not for others.

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

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_{exp} that will be observed in the measurement, and what is the uncertainty σ 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, \dots the masses of the other lines. For a given composition of the mixture, the resulting mass m is given by

$$m = \left(1 - \sum_{i=1}^n x_i\right)M_0 + \sum_{i=1}^n x_i M_i \quad \text{with} \quad \begin{cases} 0 \leq x_i \leq 1 \\ \sum_{i=1}^n x_i \leq 1 \end{cases} \quad (9)$$

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

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

$$\bar{M} = \int P(m) m dm \quad (10)$$

$$\text{and } \sigma^2 = \int P(m) (m - \bar{M})^2 dm \quad (11)$$

It is thus assumed that the experimentally measured mass will be $M_{exp} = \bar{M}$, and that σ , 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

$$m = (1 - x_1)M_0 + x_1 M_1 \quad \text{with} \quad 0 \leq x_1 \leq 1 \quad (12)$$

The relation between m and x_1 is biunivocal so that

$$P(m) = \begin{cases} 1/(M_1 - M_0) & \text{if } M_0 \leq m \leq M_1, \\ 0 & \text{elsewhere} \end{cases} \quad (13)$$

i.e. a rectangular distribution (see Fig. 4a), and one obtains :

$$\begin{aligned} M_{exp} &= \frac{1}{2}(M_0 + M_1) \\ \sigma &= \frac{\sqrt{3}}{6}(M_1 - M_0) = 0.290 (M_1 - M_0) \end{aligned} \quad (14)$$

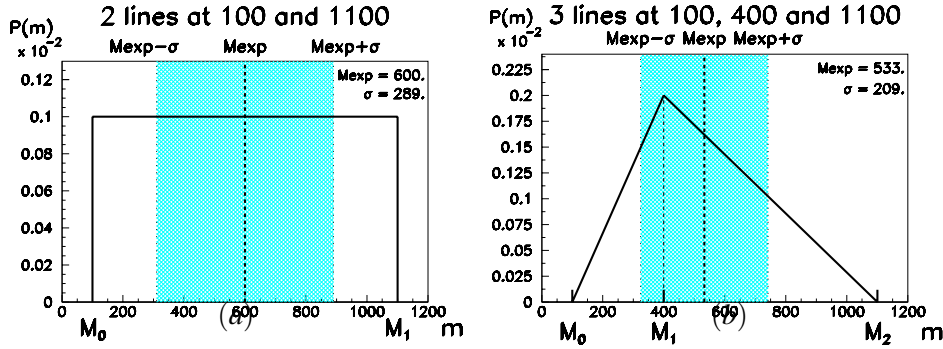


Figure 4: Examples of probabilities to measure m according to an exact calculation in cases of the mixture of two (a) and three (b) spectral lines.

B.2. Case of 3 spectral lines

In the case of three spectral lines, we derive from Eq. 9:

$$m = (1 - x_1 - x_2)M_0 + x_1M_1 + x_2M_2 \quad (15)$$

$$\text{with } \begin{cases} 0 \leq x_1 \leq 1 \\ 0 \leq x_2 \leq 1 \\ 0 \leq x_1 + x_2 \leq 1 \end{cases} \quad (16)$$

The relations (15) and (16) may be represented on a x_2 vs x_1 plot (Fig. 5). The conditions (16) define a triangular authorized domain in which the density of probability is uniform. The equation (15) 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 (16). Since the density of probability is constant along this segment, the probability $P(m)$ is proportional to its length. After normalization, one gets (Fig. 4b):

$$P(m) = \frac{2k}{M_2 - M_0} \quad \text{with } \begin{cases} k = (m - M_0)/(M_1 - M_0) & \text{if } M_0 \leq m \leq M_1 \\ k = (M_2 - m)/(M_2 - M_1) & \text{if } M_1 \leq m \leq M_2 \end{cases} \quad (17)$$

and finally:

$$\begin{aligned} M_{exp} &= \frac{1}{3}(M_0 + M_1 + M_2) \\ \sigma &= \frac{\sqrt{2}}{6} \sqrt{M_0^2 + M_1^2 + M_2^2 - M_0M_1 - M_1M_2 - M_2M_0} \end{aligned} \quad (18)$$

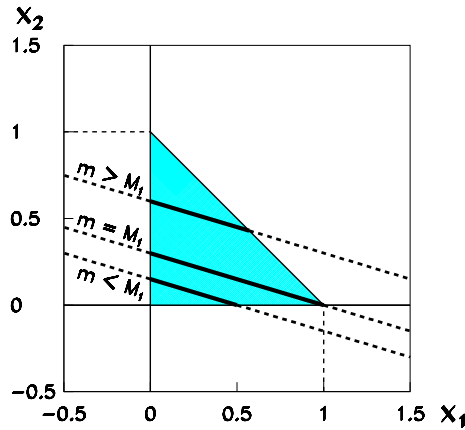


Figure 5: Graphic representation of relations 15 and 16. The length of the segments (full thick lines) inside the triangle are proportional to the probability $P(m)$. Three cases are shown corresponding respectively to $m < M_1$, $m = M_1$, and to $m > M_1$. The maximum of probability is obtained when $m = M_1$.

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 σ 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. 6). Calling $nbin$ the number of bins of the histogram, one gets :

$$\begin{aligned}
 P(m_j) &= \frac{N_j}{\sum_{j=1}^{nbin} N_j} & (19) \\
 M_{exp} &= \sum_{j=1}^{nbin} P(m_j) m_j \\
 \sigma^2 &= \sum_{j=1}^{nbin} P(m_j) (m_j - M_{exp})^2
 \end{aligned}$$

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, \dots 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

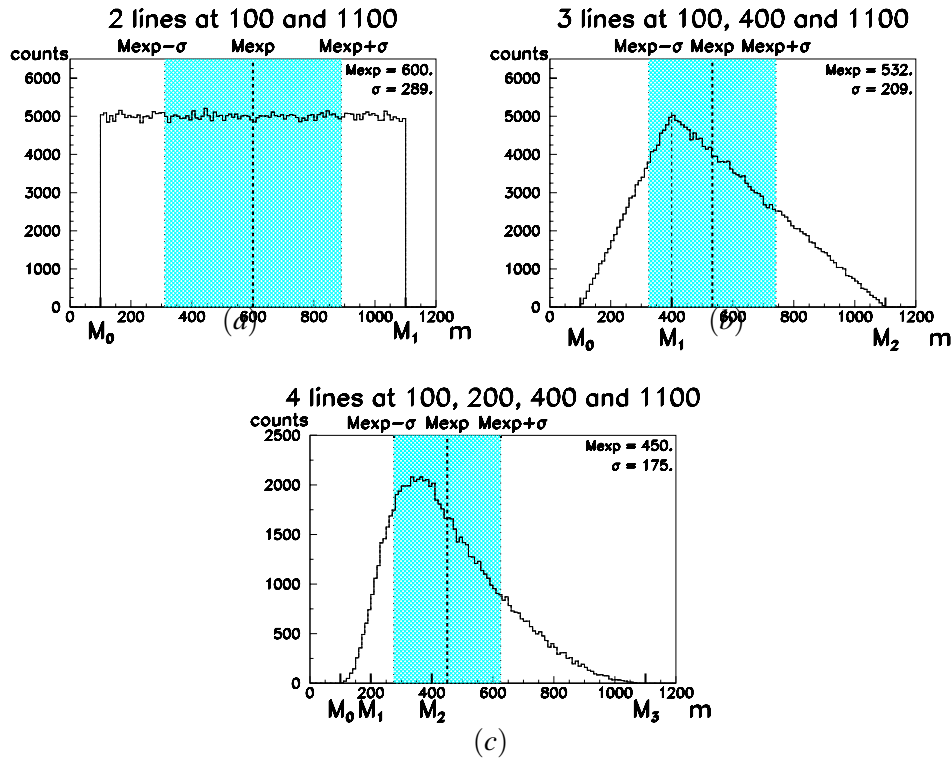


Figure 6: Examples of Monte-Carlo simulations of the probabilities to measure m in cases of two (a), three (b) and four (c) spectral lines.

in Figure 7 for the cases of two, three and four lines. The results are presented in Figure 6.

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. 4a and 6a) and three lines (see Fig. 4b and 6b).

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 $M_{exp} \pm \sigma_{exp}$ and the knowledge of the excitation energies $E_1 \pm \sigma_1, E_2 \pm \sigma_2, \dots$

With the above notation, we have $M_1 = M_0 + E_1, M_2 = M_0 + E_2, \dots$

```

program isomers
-----
c-   October 15, 2003                C.Thibault
c-   Purpose and Methods : MC simulation for isomers (2-4 levels)
c-   Returned value      : mass distribution histograms
-----
      parameter (nwpawc=10000)
      common/pawc/hmemor(nwpawc)
      parameter (ndim=500000)
      dimension xm(3,ndim)
      data e0,e1,e31,e41,e42/100.,1100.,400.,200.,400./
      call hlimit(nwpawc)
c histograms 2, 3, 4 levels
      call hbook1(200,'',120,0.,1200.,0.)
      call hbook1(300,'',120,0.,1200.,0.)
      call hbook1(400,'',120,0.,1200.,0.)
      call hmaxim(200,6500.)
      call hmaxim(300,6500.)
      call hmaxim(400,2500.)
      w=1.
c random numbers [0,1]
      ntot=3*ndim
      iseq=1
      call ranecq(iseed1,iseed2,iseq,' ')
      call ranecu(xm,ntot,iseq)
      do i=1,ndim
c 2 levels :
          t=1-xm(1,i)
          e = t*e0 + xm(1,i)*e1
          call hfill(200,e,0.,w)
c 3 levels :
          if ((xm(1,i)+xm(2,i)).le.1.) then
              t=1.-xm(1,i)-xm(2,i)
              e= t*e0 + xm(1,i)*e31 + xm(2,i)*e1
              call hfill(300,e,0.,w)
          end if
c 4 levels
          if ((xm(1,i)+xm(2,i)+xm(3,i)).le.1.) then
              t=1.-xm(1,i)-xm(2,i)-xm(3,i)
              e = t*e0 + xm(1,i)*e41 + xm(2,i)*e42 + xm(3,i)*e1
              call hfill(400,e,0.,w)
          end if
      end do
      call hrput(0,'isomers.histo','N')
end

```

Figure 7: Fortran program used to produce the histograms of Figure 6.

For a single excited isomer, equations (14) lead to :

$$\begin{aligned} M_0 &= M_{exp} - \frac{1}{2}E_1 \\ \sigma^2 &= \frac{1}{12}E_1^2 \quad \text{or} \quad \sigma = 0.29E_1 \\ \sigma_0^2 &= \sigma_{exp}^2 + \left(\frac{1}{2}\sigma_1\right)^2 + \sigma^2 \end{aligned}$$

For two excited isomers, equations (18) lead to :

$$\begin{aligned} M_0 &= M_{exp} - \frac{1}{3}(E_1 + E_2) \\ \sigma^2 &= \frac{1}{18}(E_1^2 + E_2^2 - E_1E_2) \quad \text{or} \quad \sigma = 0.236\sqrt{E_1^2 + E_2^2 - E_1E_2} \\ \sigma_0^2 &= \sigma_{exp}^2 + \left(\frac{1}{3}\sigma_1\right)^2 + \left(\frac{1}{3}\sigma_2\right)^2 + \sigma^2 \end{aligned}$$

If the levels are regularly spaced, *i.e.* $E_2 = 2E_1$,

$$\sigma = \frac{\sqrt{6}}{12}E_2 = 0.204E_2$$

while for a value of E_1 very near 0 or E_2 ,

$$\sigma = \frac{\sqrt{2}}{6}E_2 = 0.236E_2$$

For three excited isomers , the example shown in Figure 6c leads to:

$$\begin{aligned} M_0 &= M_{exp} - \frac{1}{4}(E_1 + E_2 + E_3) = 450. \\ \sigma &= 175. \\ \sigma_0^2 &= \sigma_{exp}^2 + \left(\frac{1}{4}\sigma_1\right)^2 + \left(\frac{1}{4}\sigma_2\right)^2 + \left(\frac{1}{4}\sigma_3\right)^2 + \sigma^2 \end{aligned}$$

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