Uncertainty evaluation in the estimates of isotopic abundances and atomic weight of any element: a unique application of the theory of uncertainty for derived results

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Abstract

It has been previously shown that any measurement system specific relationship (SSR)/mathematical-model \( Y_d = f_d(\{X_m\}_m^{N}) \) or so is bracketed with certain parameters which should prefix the achievable-accuracy/uncertainty \( (\epsilon_d^Y) \) of a desired result \( y_d \). Here we clarify how the element-specific-expressions of isotopic abundances and/or atomic weight could be parametrically distinguished from one another, and the achievable accuracy \( (\epsilon_d^Y) \) be even a priori predicted. It is thus signified that, irrespective of whether the measurement-uncertainty \( (u_m) \) could be purely random by origin or not, \( \epsilon_d^Y \) should be a systematic parameter.

Further, by property-governing-factors, any SSR should belong to either variable-independent (F.1) or -dependent (F.2) family of SSRs/models. The SSRs here are shown to be the members of the F.2 family. That is, it is pointed out that, and explained why, the uncertainty \( (\epsilon) \) of determining an either isotopic abundance or atomic weight should vary, even for any given measurement-accuracy(s) \( u_m(s) \), as a function of the measurable-variable(s) \( X_m(s) \). However, the required computational-step has been shown to behave as an error-sink in the overall process of indirect measurement in question.

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1. Introduction

The fractional isotopic abundances ($Y_d^{N}_{m=1}$) and atomic weight ($A_E$) of any desired multi ($N$) isotopic element ($E$) are generally determined from the measurable mass spectrometric values of the corresponding “($N-1$)” isotopic-abundance-ratios ($\{X_m = \frac{Y_m}{Y_1} \}_{m=2}$), with $Y_1$ as the highest cum reference isotopic abundance, and hence: $X_1 = 1$:

$$Y_d = f_d(\frac{X_m^N}{m=1}) = \frac{X_d}{\sum_{m=1}^{N} X_m} = \frac{X_d}{1 + \sum_{m=2}^{N} X_m}; \text{with } d = 1, 2 ... N$$

And:

$$A_E = f_E(\{M_d, Y_d^N\}_{d=1}^N) = \sum_{d=1}^{N} (M_d \times Y_d) = \sum_{d=1}^{N} \left(M_d \times \frac{X_d}{1 + \sum_{m=2}^{N} X_m}\right)$$

where $M_d$ stands for the $d^{th}$ isotopic mass.

However, a measured estimate “$x_m$” should (even after correcting for mass fractionation and, if any, other detected method specific biases) be subject to certain uncertainty “$u_m$” [1]. Therefore, the derived estimates ($\{Y_d^N\}_{d=1}^N$ and $a_E$) should also be at certain uncertainties ($\{\varepsilon_d^Y\}_{d=1}^N$, and $\varepsilon_E^A$, respectively), i.e. for a practical purpose, Eqs. (1) and (2) could be rewritten as:

$$(Y_d \pm \varepsilon_d^Y) = f_d(\{x_m \pm u_m\}_{m=1}^N) = \frac{(x_d \pm u_d)}{1 + \sum_{m=2}^{N} (x_m \pm u_m)}; \text{with } d = 1, 2 ... N$$

And:

$$(a_E \pm \varepsilon_E^A) = f_E(\{[m_d \pm u_d^M], [Y_d \pm \varepsilon_d^Y]\}_{d=1}^N)$$

$$= \sum_{d=1}^{N} \left([m_d \pm u_d^M] \times \frac{(x_d \pm u_d)}{1 + \sum_{m=2}^{N} (x_m \pm u_m)}\right)$$

where $u_d^M$ stands for the uncertainty in the mass of the $d^{th}$ isotope.

It may, however, be enquired: what is meant by the term uncertainty? And, how should the direct and indirect measurement uncertainties “$u$” and “$e$”, respectively, be correlated and/ or estimated?

As indicated by e.g. Eq. (1) and Eq. (1a), the estimate “$x_m$” should be equal to its unknown true value “$X_m$” provided that “$u_m = 0$”. Otherwise ($u_m \neq 0$), the estimate can turn
out to be so high that: \( x_m = (X_m + u_m) \) or even as low as: \( x_m = (X_m - u_m) \). That is, the uncertainty “\( u_m \)” should represent the possible (and hence, the highest and unaccountable) error in the measured estimate “\( x_m \)” (cf. Section 0.2 in [1]). Clearly, “\( u_m \)” (which, as well known, may itself turn out to be measurement method specific or even the isotopic abundance specific, and which should account for the possible errors due to small undetectable biases and/or bias correction processes employed) has to be ascertained, with the aid of relevant standards, by the experimenting lab.

Furthermore, the method of any real world (here, \( X_m \)) measurement is generally so developed that the uncertainty “\( u_m \)” should be restricted by its limiting (random) value, i.e. “\( u_m = \sigma_m \)” (with \( \sigma_m \) as the standard deviation of repetitive measurements [1]). Possibly, that is why, any derived result as “\( y_d \)” and/or even the estimated atomic weight (\( a_E \)) is usually validated in terms of its predicted scatter “\( \rho_E \)” (cf. e.g. Refs. [2-7] and the references therein). “\( \rho \)” is generally referred to as the combined standard [1] or probable [8] uncertainty, and is computed here as:

\[
\rho_d = \frac{1}{y_d} \left[ \sum_{m=1}^{N} \left( \frac{\partial y_d}{\partial x_m} \right)^2 \sigma_m^2 \right]^{1/2} \tag{3}
\]

It may here be mentioned that: (i) variation due to a small measurement-bias can be overshadowed by even the random variation, i.e. “\( \sigma_m \)” might not be a measure of purely statistical variation; (ii) the classification of errors as random and systematic is required for rather the detection of possible error-sources and/or for employing appropriate bias-correction; (iii) the magnitude of error/uncertainty of a derived result, and hence the result itself, cannot vary for whether the cause of the error(s) in the corresponding measured cum input estimate(s) is purely statistical or not; (iv) by any true value, it should bound to mean a relative truth, i.e. with reference to something as an attributed truth. Moreover, unless relate to something as rather the common reference cum truth, the term as either measurement or
error or uncertainty or accuracy or so should have no meaning. Thus, simply for avoiding unnecessary confusions of terminologies, the possible variation of any directly or indirectly measured (and hence accepted/reported) estimate is referred [9] to as either uncertainty or inaccuracy or accuracy.

Above all, the desired result is shaped through its either pre-established system specific relationship (SSR) or a proposed mathematical model, e.g.: \( y_d = f_d(\{x_m\}_{m=1}^N) \); which could be rewritten as: \( (Y_d \pm \Delta_d^Y) = f_d(\{X_m \pm \Delta_m\}_{m=1}^N) \) and/or: \( (Y_d \pm \epsilon_d^Y) = f_d(\{X_m \pm u_m\}_{m=1}^N) \). That is, not only the result-shaping “\( x_m(s) \rightarrow y_d \)” but also the (unknown) true-error “\( \Delta_m(s) \rightarrow \Delta_d^Y \)” or the uncertainty “\( \Delta_m(s) \rightarrow \epsilon_d^Y \)” transformation should have to be accomplished in terms of the SSR “\( f_d \)” [9]. In other words, the uncertainty “\( \epsilon_d^Y \)” should, like the desired result “\( y_d \)”, be the SSR “\( f_d \)” governed systematic parameter. Moreover, the desired estimate “\( y_d \)” should depend on only the magnitude of, and not the nature and/or process of deciding, “\( x_m \)”. Similarly, the output-uncertainty “\( \epsilon_d^Y \)” should be independent of whether the measurement-uncertainty “\( u_m \)” is purely random in nature or not. Furthermore, even two similar SSRs/ functions “\( f_d(\{X_m\}_{m=1}^N) \)” and “\( f(\{X_m\}_{m=1}^N) \)” cannot be expected to yield (by magnitude) the same result. Similarly, it is the intrinsic (input-to-output variation) property [9] of the required evaluation-step as Eq. (1), which should preset whether Eq. (1) will act as either an error-source or even a -sink or a non-interfering-step in the process of shaping the desired result (\( y_d \)), and hence in defining the resultant error (\( \Delta_d^Y \)). Thus, the purpose of this work is simply to exemplify the characteristic parameters of Eq. (1) and/or Eq. (2), which should, in turn, define the corresponding output error/uncertainty “\( \epsilon \)”.

2. Evaluation of Output Uncertainty

It has been shown previously [9-11] that, irrespective of whatever might a required SSR or proposed measurement-model (say: \( f_d \), cf. Eq.(1)) represent, the output uncertainty
“ε” should best (in fact, in the case of a linear SSR/ model, exactly) be accountable/predictable as:

$$\varepsilon_d^Y = \sum_{m=1}^{N} (|MF|^d_m \times u_m) = \sum_{m=1}^{N} (|MF|^d_m \times F_m) \times G_u = ([UF]_d \times G_u)$$ (4)

And/ or, the true error ($\Delta_d^Y$) in a desired result ($y_d$) should get accounted for as:

$$\Delta_d^Y = \sum_{m=1}^{N} (|MF|^d_m \times \Delta_m)$$ (4a)

where (as only the relative errors should be inter comparable, the true-errors “$\Delta_m$ and $\Delta_d^Y$” as well as the uncertainties “$u_m$ and $\varepsilon_d^Y$” are referred to here as relative, i.e.: $u_m = \text{Max} |\Delta_m| = \text{Max} \frac{\Delta X_m}{X_m}$; and $\varepsilon_d^Y = \text{Max} |\Delta_d^Y| = \text{Max} \frac{\Delta Y_d}{Y_d}$; $[MF]^d_m$ is a theoretical constant, representing the SSR/ model “$f_d$” specific relative-rate of variation of the desired/modelled variable “$Y_d$” as a function of the measurable variable “$X_m$”:

$$[MF]^d_m = \left( \frac{\partial Y_d}{\partial X_m} \right)_{Y_d} \left( \frac{X_m}{Y_d} \right), \quad m = 1, 2 \ldots N$$ (5)

And, $F_m = (u_mG_u)$; so that:

$$[UF]_d = (\varepsilon_d^Y/G_u) = \sum_{m=1}^{N} (|MF|^d_m \times F_m)$$ (6)

where $G_u$ stands for any $u_m$-value, viz. the measurement accuracy which could be preset to be achieved before developing the required experimental-methodology and/ or establishing (if it happens to be so) the $X_m$ specific “$u_m$”. However, if all $X_m$-measurements should be subject to equal uncertainty ($u_\text{m} = G_u$, i.e. if: $F_m = 1$, with: $m = 1, 2 \ldots N$), then:

$$[UF]_d = \sum_{m=1}^{N} (|MF|^d_m \times F_m) = \sum_{m=1}^{N} |MF|^d_m$$ (6a)

Clearly, “[UF]_d” should give (at least, in a case where “$F_m \neq 1$”, a measure of) the relative-rate of variation of $Y_d$ as a function of all the measurable variables ($\{X_m\}_{m=1}^{N}$; of course, in our specific case of Eq. (1): $m = 2, 3 \ldots N$) collectively. Therefore the smaller be the $[UF]_d$ (viz.: $[UF]_d < 1$, rather: $[UF]_d \ll 1$), the better representative the desired result “$y_d$” (and/ or the evaluation model “$f_d$”) should be. However should really, in our case of either or both Eq.(1) and Eq.(2), “[UF]” be <1? The point is returned to below. The “[UF]_d”
may be called as the SSR/ model “$f_d$” specific-uncertainty-factor, and the “$[MF]^d_m$” (which numerically equals the relative error magnification factor [12,13] of determining $Y_d$ with respect to the $m^{th}$-measurable variable $X_m$, cf. Eq. 5) as the -individual-error-magnification-factor.

2.1 Family characteristics of SSRs/ Models

Different possible SSRs/ models should, depending upon their gross properties, belong to two different families [9,11] only: — an “$f_d$ with: $|[MF]^d_m| = 1^{N_{m=1}}$” and the “$f_d$ with: $|[MF]^d_m| \neq 1$ (for, at least, any single $m$)” be the members of variable-independent (F.1) and -dependent (F.2) families, respectively. Clearly, for a F.1 family member, Eq. (4) should reduce as:

$$\epsilon^Y_d = \sum_{m=1}^{N} ([MF]^d_m \times u_m) = \sum_{m=1}^{N} u_m = [\sum_{m=1}^{N} F_m] \times G = ([UF]_d \times G_u) \quad (4.F.1)$$

And, thus:

$$[UF]_d = (\epsilon_d / G_u) = \sum_{m=1}^{N} F_m \quad (6.F.1)$$

Further, if the uncertainty “$u_m$” should be independent of the measurable-variable “$X_m$” (viz. $u_m = G_u$, i.e. if: $F_m = 1$, with: $m = 1, 2 \ldots N$), then:

$$\epsilon^Y_d = \sum_{m=1}^{N} u_m = (N \times u_m) = (N \times G_u) = ([UF]_d \times G_u) \quad (4.F.1a)$$

And:

$$[UF]_d = N \quad (6a.F.1)$$

Thus say, for illustration, that “$f_d$, (cf. Eq. 1)” to be a F.1 family member. Then the uncertainty ($\epsilon^Y_d$) of determining an atom fraction ($Y_d$) should solely be governed by the measurement-uncertainties, namely, as: $\epsilon^Y_d = \sum_{m=2}^{N} u_m$. Clearly, the desired estimate ($y_d$) should never then be, it may be emphasized, better accurate than a measured estimate ($x_m$), i.e. $\epsilon^Y_d$ should be $\geq u_m$ and may turn out as high as “$(N - 1)u_m$”.

If “$f_d$” should belong to the F.2 family, then “$[MF]^d_m$” should however be dependent on the specific nature of the “SSR-$f_d$” and even vary with the value(s) of $X_m(s)$.
That is, on the one, a F.2 SSR and/or careful F.2-modelling can help achieve “[\(UF\)]_d < 1” and hence, “\(\varepsilon^Y_d < u_m\)” On the other, another F.2 member may turn out to be characterized by “[\(UF\)]_d > 1” or even “[\(UF\)]_d \gg 1”. Thus e.g. while the SSR “\(Y_R = f_R(X_S, X_W) = \frac{x_S}{x_W}\)” should belong to F.1, the apparently similar SSR “\(Y_\delta = f_\delta(X_S, X_W) = \left(\frac{x_S}{x_W} - 1\right)\)” is a F.2 member [11]. Clearly, for “\(|X_S - X_W| \to 0\)”, the estimate \(y_R\) could be expected to be increasingly accurate but the differential estimate \(y_\delta\) will, one can verify, be increasingly erroneous [11,14,15]; that is that: \(\varepsilon^Y_R = [u_S + u_W]\); but: \(\varepsilon^Y_\delta = \left(|\frac{x_S}{x_S - x_W}| \times [u_S + u_W]\right) = \left(|\frac{x_S}{x_S - x_W}| \times \varepsilon^Y_R\right). \) These should explain why in IRMS, where “\(|X_S - X_W| \to 0\)” is rather a requirement, the modelling of the IRMS measurement cum evaluation as “\(f_\delta\)” rather than as “\(f_R\)” is illogical, and/or why there should be confusion [7] in dealing with IRMS data. Moreover, such a fact has made us to be interested in studying the behaviour of the other isotopic SSRs as those represented by Eqs. (1) and (2).

3. Results and Discussion

We consider the Table [16] isotopic abundances of a somewhat simpler system, oxygen, for illustrating the implications of the uncertainty theory (Eq. (4)). The oxygen isotopes, their masses (true \(M_d\)-values), relative abundances (i.e. the true values of the measureable \(X_m\)-variables), atom fractions (true \(Y_d\)-values) and the corresponding Eq.(1) specific parameters (\([MF]_m^d\), \([UF]_d\) and \(\varepsilon^Y_d\)-values, cf. Eqs. (4-6a)) are furnished in Table 1. Similarly, the true atomic weight of oxygen (\(A_O\)) and the evaluated parameters of corresponding Eq. (2) are tabulated in Table 2.

It could be our interest to note the following features of the predictions (cf. Table 1 and Table 2).

i) Irrespective of whether the measurement accuracy (\(u_m\)) should be the ratio “\(X_m\)” (i.e. isotope) specific or not, the achievable accuracy (\(\varepsilon^Y_d\)) of determining an atom fraction
“Y_d” should be the isotope “d” and/or the SSR “f_d” specific (comparison between the rows in Table 1).

ii) Eq. (1) should belong to the F.2 family of SSRs, i.e. the relative-rate of \((Y_d \text{ vs. } X_m)\) variation \(\frac{d\{MF\}}{d_m}\), and thus the uncertainty \(\epsilon_d^Y\), should vary even with the magnitude of the measurable variable “\(X_m\)”.

iii) By and large, the uncertainty-factor \([UF]_d\), and hence the uncertainty \(\epsilon_d^Y\), should be inversely proportional to the isotopic abundance, \(Y_d\), to be determined.

iv) (The determination of either an atom fraction, \(Y_d\), or the atomic weight, \(A_E\), should require the \((N-1)\) different ratio (\(X_m\)) measurements. In addition, any isotopic mass \((M_d)\) should be subject to certain error/uncertainty, cf. Eq.2). However, Table 1 and also Table 2 show that, without exception: \(|\{MF\}| < 1\). That is, the SSRs “\(f_d\)” and “\(f_E\)” should, at least with respect to any relevant individual input variable (\(X_m\), or even, in the case of Eq. 2, \(M_d\)) and hence, as a whole, behave as error-sinks.

v) \(\text{Highest } [UF]_d \approx 1\) (cf. Table 1, for \(^{17}\)O), and also: \([UF]_{A_0} \approx 1\) (cf. Table 2), i.e. although the above mentioned F.2 family member “IRMS-model-\(f_{\delta}\)” had been shown \([11,14,15]\) to act as an error-source in the overall process of indirect measurement, the present F.2 members (SSRs “\(f_d\)” and “\(f_E\)” should behave as rather good error-sinks.

vi) The isotopic mass dependent error-magnification-factors \(\left\{\frac{\{MF\}_{A_0}^{M_d}}{3}_{d=1}\right\}\) actually represent, one can verify, the corresponding mass fractions, and thus: \(\sum_{d=1}^{3}[MF]_{M_d}^{A_0} = 1\), which should in turn imply that (cf. Table 2): \(\sum_{m=2}^{3}[MF]_{X_m}^{A_0} = 0.00028\). That is to say that the atomic weight should be more susceptible towards variation for a given error in isotopic-masses than in –ratios. Therefore, if the isotopic-masses (with insignificant uncertainties) should be considered to be invariable, then (cf. Table 2): \([UF]_{A_0} = (\sum_{m=2}^{3}[MF]_{X_m}^{A_0}) = 0.00028\), and thus for “\(\mu = 1\%\)”: \(\epsilon^A_{\delta} = ([UF]_{A_0}\)
\[ \times G(w) = 0.00028\%, \text{ i.e. the evaluation of atomic weight (cf. Eq. 2) should lead to} \]

significant reduction of experimental-errors.

At this point, it may be kept in mind that Eq. (1) and Eq. (2) are non-linear. However Table 3 (which presents the evaluated estimates of atom fractions, \( \{y_d\}_{d=1}^3 \), and atomic weight, \( a_O \), of oxygen from, presumably, the corresponding input estimates (i.e. isotopic-ratios \( \{x_m\}_{m=2}^3 \) and also, in case of latter, -masses \( \{m_d\}_{d=1}^3 \) with known errors) verifies that the above predictions are correct for not only \( \pm 0.01\% \) (cf. example nos. 1 and 2) but also as high as \( \pm 1.0\% \) (cf. example nos. 3 and 4) input errors. Thus, for example, the observed output errors are different for different isotopes (comparison, for a given example, between columns nos. 3, 4 and 5), and are in agreement with their predicted values (e.g.: \( \Delta Y_{16} = \text{Pred} \Delta Y_{16} \), and/ or: \( \Delta Y_{16} \leq \text{Pred} \varepsilon Y_{16} \)). Even the observed error in the evaluated atomic weight (\( a_O \)) is, it may be emphasized, the same as its predicted value (\( \Delta A_O = \text{Pred} \Delta A_O \)), and/ or: \( \Delta A_O \leq \text{Pred} \varepsilon A_O \); cf. column 7). Above all, example no.4 (for which the isotopic masses are considered to be constant) confirms that Eq. (2) does act as a very good error-sink (namely, the sum of input-error is 2\%, but the output error has turned out to be 0.00028\% only. Moreover, it may be pointed out that an output error has in no case, numerically, exceeded the predicted uncertainty. The output error in Table 3 has been emboldened, however, in only those cases where it has acquired its highest predicted value (e.g. in the case where: \( |\Delta Y_{17}| = \text{Pred} |\Delta Y_{17}| = \text{Pred} \varepsilon Y_{17} \); cf. example no. 2).

Let us now consider an abundance spectrum from the literature for discussion. The measured [4] isotopic abundance ratios of xenon (\( x_m \)-values) and their reported [4] uncertainties (the absolute values are referred to as “\( \text{Max} |\Delta X_m| \)”, and the relative values as “\( \mu_m \)”), the correspondingly reported atom fractions (\( y_d \)-values) cum probable errors (\( \rho_d \)-values) and the atomic weight (\( a_{Xe} \)) cum probable error (\( \rho_{Xe} \)), are reproduced in Table 4 (cf. cols. 4 and 5, and bottom leftmost box). Moreover, for examining whether our computations
lead to any discrepancy in results, we have also furnished our evaluated \( y_d \) and \( a_{\chi e} \)-values, along with the respective probable errors (\( \rho_d \)- and \( \rho_{\chi e} \)-values, cf. Eq. 3) and also the predicted uncertainties (cf. Eq. 4, i.e. \( \text{pred}\epsilon_{d}Y \) and \( \text{pred}\epsilon_{\chi e}A \)-values corresponding to the reported \([4] u_m\)-values), in Table 4 (cf. col. 6, and bottom side middle box). Clearly the discrepancy in results and/or in their probable errors (comparison between cols. 5 and 6, also between the bottom blocks for atomic weight), if there seems at all to be any, should be due to truncation of data.

It may also be mentioned that, for our prediction (cf. Eq. 4), we have considered the reported \([4] x_m\)-values as their true values (i.e.: \( X_m = x_m \)\( _{m=2}^9 \)) and hence: \( y_d = y_d \)\( _{d=1}^9 \), and: \( A_{\chi e} = a_{\chi e} \) and evaluated the individual ([MF], cf. Eq.5) and collective ([UF], cf. Eq. 6a) rates of “\( Y_d \) vs. \( X_m \)” , “\( A_{\chi e} \) vs. \( X_m \)” and even “\( A_{\chi e} \) vs. (\( X_m, M_d \))” variations. However, for simplicity, only the “\( \text{highest-}[MF]_{m}^d \)” , [UF]\( _d \) and [UF]\( _{\chi e} \) values are tabulated in Table 4 (cf. cols. 7 and 8, and the bottom rightmost box).

However, both “\( \text{Max.}[MF]_{m}^d \)” and “\( [UF]_{d} \)” vary from isotope \( (d) \) to isotope, and “\( \text{Max.}[MF]_{m}^d \)” is <1, thereby reinforcing our above finding that Eq. (1) behaves as an isotope specific error-sink. Similarly, Eq. (2) is once again predicted to behave as an error-sink, specifically in terms the ratio \( (X_m) \) variables (cf. the end row in Table 4).

Moreover, the isotopic mass \( (M_d) \) dependent relative-rate of variation of atomic weight “\( \text{[MF]}_{M_d}^{A_{\chi e}} \)” could like the oxygen case above be shown to equal the corresponding \( (d^{th}) \) isotopic mass fraction (e.g.: \( [MF]_{M_{124}}^{A_{\chi e}} = 0.00089796 \); or: \( [MF]_{M_{129}}^{A_{\chi e}} = 0.25920437 \)). That is to say that the effect of an isotopic-mass-error on the estimate of atomic weight should be reduced by a factor equalling the isotopic mass fraction. And, of course, it could be shown that: \( \sum_{d=1}^9 [MF]_{M_d}^{A_{\chi e}} = 1.0. \)
What should however be significant to note in Table 4 is that the uncertainty of determining an atom fraction “\(Y_d\)” or even the atomic weight “\(A_{Xe}\)” is predicted to be higher than the corresponding probable error: \(\text{pred.}\epsilon_d^Y > \rho_d\), and even: \(\text{pred.}\epsilon_{Xe}^A > \rho_{Xe}\). Nevertheless, that the uncertainties in even the present [4] cases of outputs are accountable by Eq. (4), rather than by Eq. (3), could be verified from Table 5, which furnishes the results of “\(Y_d\) vs. \(X_m\)” and “\(A_{Xe}\) vs. \(X_m\)” and even “\(A_{Xe}\) vs. (\(X_m\) and \(M_d\))” variations by considering certain sets of relevant input-estimates (\(\{x_m\}_m=2\), and \(\{m_d\}_d=1\)) of known errors (\(\{\Delta_m\}_m=2\), and \(\{\Delta_d\}_d=1\), respectively): (i) Example Nos. 1 and 2 refer to “\(\Delta_m\) and \(\Delta_d^M\)” as the measurement [4] and the mass-uncertainties “\(\pm u_m\) and \(\pm u_d^M\)” tabulated in Table 4, respectively; (ii) Example Nos. 2a and 3 correspond to “\(\{\Delta_m = \pm u_m\}_m=2\), and \(\{\Delta_d^M = 0.0\}_d=1\)” ; (iii) Example No. 4 gives the results for “\(\{\Delta_m = \pm 1.0\%_m\}_m=2\), and \(\{\Delta_d^M = 0.0\}_d=1\)” ; and (iv) Example No. 5 refers all the measurement and mass errors as \(\pm 1.0\%\). Of course, for simplicity, the results of “\(Y_d\) vs. \(X_m\)” variations are shown for only three typical isotopes, namely, the lower, highest and middle abundant \(^{124}\text{Xe}\), \(^{132}\text{Xe}\) and \(^{136}\text{Xe}\), respectively. However it should be noted that, irrespective of whether the input-errors are as small as the measurement [4] uncertainties (cf. Example Nos. 1-3) or as high as \(\pm 1.0\%\) (cf. Example Nos. 4 and 5), the output-errors of both Eq. (1/1a) and Eq. (2/2a) are in agreement with their predicted (cf. Eq. 4a) values (e.g.: \(\Delta^Y_{124} = \text{pred.}\Delta^Y_{124}\), and: \(\Delta^A_{Xe} = \text{pred.}\Delta^A_{Xe}\)) and of course, in no case exceeded the corresponding predicted (cf. Eq. 4) uncertainties (i.e.: \(|\Delta^Y_{124}| \leq \text{pred.}\epsilon^Y_{124}\); and also: \(|\Delta^A_{Xe}| \leq \text{pred.}\epsilon^A_{Xe}\)).

We may now examine our considerations in terms of some other isotopic data from the literature. As indicated in Table 6, we assume the TIMS-measured [6] estimates of the isotopic abundance ratios of neodymium (\(\{x_m\}_m=2\), cf. col. 4), the reported [6] isotopic abundances (\(\{y_d\}_d=1\), col. 5) and atomic weight (\(a_{Nd}\), cf. leftmost box at the bottom) of neodymium as their respective true values: (\(\{X_m = x_m\}_m=2\), \(\{Y_d = y_d\}_d=1\), and \(A_{Nd} = a_{Nd}\)). Similarly we consider, but irrespective of whether the authors’ [6] had really so meant
or not, the uncertainty values shown there in column 4 as the ratio-specific measurement-uncertainties, and evaluate the uncertainties as Eq. 4 and the probable errors (cf. Eq. 3) to be expected in the outputs of Eqs. (1) and (2); and furnish the same also in Table 6. Of course, the output-characteristics are tabulated along with our evaluated outputs (see, for the atom fractions, col.6 and, for the atomic weight, see the 2nd box at the bottom of Table 6).

Clearly, our evaluated atom fractions $\{Y_d\}_{d=1}^7$ and atomic weight $\langle A_{Nd} \rangle$ are not really different from the respective reported results (comparison between the cols. 5 and 6; and between the 1st and 2nd boxes at the bottom of Table 6). Moreover, for three different combinations of known measurement-errors “$\pm u_m$” (i.e. for: $x_m = (X_m \pm u_m)$ with $u_m$-values shown in column 4), we have evaluated the atom fractions and atomic weight and furnished the results along with their observed and predicted (cf. Eq. 4a) errors in Table 6 (cf. examples 1, 2 and 3). Thus, it may be noted that, in general: “$\Delta^Y_d = \text{Pred.} \Delta^Y_d$” and/or: “$|\Delta^Y_d| \leq \text{Pred.} \epsilon^Y_d$” (cf. col. 6 for: $\text{Pred.} \epsilon^Y_d$)”; and similarly “$\Delta^A_{Nd} = \text{Pred.} \Delta^A_{Nd}$” and/or: “$|\Delta^A_{Nd}| \leq (\text{Pred.} \epsilon^A_{Nd} = 0.0005437\%)$”. Of course, the example no. 1 shows that: $|\Delta^Y_{144}| = \text{Pred.} |\Delta^Y_{144}| = \text{Pred.} \epsilon^Y_{144} = 0.0333\%$. Similarly, the error-combination as the example no. 2 makes the error in atomic weight to attain the corresponding highest possible value: $|\Delta^A_{Nd}| = \text{Pred.} |\Delta^A_{Nd}| = \text{Pred.} \epsilon^A_{Nd} = 0.0005437\%$; and the combination no. 3 causes: $|\Delta^Y_{150}| = \text{Pred.} |\Delta^Y_{150}| = \text{Pred.} \epsilon^Y_{150} = 0.1007\%$; but the observed error has in no case exceeded the corresponding predicted (cf. Eq. 4) uncertainty, however. Above all, the present findings also make it a point that both Eqs. (1) and (2) should cause isotope-specific and element-specific reduction of net measurement error in the results (here: $y_d$ and $a_{Nd}$, respectively). That is, the individual relative error magnification factors could here again be shown to be numerically $<1$. Thus, for example, one can verify that the Eq. (2) specific “MFs” take values as: $[MF]_{X2}^{A_{Nd}} = -0.004393$, 

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\[ MF_{X_3}^{\text{Nd}} = -0.001124, \quad MF_{X_4}^{\text{Nd}} = 0.0003858, \quad MF_{X_5}^{\text{Nd}} = 0.001992, \quad MF_{X_6}^{\text{Nd}} = 0.0014666 \]
and, \[ MF_{X_7}^{\text{Nd}} = 0.002220. \]

4. Conclusions

The input-output behaviour of certain system specific relationships (SSRs: Eqs. (1) and (2)), enabling the determination of isotopic abundances and/or atomic weight from measured isotopic abundance ratios of any possible poly-isotopic element, is discussed above. The study emphasizes rather a previous finding [9] that the relative-rate of any input to output variation should always be prefixed by the SSR in question. The relative rate(s) should in turn dictate the output-characteristics (error/uncertainty), corresponding to any possible input-error, to be expected. That is to say that, irrespective: (i) whether the input (measurement) error(s)/uncertainty(s) should be purely statistical or not, and (ii) whatever might the investigating-SSR stand for; the output error/uncertainty is confirmed above to be the SSR governed systematic parameter. It is outlined above how should the output uncertainty (\( \epsilon \)) be evaluated, or even be ‘a priori’ predicted as a multiplying factor (called as the uncertainty factor “[UF]”) of the possible measurement uncertainty (\( \sigma_u \)).

Both Eq. (1) and Eq. (2) have been shown to belong to the F.2 family of the two [9] possible, i.e. input-variable-independent “F.1” and –dependent “F.2”, families of SSRs cum mathematical models. The well-known F.2 SSR cum IRMS-measurement-model “\( Y_\delta = \left( \frac{x_s}{x_w} - 1 \right) \)” had previously been shown [11,14,15] to cause the enhancement of possible “\( x_s \) and \( x_w \)” measurement errors in the estimated ratio “\( y_\delta \)”. However, in contrast, both Eq. (1): \( Y_d = f_d(\{X_m\}_{m=1}^N) \) and Eq. (2): \( A_E = f_E(\{M_d,Y_d\}_{d=1}^N) \) are shown above to act as the error-sinks in the overall processes of indirect measurements (here, of any desired atom fraction “\( Y_d \)” and atomic weight “\( A_E \)”, respectively). The reason is, as also clarified above, that any relevant relative-rate of input-to-output variation (i.e. any individual error magnification
factor \( [MF]_{m}^{d}, \) cf. Eq. (1)” or “\([MF]_{X m}^{A E}, \) or “\([MF]_{M d}^{A E}, \) cf. Eq. (2)” should numerically be a fraction.

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Exemplifying oxygen isotopic details and the correspondingly predicted individual error magnification factors \((\{MF\}^d_{m=2})\), uncertainty-factor \((UF)_{d}\) and the uncertainty \((\epsilon_d^Y)\) of determining any of the three oxygen-isotope-fractions \((Y_d)_{d=1}\), cf. by Eq.(1))

| Isotope \((d)\) | Isotopic Mass \((M_d)\) | \(m\) | Relative Abundance (i.e. the measurable ratio: \(X_m\)) | Atom/Isotope Fraction \((Y_d)\) | \([MF]_2^d\) (cf. Eq.(5)) | \([MF]_3^d\) (cf. Eq.(5)) | \([UF]_d\) \(^{1}\) |
|----------------|-----------------|-----|-----------------|-----------------|-----------------|-----------------|-----------------|
| \(^{16}\text{O}\) | 15.99491462 | 1 | 1.0 | 0.99757 | \(-X_2\) \[
1 + X_2 + X_3 = -0.00038 \]
| \(^{17}\text{O}\) | 16.99913150 | 2 | 38.092565×10\(^{-5}\) | 0.00038 | \(1 + X_3\) \[
1 + X_2 + X_3 = 0.99962 \]
| \(^{18}\text{O}\) | 17.99916040 | 3 | 20.549936×10\(^{-4}\) | 0.00205 | \(-X_2\) \[
1 + X_2 + X_3 = -0.00038 \]

Atomic weight \((A_O) = 15.99940493\)

\(^{1}\) \([UF]_d = (\{MF\}^d_2 + \{MF\}^d_3)\), i.e. for “\(u_2 = u_3 = G_u\)”; cf. Eq. (6a)
Table 2
The predicted relative-rates of variations \( \{[MF]_{M_d}^{A_o}\}_{d=1}^3 \) and \( \{[MF]_{X_m}^{A_o}\}_{m=2}^3 \) of the atomic weight variable “\( A_o \) (cf. Eq.2)” as a function of the oxygen isotopic mass and abundance variables (\( M_d \) and \( X_m \), respectively)

| Atomic weight \( (A_o) \) | \( [MF]_{M_1}^{A_o} = \frac{M_1}{D} = \frac{M_1}{M_1 + M_2X_2 + M_3X_3} \) | \( [MF]_{M_2}^{A_o} = \frac{M_2X_2}{M_1 + M_2X_2 + M_3X_3} \) | \( [MF]_{M_3}^{A_o} = \frac{M_3X_3}{M_1 + M_2X_2 + M_3X_3} \) | \( [MF]_{X_2}^{A_o} = \frac{N_2}{D_{X_2}} \) where *1 | \( [MF]_{X_3}^{A_o} = \frac{N_3}{D_{X_3}} \) where *2 | \( [UF]_{A_o} \) where *3 |
|-----------------------------|---------------------------------|---------------------------------|---------------------------------|-----------------------------|-----------------------------|-----------------------------|
| 15.999405                   | 0.99729                         | 0.0004037                       | 0.0023062                       | 0.0000237                   | 0.0002562                   | 1.00028                     |

*1: \( N_2 = X_2 \times (M_2 - M_1 + X_3 \times [M_2 - M_3]) \) &: \( D_{X_2} = (1 + X_2 + X_3) \times (M_1 + M_2X_2 + M_3X_3) \).

*2: \( N_3 = X_3 \times (M_3 - M_1 + X_2 \times [M_3 - M_2]) \).

*3: (Assuming the estimates of “\( M_d \) and \( X_m \)” to be equally accurate, i.e. for “\( u_1^M = u_2^M = u_3^M = u_2^u = u_3^u = G_u \)” , cf. Eq. (6a)):

\[
[UF]_{A_o} = ([MF]_{M_1}^{A_o} + [MF]_{M_2}^{A_o} + [MF]_{M_3}^{A_o} + [MF]_{X_2}^{A_o} + [MF]_{X_3}^{A_o}) = 1.00028.
\]

And (if “\( G_u = 1\% \)” , then the uncertainty (cf. Eq. (4)):

\[
\epsilon_{\Delta} = ([UF]_{A_o} \times G_u) = 1.00028\%.
\]
Table 3
Output estimates (i.e. the atom fractions: \([y_d \pm \Delta_d^Y]_{d=1}\), cf. Eq.(1a)) and the atomic weight \([a_O \pm \Delta_O^A]\), cf. Eq.(2a) of oxygen obtained against the relevant input estimates with known errors/uncertainties \((x_m = [X_m \pm \Delta_m]_{m=2}^3, \text{and } m_d = [M_d \pm \Delta_d^A]_{d=1}^3)\)

| Ex. No. | Input ratios: \(\{x_m\}_{m=2}^3\) (for given: \(6u\)) | Output of Eq. (1a): \(y_d\) and its Observed & Predicted Errors cum uncertainty | Input masses: \(\{m_d\}_{m=1}^3\) | Output of Eq. (2a): \(a_O\) \((\Delta_O^A \times 10^2)\) \([\text{Pred.}\Delta_O^A \times 10^2; \text{Eq. (4a)}] \) |
|---------|-------------------------------------------------|-------------------------------------------------|-----------------------------|-----------------------------------------------|
| 1       | i) \(x_2\) \((\Delta_2 \times 10^2)\) \(0.01\) \((0.01)\) \(0.00038096\) \((0.01)\) ii) \(x_3\) \((\Delta_3 \times 10^2)\) \(0.00205520\) \((0.01)\) | \(y_{16} \times 10^2 \) \((\Delta_{16}^Y \times 10^2)\) \(\text{cf. Eq. 4a[16]}\) \(\{\text{Pred.}\Delta_{16}^Y \times 10^2; \text{cf. Eq. 4a[17]}\) \(0.038003791\) \((0.00997975)\) \(0.000000243\) \% \(\text{Pred.}\Delta_{17}^Y \times 10^2\) \(0.00100167\) \% \(\text{Pred.}\Delta_{18}^Y \times 10^2\) \(0.205020447\) \((0.0099757)\) \(0.000000280\) \% | \(m_{i16}\) \((\Delta_{16}^M \times 10^2)\) \(15.99651411\) \((0.01)\) ii) \(m_{i17}\) \((\Delta_{17}^M \times 10^2)\) \(17.00083141\) \((0.01)\) iii) \(m_{i18}\) \((\Delta_{18}^M \times 10^2)\) \(18.00096032\) \((0.01)\) | \(16.00100532\) \((0.000100208)\) \((0.000100208)\%\) |
| 2       | i) \(6u = 0.01\%\) \((0.01)\) \(-0.00038089\) \((0.01)\) ii) \(6u = 0.01\%\) \((0.01)\) \(0.00205520\) \((0.01)\) | \(99.756983\) \(-0.000001670\) \(-16.70 \times 10^{-6}\) \(0.00000243\) \% | \(0.037996194\) \((-0.00100167)\) \((-0.00100167)\) \% | \(0.205020462\) \((0.0099833)\) \((0.0099833)\) \% | \(15.99331513\) \(-0.00999515\) \((-0.00999516)\) \% | \(15.9978127\) \((-0.00999515\) \((-0.00999516)\) \% | \(0.0100028\) \% |
| 3       | i) \(6u = 1\%\) \((1.0)\) \(0.0038473\) \((1.0)\) ii) \(6u = 1\%\) \((1.0)\) \(0.00207554\) \((1.0)\) | \(99.754576\) \((-0.0002430)\) \(-0.002430\) \(0.00243\) \% | \(0.03837907\) \((0.997546)\) \((0.997560)\) \(1.00167\) \% | \(0.20704497\) \((0.997546)\) \((0.997570)\) \(0.99833\) \% | \(16.15486377\) \((1.0)\) \(17.169122815\) \((1.0)\) \(18.179152004\) \((1.0)\) | \(16.15944422\) \((1.000283)\) \((1.000280)\) \% | \(1.000280\) \% |
| 4       | i) \(6u = 0.0037712\) \((-1.0)\) ii) \(6u = 0.0037712\) \((-1.0)\) | \(99.759424\) \((0.002430)\) \(0.002430\) \(0.00243\) \% | \(0.0376209\) \((-0.997594)\) \((-0.997570)\) \(1.00167\) \% | \(0.20295493\) \((-0.997594)\) \((-0.997570)\) \(0.99833\) \% | \(15.99936013\) \((-0.0000280)\) \((-0.0000280)\) \% | \(0.0000280\) \% |
Table 4

| Isotope (d) | Isotopic Mass: $M_d$ (Max. $|\Delta M_d|$, $[\mu_d^N (%)$] | $m$ | Inputs and Outputs of Eq. (1/1a) | Predicted parameters |
|-------------|---------------------------------------------------------------|-----|----------------------------------|----------------------|
|             | Reported: $x_m$ (Max. $|\Delta X_m|$, $[\mu_m^N (%)$] | Reported: $y_d \times 10^2$ (Max. $|\Delta Y_d|$, $[\rho_d (%)$] | Our evaluated: $\gamma_d \times 10^2$ (Max. $|\rho_d|$, $[\rho_d (%)$] | Max $[MF]_m^N$ = (cf. Eq. (5)) |
| $^{132}$Xe | $131.904154$ (0.000001) $[75.8 \times 10^{-8}]$ | 1 | 1.0 | 26.9086 (0.0033) | 26.908653 (0.01226) | $0.02207$ | $0.26401$ |
| $^{124}$Xe | $123.905896$ (0.000002) $[16.1 \times 10^{-8}]$ | 2 | 0.003536 (0.000012) | 0.0952 (0.0003) | 0.095149 (0.03393) | $0.368$ | $0.99905$ |
| $^{126}$Xe | $125.904269$ (0.000007) $[55.6 \times 10^{-8}]$ | 3 | 0.0030277 (0.000072) | 0.0890 (0.0002) | 0.089006 (0.02178) | $0.2394$ | $0.99911$ |
| $^{128}$Xe | $127.903530$ (0.000002) $[15.6 \times 10^{-7}]$ | 4 | 0.070989 (0.000029) | 1.9102 (0.0008) | 1.910218 (0.0419) | $0.0614$ | $0.98090$ |
| $^{129}$Xe | $128.9047794$ (0.000009) $[69.8 \times 10^{-8}]$ | 5 | 0.9811 (0.00041) | 26.4006 (0.0082) | 26.4000618 (0.03126) | $0.0418$ | $0.73599$ |
| $^{130}$Xe | $129.903508$ (0.000001) $[77.0 \times 10^{-8}]$ | 6 | 0.15129 (0.000047) | 4.0710 (0.0013) | 4.071001 (0.03224) | $0.0506$ | $0.95929$ |
| $^{131}$Xe | $130.905082$ (0.000001) $[76.4 \times 10^{-8}]$ | 7 | 0.789055 (0.000076) | 21.2324 (0.0030) | 21.232407 (0.01441) | $0.0276$ | $0.78768$ |
| $^{134}$Xe | $133.9053945$ (0.000009) $[67.2 \times 10^{-8}]$ | 8 | 0.387819 (0.000069) | 10.4357 (0.0021) | 10.435687 (0.02008) | $0.03615$ | $0.89564$ |
| $^{136}$Xe | $135.907220$ (0.000008) $[58.9 \times 10^{-7}]$ | 9 | 0.32916 (0.000017) | 8.8573 (0.0044) | 8.857252 (0.04845) | $0.06457$ | $0.91143$ |

Reported [4] atomic weight ($\alpha_{xe}$) = 131.292755
Max $|\Delta A| = 0.00034$
$\rho_{xe} (%) = 0.00026$

$\alpha_{xe} = 131.292761$
$\rho_{xe} (\%) = 0.000261$
$\epsilon_{xe} (\%) = 0.004653$ *2

*1 (cf. Eq. 6a); $[UF]_d = \sum_{m=2}^{n} [MF]_m^N$; i.e. for $m = 2, 3, \ldots 9$.

For the estimates of "$M_d$ and $x_m$" to be equally accurate, i.e. for "$u_m = u_d^N$ = $G_m$" (with: $m = 2, 3, \ldots 9$), Eq. (6a) predicts that:

$[UF]_x = \sum_{m=2}^{9} [MF]_x^N + \sum_{d=1}^{9} [MF]_d^N = 1.0116323$; and: $\epsilon_{xe} = (0.0116323 \times G_u)$.  $\epsilon_{xe} = (0.0116323 \times G_u)$.
Table 5

Typical outputs (atom fractions: \( \{ y_d \pm \Delta y_d \} \)), with: \( d = ^{124}\text{Xe}, ^{132}\text{Xe} \) and \( ^{136}\text{Xe} \); and the atomic weight of Xenon: \( [a_o \pm \Delta a_o \{ ^{124}\text{Xe} \}] \) of Eq. (1a) and Eq. (2a) obtained using the relevant input estimates with known errors (\( \{ \pm \Delta m \}_{m=2} \)) and \( \{ \pm \Delta a \}_{d=1} \), cf. columns 4 and 2, respectively, in Table 4

| Ex. No. | Input ratio errors | Output (cf, Eq. 1a): \( y_d \) and its Observed & Predicted Errors cum uncertainty | Input mass-errors | Output of Eq. 2a: \( \Delta A_{\text{Xe}} \)
\( (\Delta A_{\text{Xe}} \times 10^2) \)
\( [\text{Pred.} A_{\text{Xe}} \times 10^2; \text{cf. Eq. (4a)}] \)
|---|---|---|---|---|
| 1 | i) \(-0.339367\) ii) \(0.217674\) iii) \(0.040851\) iv) \(0.041789\) v) \(0.031066\) vi) \(0.009362\) vii) \(0.017792\) viii) \(0.051647\) (see also Table 4) | \( y_{124} \times 10^2 \) (\( \Delta y_{124} \times 10^2 \)) \[\text{Pred.} \Delta y_{124} \times 10^2, \text{cf. Eq. 4a}\] \( y_{132} \times 10^2 \) (\( \Delta y_{132} \times 10^2 \)) \[\text{Pred.} \Delta y_{132} \times 10^2, \text{cf. Eq. 4a}\] \( y_{136} \times 10^2 \) (\( \Delta y_{136} \times 10^2 \)) \[\text{Pred.} \Delta y_{136} \times 10^2, \text{cf. Eq. 4a}\] | i) \(-75.81 \times 10^{-8}\) ii) \(-16.14 \times 10^{-7}\) iii) \(-55.6 \times 10^{-7}\) iv) \(-15.6 \times 10^{-7}\) v) \(-69.8 \times 10^{-8}\) vi) \(-77.0 \times 10^{-8}\) vii) \(-76.4 \times 10^{-8}\) VIII) \(-67.2 \times 10^{-8}\) ix) \(-58.9 \times 10^{-9}\) | i) \(-131.292717\) \((33.51 \times 10^{-6})\) ii) \(-131.293372\) \((0.0004653)\) |
(Table 5 continued)

| Ex. No. | Input ratio-errors | Output (cf, Eq. 1a): $y_d$ and its Observed & Predicted Errors cumulative uncertainty | Input mass-errors | Output of Eq. 2a: $\alpha_{\text{Xe}}$ |
|---------|-------------------|---------------------------------------------------------------------------------|------------------|-------------------------------|
| 2a      | Errors are exactly the same as shown for the Example No. 2 | | (i) to (ix): 0.0, i.e. $\{\Delta^M_d = 0.0\}_{d=1}^9$ (Isotopic masses are treated as constants) | 131.293370 $\pm$ 0.004641 |
|         | $0.3608\%$ | $26.911131 \pm 0.009209$ | $8.862643 \pm 0.060855$ | 131.293370 $\pm$ 0.004641 |
| 3       | i) $0.339367\%$ | (ii) to (ix): Errors are exactly the same as shown for the Example No. 1 | Isotopic masses are treated as constants | 131.29267065 $\pm$ 68.61 $\times$ 10^{-6} |
|         | $0.3608\%$ | $26.902715 \pm 0.022070$ | $8.859871 \pm 0.029576$ | 131.29267065 $\pm$ 68.61 $\times$ 10^{-6} |
| 4       | (for: $\nu = 1\%$) | (i) to (vi): +1.0, i.e. $\{(\Delta_m = 1\%)_{m=2}^9$ vii) $-1.0$ viii) $-1.0$ | See the Example No. 2a (Isotopic masses are treated as constants) | 131.27754086 $\pm$ 0.011592 |
|         | $1.7290\%$ | $26.816123 \pm 0.3439$ | $8.738527 \pm 1.3451$ | 131.27754086 $\pm$ 0.011592 |
| 5       | (for: $\nu = 1\%$) | (i) to (viii): +1.0, i.e. $\{(\Delta_m = 1\%)_{m=2}^9$ ix) $-1.0$ | (i) to (ix): $-1.0$, i.e. $\{\Delta^M_d = -1.0\}_{d=1}^9$ | 129.97016539 $\pm$ 1.007479 |
|         | $1.7290\%$ | $26.760462 \pm 0.5507$ | $8.720389 \pm 1.5538$ | 129.97016539 $\pm$ 1.007479 |
| Isotope (d) | Isotopic Mass: M_d | m | Let: [X_m = x_m^7_{m=2}] & [Y_d = y_d^10_{d=1}] | Example No. 1 | Example No. 2 | Example No. 3 |
|------------|-------------------|---|---------------------------------|---------------|---------------|---------------|
| 143Nd      | 143.910083        | 1 | 23.798(12)                      | 23.789812     | 23.798418     | 23.791850     |
|            |                   |   | [0.01458]                      | (-0.033306)   | (0.002856)    | (-0.024744)   |
|            |                   |   | [0.03332]                      |                 | (0.002856)    |               |
| 142Nd      | 141.907719        | 2 | 27.153(19)                      | 27.150837     | 27.160658     | 27.153162     |
|            |                   |   | [0.02164]                      | (-0.009650)   | (0.026520)    | (-0.001086)   |
|            |                   |   | [0.4413]                       |                 | (0.026519)    |               |
| 143Nd      | 142.90981          | 3 | 12.173(18)                      | 12.178243     | 12.182648     | 12.179286     |
|            |                   |   | [0.06458]                      | (0.039001)    | (0.075188)    | (0.047575)    |
|            |                   |   | [0.08804]                      |                 | (0.075186)    |               |
| 145Nd      | 144.912569        | 4 | 8.293(7)                       | 8.293129      | 8.290421      | 8.293839      |
|            |                   |   | [0.03466]                      | (0.001118)    | (-0.031580)   | (0.009683)    |
|            |                   |   | [0.06204]                      |                 |                 | (0.009686)    |
| 146Nd      | 145.913112        | 5 | 17.189(17)                      | 17.190280     | 17.181744     | 17.191753     |
|            |                   |   | [0.03770]                      | (0.009600)    | (-0.040065)   | (0.018165)    |
|            |                   |   | [0.06148]                      |                 |                 | (0.018170)    |
| 148Nd      | 147.916889        | 6 | 5.756(8)                       | 5.753732      | 5.752316      | 5.757866      |
|            |                   |   | [0.06013]                      | (0.028703)    | (0.059164)    | (0.03726)     |
|            |                   |   | [0.08820]                      |                 |                 | (0.03727)     |
| 150Nd      | 149.920887        | 7 | 5.637922                       | 5.640327      | 5.637999      | 5.632245      |
|            |                   |   | [0.07304]                      | (0.042647)    | (0.073125)    | (0.10070)     |
|            |                   |   | [0.10073]                      |                 |                 | (0.10073)     |

Reported [6] atomic weight (A_Nd) = 144.2415

(Our evaluated) A_xc = 144.241539

\[
\rho_{x_c} = 0.0002482 \\
\text{Pred.}_{x_c} = 0.0005437
\]

\[
\Delta_{\text{Nd}}^d = 0.00017308\% \\
\text{Pred.}_{\Delta_{\text{Nd}}^d} = 0.00054367\%
\]

\[
\Delta_{\text{Nd}}^A = -0.00016141\% \\
\text{Pred.}_{\Delta_{\text{Nd}}^A} = -0.00016148\% \text{Eq. (4a)}
\]