Research Square

Preprints are preliminary reports that have not undergone peer review.
They should not be considered conclusive, used to inform clinical practice,
or referenced by the media as validated information.

Evaluation of uncertainties in the estimates of correlated variables as the elemental-isotopic-abundances: properties of corresponding indirect-measurement system-specific-relationships

B. P. Datta

bibeknrdgpd@gmail.com

Bhabha Atomic Research Centre

Research Article

Keywords: Isotopic abundance, Atomic weight, Direct-measurement (input) uncertainty, Indirect-measurement (output) uncertainty, Input-to-output variation rate

Posted Date: November 26th, 2026

DOI: https://doi.org/10.21203/rs.3.rs-11771191/v1

License: This work is licensed under a Creative Commons Attribution 4.0 International License.
Read Full License

Additional Declarations: No competing interests reported.

Evaluation of uncertainties in the estimates of correlated variables as the elemental-isotopic-abundances: properties of corresponding indirect-measurement system-specific-relationships

B. P. Datta[1]
Radiochemistry Laboratories (BARC), Variable Energy Cyclotron Centre, Department of Atomic Energy, 1/AF Bidhan Nagar, Kolkata 700064, India

Key words: Isotopic abundance; Atomic weight; Direct-measurement (input) uncertainty; Indirect-measurement (output) uncertainty, Input-to-output variation rate

ABSTRACT

Usually, by *uncertainty*-evaluation, it is meant the assessment of certain desired-variable ($\boldsymbol{Y}$) specific indirect-measurement-uncertainty ($\boldsymbol{\epsilon^{Y}}$) from the corresponding lab-measurable-($\boldsymbol{X_m}$)-variable(s) specific uncertainty(s), $\boldsymbol{u_m(s)}$, by the error propagation law. However, the propagation-law requires the "$\boldsymbol{u_m(s)}$" to be purely accidental-in-nature, and implies the "$\boldsymbol{\epsilon^{Y}}$" also as random-by-origin. Moreover in the case, where either or both of the measurable (*input*) and the desired (*output*) variables should be correlated as the isotopic-abundance-ratios and atom-fractions ($\{\boldsymbol{X_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$, and: $\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}$, respectively) of any multi-($\boldsymbol{N}$)-isotopic element ($\boldsymbol{E}$), any output-specific-uncertainty ($\boldsymbol{\epsilon_d^Y}$) is used to be evaluated by incorporating certain inter-variables-correlation correction-factor(s) in the error propagation formula.

However, it is here clarified that: (i) $\boldsymbol{u_m(s)}$ may not, in reality, be purely statistical by origin; (ii) any output-uncertainty ($\boldsymbol{\epsilon}$) should be the exactly-corresponding *input(s)-output* system-specific-relationship (**SSR**) governed (i.e. a *systematic*) parameter, irrespective of whether $\boldsymbol{u_m(s)}$ be purely *random*-in-nature; and (iii) the uncertainty ($\boldsymbol{\epsilon_d^Y}$) of determining a correlated-quantity ($\boldsymbol{Y_d}$) should, like the desired-estimate ($\boldsymbol{y_d}$) itself, be independent of whether the desired-output (and/ or, input) variables be correlated. That is, like *non-*

[1]: The author had carried out this work as an employee (Scientific Officer) of the Bhabha Atomic Research Centre, Department of Atomic Energy, Government of India. However, the author has retired from the service. His present address is as follows: VILLAGE: Ramnagar, POST OFFICE: Hatgobindapur, DISTRICT: Purba Bardhaman, West Bengal, INDIA, Pin code: 713407.

correlated cases discussed elsewhere, any **SSR** ($\boldsymbol{Y_d = f_d(\{X_m\}_{m=2}^N)}$) here is shown to be bracketed with certain input(s)**-to-**output variation-parameter(s)**:** $\boldsymbol{[MF]_m^d(s)}$. And it is the "$\boldsymbol{[MF]_m^d(s)}$" which should, for given the lab-established input-estimate(s) $\boldsymbol{x_m(s)}$ and uncertainty(s) $\boldsymbol{u_m(s)}$, decide the corresponding output-estimate ($\boldsymbol{y_d}$) and -uncertainty ($\boldsymbol{\epsilon_d^Y}$). Thus, an 'a priori' study of only the **SSR-**characterizing-"**[*MF*]*(s)***" should help to predict the corresponding output-uncertainty ($\boldsymbol{\epsilon}$) and, to enable proper experimental-preplanning (or, where the **SSR** itself should be a *proposed*-model, to ascertain whether the modelling is being worth). We exemplify how 'a priori' predicted output-uncertainties (here, for determining the usually unknown isotopic-abundances and atomic-weight) should be authenticated.

However the uncertainties ($\boldsymbol{\epsilon_d^Y}$, and say, $\boldsymbol{\epsilon_E^A}$) of determining any desired-isotopic-abundance ($\boldsymbol{Y_d}$) and the corresponding-atomic-weight ($\boldsymbol{A_E}$) are shown to vary as a function of the measurable-($\boldsymbol{X_m}$)-variable(s). Actually, by intrinsic *input(s)***-to-***output* variation-behaviour, all conceivable **SSRs** and **models** have been classified elsewhere into the two, measurable-variable [as**:** $\boldsymbol{X_m}$] *independent* (**F.1**) and $\boldsymbol{X_m}$*-dependent* (**F.2**), families. Thus, the isotopic-**SSRs** here belong to the **F.2** family. However, the point of interest is that, whereas certain other (isotopic) **F.2**-family member as the popular-**delta-**measurement-**model** is clarified elsewhere to behave as an extraneous *error-source* in any **delta**-measurement, the $\boldsymbol{Y_d}$ and the $\boldsymbol{A_E}$ specific-**SSRs** are even exemplified to act as the (isotope, ***d***, and the element, ***E***, specific) *sinks* of corresponding experimental-(input)-error-sums (respectively).

1. INTRODUCTION

Isotopic-abundances $\left(\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}\right)$ of any multi-(***N***)-isotopic-element (***E***) are *interdependent*. Therefore the measurement of isotopic-abundances (and thus of atomic-weight $\boldsymbol{A_E}$), of an element as ***E***, is usually carried out indirectly from the, rather accurately measurable, corresponding ($\boldsymbol{N-1}$) abundance-ratios ($\{\boldsymbol{X_m = \frac{Y_m}{Y_1}}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$). The measurement-process involves, grossly, two-steps**: (i)** real-world-(mass-spectrometric)-measurements of

the ratio(s) $\boldsymbol{X_m(s)}$; and**: (ii)** computations of $\boldsymbol{Y_d}$*-values*, and/ or $\boldsymbol{A_E}$*-value*, from measured-$\boldsymbol{X_m}$*-value(s)*, using the corresponding (desired-*output*-variable versus measureable-*input*-variables) system-specific-relationship (**SSR**) as:

$$Y_d = f_d(\{X_m\}_{m=1}^N) = \frac{X_d}{\sum_{m=1}^N X_m} = \frac{X_d}{1+\sum_{m=2}^N X_m}; with: d = 1, 2 \dots N \qquad (1)$$

And:

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

where $\boldsymbol{Y_1}$ is, for the convenience of representation, referred to as the *reference*-isotopic-abundance (and thus**:** $\boldsymbol{X_1 = 1}$); and $\boldsymbol{M_d}$ stands for the $\boldsymbol{d^{th}}$-isotopic-mass.

However, any estimated-ratio ($\boldsymbol{x_m}$) should, even after correcting for the possible mass-fractionation and/ or other detected method-specific-biases, be subject to certain uncertainty [1], i.e.**:** $\boldsymbol{X_m} = (\boldsymbol{x_m} \pm \boldsymbol{u_m})$ and/ or**:** $\boldsymbol{x_m} = (\boldsymbol{X_m} \mp \boldsymbol{u_m})$; with $\boldsymbol{u_m}$ as, generally, the lab-established $\boldsymbol{X_m}$-measurement (also called *input*) uncertainty. Therefore the desired estimates ($\{\boldsymbol{y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}$, and $\boldsymbol{a_E}$) should also be at certain uncertainties (say: $\{\boldsymbol{\epsilon_d^Y}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}$, and: $\boldsymbol{\epsilon_E^A}$, respectively)**:** $\boldsymbol{Y_d} = (\boldsymbol{y_d} \pm \boldsymbol{\epsilon_d^Y})$ or**:** $\boldsymbol{y_d} = (\boldsymbol{Y_d} \mp \boldsymbol{\epsilon_d^Y})$, and**:** $\boldsymbol{A_E} = (\boldsymbol{a_E} \pm \boldsymbol{\epsilon_E^A})$ or**:** $\boldsymbol{a_E} = (\boldsymbol{A_E} \mp \boldsymbol{\epsilon_E^A})$. That is, for practical usages, the Eqs. (1) and (2) should be re-represented as:

$$(y_d \pm \epsilon_d^Y) = f_d(\{x_m \pm u_m\}_{m=1}^N) = \frac{(x_d \pm u_d)}{1+\sum_{m=2}^N (x_m \pm u_m)}; with d = 1, 2 \dots N \qquad (1a)$$

And:

$$(a_E \pm \epsilon_E^A) = f_E(\{[m_d \pm u_d^M], [y_d \pm \epsilon_d^Y]\}_{d=1}^N)$$

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

where $\boldsymbol{u_d^M}$ stands for the uncertainty in the *estimate* ($\boldsymbol{m_d}$) of the $\boldsymbol{d^{th}}$*-true*-isotope-mass (**$\boldsymbol{M_d}$**; *see* also the **Appendix 1**, which gives a clarification on the notations used in this paper**)**. However, it may here be mentioned that "$\boldsymbol{m_d}$ [cf. Eq. (2a)]" is, in practice, used as its recommended-Table-data, i.e. different possible measuring-lab-results ($^{Lab1}\boldsymbol{a_E}$, $^{Lab2}\boldsymbol{a_E}$, **…**), for a given sample-source, cannot get varied for mass-dependent uncertainties.

Eqs. (1a) and (2a) clarify that whether the output-estimates $\boldsymbol{y_d(s)}$ and $\boldsymbol{a_E}$ should, at least acceptably, represent their desired-true-values ($\boldsymbol{Y_d(s)}$ and $\boldsymbol{A_E}$) be indicated by the respective uncertainties, $\boldsymbol{\epsilon_d^Y(s)}$ and $\boldsymbol{\epsilon_E^A}$, only. Thus, correct knowledge of the output-uncertainties should be a part and parcel of the desired indirect measurements. However, how should the said-requirement be truly fulfilled?

Of course, the 2nd-stage-task **(**computation of a desired result**:** $\boldsymbol{y_d}$, or $\boldsymbol{a_E}$**)** should in practise be accomplished by simply replacing the ratio-variable(s), $\boldsymbol{X_m(s)}$, in the corresponding **SSR (**Eq.(1), or Eq.(2)**)** by their estimate(s), $\boldsymbol{x_m(s)}$, and therefore, without involving any extraneous **(**i.e. other than the ratio-$\boldsymbol{X_m}$-measurement**)** *source-of-error* in the overall process of the desired (indirect) measurement. Yet, a question is raised**:** should the acceptably accurate ratio-estimate(s), $\boldsymbol{x_m(s)}$, ensure the desired-results ($\{\boldsymbol{y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}$, and $\boldsymbol{a_E}$) also to be so accurate? That is, shouldn't the computational-process (**SSR**) play a role in deciding the (magnitude of the corresponding) output-estimate ($\boldsymbol{y_d}$, or $\boldsymbol{a_E}$) and/ or true output-error or -uncertainty? Thus, let's consider e.g. any possible **bi-**isotopic (i.e. *single*-ratio) measurement-system ($\boldsymbol{d = 1}$ and $\boldsymbol{2}$; $\boldsymbol{m = [N-1] = 1}$). Then, should the output-uncertainties be *necessarily* equal to the corresponding (single) input-uncertainty ($\boldsymbol{\epsilon_1^Y = \epsilon_2^Y = \epsilon_E^A = u_{m=(N-1)=1}}$)? How should the case, for '$\boldsymbol{N \geq 2}$'**,** get governed? Above all, can we 'a priori' predict any resultant-uncertainty **(**$\boldsymbol{\epsilon_d^Y}$, viz. as a factor, $\boldsymbol{[UF]_d}$, of a given measure, $\boldsymbol{^G u}$, of achievable measurement-[input]-uncertainty, i.e. as**:** $\boldsymbol{\epsilon_1^Y = ([UF]_d \times {}^G u)}$**)**, thereby enabling the required possible development of the method of ratio-measurement(s)?

However, it may be pointed out that if the ratio-uncertainty(s) can somehow be ensured to be nil (i.e. if**:** $\boldsymbol{u_m(s) = 0}$), then any resultant-uncertainty should have to be nil ($\boldsymbol{\epsilon(s) = 0}$). Moreover, a result cannot vary for whether the computations be carried out manually or by off-line/ on-line software. Therefore, the basic question raised and/ or to be

resolved here is**:** how exactly the uncertainty-*translation* as either**:** $(\{\boldsymbol{u_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}) \rightarrow \boldsymbol{\epsilon_d^Y}$; or**:** $(\{\boldsymbol{u_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}) \rightarrow \boldsymbol{\epsilon_E^A}$; or even**:** $(\{\boldsymbol{u_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}, \{\boldsymbol{u_d^M}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}) \rightarrow \boldsymbol{\epsilon_E^A}$, should take place?

However, what exactly the term, uncertainty, should mean?

2. UNCERTAINTY

As indicated by e.g. Eq. (1) and Eq. (1a), any input-estimate ($\boldsymbol{x_m}$) should be equal to its unknown-true-value ($\boldsymbol{X_m}$) provided that (the input**-**uncertainty)**:** $\boldsymbol{u_m} = \mathbf{0}$. Otherwise (i.e. for**:** $\boldsymbol{u_m} \neq \mathbf{0}$), the estimate "$\boldsymbol{x_m}$" may turn out to be so much *higher* than its true-value "$\boldsymbol{X_m}$" that**:** $\boldsymbol{x_m} = \boldsymbol{(X_m + u_m)}$ or even so much *lower* that**:** $\boldsymbol{x_m} = \boldsymbol{(X_m - u_m)}$. That is to say, the uncertainty "$\boldsymbol{u_m}$" should stand for the **possible (**and therefore the *highest* and *unaccountable*), **error** in the **(**directly**-**measured, and hence the mass-fractionation and all other detected biases corrected, input**)** estimate**:** $\boldsymbol{x_m}$ (cf. the Section 0.2 in [1]). Thus, as a natural consequence, the resultant-uncertainty ($\boldsymbol{\epsilon_d^Y}$, cf. Eq. 1a) should also stand for the *highest***-***possible*-error in the desired-result**:** $\boldsymbol{y_d}$. Similarly, $\boldsymbol{\epsilon_E^A}$ (cf. Eq. 2a) should represent the highest-possible-error in the estimate $\boldsymbol{a_E}$ (of the desired true atomic weight $\boldsymbol{A_E}$).

Here, it may also be re-noted that the ratio-uncertainty "$\boldsymbol{u_m}$" **(**which may itself turn out to be the measurement method specific and/ or the isotopic-abundance-ratio specific, and which should account for the *possible* errors due to**:** (i) detected-biases-correction *processes* employed, and even**:** (ii) small **undetectable** biases**)** should have no alternative to getting ascertained, with the aid of relevant standards, by the experimenting-lab. Therefore, the idea here is to simply explore the fact as to how really, for given the input-uncertainty(s) $\boldsymbol{u_m(s)}$, the output-uncertainty(s) $\boldsymbol{\epsilon(s)}$ should get decided and/ or be evaluated/ predicted.

However the central *cause*, behind the *effect* called (input/ output) uncertainty, is *measurement*. Thus, to begin with, it may be worth evaluating (cf. **Appendix 2**) the points**: (i)** purpose of any required (direct/ indirect) measurement, and**: (ii)** difference, if should be any, between *uncertainty* and *accuracy* (of an estimate).

2.1 Output-uncertainty: conventional concept of evaluation

It could, perhaps without an exception, be shown that the evaluation of rather any kind of indirect-measurement-variable ($\boldsymbol{Y}$) specific uncertainty is meant by the established literature until today as truly the assessment of corresponding *predicted-scatter* ($\boldsymbol{\rho_Y}$) laid down by the popular error propagation law itself, or by the measurement system specific implemented formulation (and/ or by certain specific method but based on the implications) of the propagation law **(**cf. e.g. [1-12], and the references therein**)**. The predicted-scatter is also called as the combined standard [1] or probable [13] uncertainty.

However, the propagation law itself is based on the idea that, by origin, the input-uncertainty(s), and the corresponding output-uncertainty, should be purely random [13]. That is, we should here consider that the input-uncertainty**:** $\boldsymbol{u_m = \sigma_m}$ (with $\boldsymbol{\sigma_m}$ as the *standard deviation* [1] of the ratio-$\boldsymbol{X_m}$-measurements), and the output-uncertainties $\boldsymbol{\epsilon_d^Y}$ and $\boldsymbol{\epsilon_E^A}$ (for determining the $\boldsymbol{d^{th}}$**-**isotopic-abundance, $\boldsymbol{Y_d}$, and atomic-weight, $\boldsymbol{A_E}$, respectively) as**:** $\boldsymbol{\epsilon_d^Y = \rho_d}$ and or**:** $\boldsymbol{\epsilon_E^A = \rho_E}$. Accordingly, the predicted-scatter, e.g. $\boldsymbol{\rho_d}$, is computed here as:

$$\rho_d = \frac{1}{y_d}\left[\sum_{m=1}^{N}\left(\frac{\partial Y_d}{\partial X_m}\right)^2 \sigma_m^2\right]^{1/2} \qquad (3)$$

However, as indicated even here above, the predicted-scatter as either "$\boldsymbol{\rho_d}$" or "$\boldsymbol{\rho_E}$" is generally being computed (cf. e.g. Refs. [8,9] and so) by incorporating suggested [1] correlation-*correction*-factor(s) in Eq. (3). That is, inter-variables-correlation is used to be considered as an uncertainty-governing-parameter.

However, we should here re-note that**:** (i) it is difficult, in practice, to ensure the input-uncertainty(s) $\boldsymbol{u_m(s)}$ as purely random in nature (cf. **Appendix 2**); (ii) it is because that the isotopic-abundances ($\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}$) are correlated, the abundance-measurements are (rather required to be) carried out indirectly from the correspondingly-estimated-ratios, $\{\boldsymbol{x_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$; and **(**as implied by the Eq. (1/ 1a) or Eq. (2/ 2a)**):** (iii) for *given* the **SSR** and the

input-estimate(s), the correspondingly desired output-*estimate* and therefore its *true*-error and/ or *uncertainty* can in no way **(**say, even be caused to**)** get affected by the factors as**: (1)** the *inter-dependency* of isotopic-abundances ($\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}$**,** and/ or of their-ratios**:** $\{\boldsymbol{X_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$); **(2)** *experimental*-methodology; and (if at all involved) *mathematical*-processes, of deciding the input-estimate(s) $\boldsymbol{x_m(s)}$; and so. The point here is also returned to the below.

2.2 On "$\boldsymbol{u_m(s) \rightarrow \epsilon}$" translation and "correlation": Predictability of"$\boldsymbol{\epsilon}$"

Any desired-result, e.g. $\boldsymbol{d^{th}}$**-**atom-fraction ($\boldsymbol{y_d}$), is *in practice* obtained (cf. Eq.(1/ 1a) as: $\boldsymbol{y_d = f_d(\{x_m\}_{m=2}^N)}$. The latter **(**$\boldsymbol{y_d = f_d(\{x_m\}_{m=2}^N)}$**)** may, in terms of **true** input- and output-*errors* ($\{\Delta_{\boldsymbol{m}}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$ and $\Delta_{\boldsymbol{d}}^{\boldsymbol{Y}}$, respectively), be rewritten as:

$$(Y_d \pm \Delta_d^Y) = f_d(\{X_m \pm \Delta_m\}_{m=2}^N) \qquad (1b)$$

And in terms of input- and output-*uncertainties* ($\{\boldsymbol{u_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$ and $\boldsymbol{\epsilon_d^Y}$, respectively) as:

$$(Y_d \pm \epsilon_d^Y) = f_d(\{X_m \pm u_m\}_{m=2}^N) \qquad (1a^{/})$$

Eq. (1b) and/ or Eq. (1a$^{/}$) clarifies that, **(**though a desired-result should need to be computed by simply replacing the concerned-input-variables ($\{\boldsymbol{X_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$) by their-estimates ($\{\boldsymbol{x_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$)**)**, the desired**-***translation* "([input-estimates(s)]**:** $\boldsymbol{x_m(s)}$ → [output-estimate]**:** $\boldsymbol{y_d}$)" and the ***hidden***-transformation "([true**-**input-error(s)]**:** $\boldsymbol{\Delta_m(s)}$ → [true-output-error]**:** $\boldsymbol{\Delta_d^Y}$)" and therefore, the *corresponding*-transformation of "**given**-input-uncertainty(s) *into* output-uncertainty**:** $[^{\mathbf{MAX.}}\boldsymbol{\Delta_m(s)} \rightarrow {}^{\mathbf{MAX.}}\boldsymbol{\Delta_d^Y}] \equiv [\boldsymbol{u_m(s)} \rightarrow \boldsymbol{\epsilon_d^Y}]$", should all be**: (i)** dictated by the $\boldsymbol{d^{th}}$**-[SSR as]-**Eq.**(1)**, and**: (ii)** be complementary and/ or be accomplished (like the well-known oxidation and reduction processes) simultaneously. That is to say that any output-uncertainty **(**e.g. "$\boldsymbol{\epsilon_d^Y}$" of determining the *correlated*-variable "$\boldsymbol{d^{th}}$-isotopic-abundance**:** $\boldsymbol{Y_d}$"**)** should, like the corresponding output-estimate (as "$\boldsymbol{y_d}$") itself, be the concerned**-SSR (**as, here, the "$\boldsymbol{d^{th}}$-abundance specific Eq.**(1),** rather the function**:** $\boldsymbol{f_d}$ "**)** *governed*-systematic-parameter. Therefore, output-uncertainty ($\boldsymbol{\epsilon}$) is likely to be **predictable** a priori.

Moreover, for a *given* set of input-estimates (as "$\{x_m\}_{m=2}^{N}$"), corresponding two different **SSRs**/ functions (viz.: $Y_d = f_d(\{X_m\}_{m=2}^{N})$, and $Y_d^{/} = f_d^{/}(\{X_m\}_{m=2}^{N})$) cannot generally yield the output-estimates (y_d, and $y_d^{/}$) of exactly the same-magnitude; and therefore corresponding *true*-(output)-errors (Δ_d^{Y}, and $\Delta_d^{Y/}$) should be different by their magnitudes. However, the said statement should be a fact provided that the functions "f_d, and $f_d^{/}$" be characterized by *different* input(s)-**to**-output variation-***rate(s)*** [14].

Thus, it is exactly the concerned-**SSR** (rather the function as "f_d"), which really preset(s) whether the **2nd**-stage process (computational-step: $[x_m(s) \rightarrow y_d]$) should **act**, effectively, as either "an *extraneous*-error-*source*" or "a kind of *sink* of net-experimental-[input]-error" or "a *non-interfering-medium*" in the overall-process of the indirect-measurement (as of "Y_d") and hence, in defining the corresponding true-output-error (as "Δ_d^{Y}") and/ or output-uncertainty (as "ϵ_d^{Y}").

Therefore, the task of evaluating/ predicting an output-uncertainty "ϵ" should reduce to identifying (cf. **Appendix 3)** the corresponding **SSR** (Eq. (1) or Eq. (2) here) *characterizing* input(s)-*to*-output *variation*-parameter(s).

2.2.1 *Evaluation of output-uncertainty (ϵ)*

A desired result, e.g. d^{th}-atom-fraction (y_d), is obtained only at the end of certain computations in terms of, however, the corresponding **SSR** as the d^{th}-isotope-specific-Eq.(1). Thus, it is not only that the **SSR** as Eq.(1) has happened to be known. It is but also that a requirement, for any indirect-measurement to be carried out, to establish the representative input-output **SSR/** model beforehand.

Again, as clarified in Appendix **3**, given an **SSR** as Eq.(1) means that the corresponding (function "f_d", specific) *individual*-input, and even the *collective*-inputs, based ***rates*** of output-*variations* ($[MF]_m^d\}_{m=2}^{N}$ and $[UF]_d$, respectively) are also given,

thereby enabling to either account for or even 'a priori' predict the corresponding output-uncertainty $\boldsymbol{\epsilon_d^Y}$ as **(**cf. Eq. (6b) and also Eqs. (7) and (7a)**)**:

$$\epsilon_d^Y = \sum_{m=2}^{N} \left(\left|[MF]_m^d\right| \times u_m\right) = \left([UF]_d \times {}^{G}u\right)$$

Thus, the evaluation/ prediction of an output-uncertainty "$\boldsymbol{\epsilon}$" should essentially mean the evaluation of corresponding *uncertainty-factor* (**[*UF*]**). However, before examining whether the "**[*UF*]**", corresponding to the isotopic **SSR** as either **Eq.(1)** or **Eq.(2)**, should be **>1** or **<1** or **1 (**i.e. whether the estimated atom-fraction $\boldsymbol{y_d}$ [cf Eq.(1a)] and/ or atomic weight $\boldsymbol{a_E}$ [cf Eq.(2a)] should, at least for any bi-isotopic element, turn out to be worse or better or equally accurate as the corresponding *single* input-estimate $\boldsymbol{x_m}$**)**, a note on the possible classification of **SSRs**/ models is believed to be useful here (cf. **Appendix 4**).

Either or both of the isotopic-**SSRs** "Eq. (1) and Eq.(2)" should be belonging to, as clarified in Appendix **4**, the **F.1** or the **F.2** family. That is the uncertainties ($\{\boldsymbol{\epsilon_d^Y}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}$, and $\boldsymbol{\epsilon_E^A}$) of determining the isotopic-abundances and atomic-weight ($\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{N}}$**,** and $\boldsymbol{A_E}$, respectively) of any possible element (***E***) **c**ould be decided **(**like the **F.1** family-case as [cf. Appendix 4] the uncertainty, $\boldsymbol{\epsilon_R^Y}$, of valuating any simple-*ratio* of two different input-estimates**)** by the isotopic-abundance-ratio ($\boldsymbol{X_m}$) *measurement*-[input]-uncertainties ($\{\boldsymbol{u_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$) only. Alternatively **(**i.e. like the **F.2** family-case [cf. Appendix 4] of the ***delta-****ratio*-uncertainty**:** $\boldsymbol{\epsilon_\delta^Y}$**)**, either or both of the uncertainties ($\boldsymbol{\epsilon_d^Y}$, and $\boldsymbol{\epsilon_E^A}$) should get governed by the ***collective-****factors* as**:** (i) ratio- $\boldsymbol{X_m}$ -variable(s) itself(s) and**:** (ii) corresponding-measurement-uncertainty(s), $\boldsymbol{u_m(s)}$.

However, we are yet to examine and/ or exemplify as to what be the facts. The *measurement*-[input]-uncertainty $\boldsymbol{u_m}$ is ascertained by real world measurement on a relevant standard. However, the evaluation of any indirect-measurement-result and/ or corresponding-uncertainty "$\boldsymbol{\epsilon}$" is a theoretical task. Therefore, we should ensure the uncertainty "$\boldsymbol{\epsilon}$" governing facts on one or more theoretical-standards (i.e. on known isotopic-compositions

(**ICs**)). Nevertheless, we should also show, below, how any possible unknown case specific output-uncertainty ($\boldsymbol{\epsilon}$) be 'a priori' predicted and, even verified.

3. RESULTS AND DISCUSSION: prediction and verification of "$\boldsymbol{\epsilon(s)}$"

The **SSRs,** Eq.(1) and Eq.(2), are isotopic-*multiplicity*-(***N***)-specific. Thus let us first consider the simplest possible isotopic-measurement-system, ***bi-****isotopic* element (***N*** **= 2**), for our investigation.

3.1 Bi-isotopic cases

Let's suppose that **(**for developing the required method of determining the isotopic composition and the atomic weight of **e.g.** natural chlorine, and hence for establishing the isotopic-ratio measurement-(*input*)-uncertainty**:** $\boldsymbol{u_m \equiv u_{37/35}}$**)** we have chosen a chlorine material of the known **^{37}Cl/^{35}Cl**-abundance-ratio**:** ($\boldsymbol{X_m \equiv X_{37/35}}$) = **0.3199578**, and interested to know *beforehand* whether an acceptable "$\boldsymbol{u_m}$" should ensure the output-uncertainties, $\{\boldsymbol{\epsilon_d^Y}\}_{\boldsymbol{d=1}}^{\boldsymbol{2}}$ and $\boldsymbol{\epsilon_{Cl}^A}$ **(**of determining the any corresponding-***unknown***, i.e. natural/ near natural chlorine, isotopic-abundances**:** $\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{2}}$ and atomic-weight**:** $\boldsymbol{A_{Cl}}$, respectively**),** to also be so restricted **(viz.** whether**:** $[\boldsymbol{\epsilon_1^Y \equiv \epsilon_{35}^Y}] = [\boldsymbol{\epsilon_2^Y \equiv \epsilon_{37}^Y}] = \boldsymbol{\epsilon_{Cl}^A = u_m}$, be *true***?)**.

3.1.1 *Prediction of output-uncertainty(s)*

One can easily verify that the abundance-ratio, ($\boldsymbol{X_m} \equiv X_{37/35}$) = **0.3199578**, should imply that the *true* ^{35}Cl and ^{37}Cl abundances ($\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{2}}$, cf. Eq. (1)) to be**:** $\boldsymbol{(Y_1 \equiv Y_{35})}$ **= 0.7576**, and**:** $\boldsymbol{(Y_2 \equiv Y_{37})}$ **= 0.2424**, respectively; and the corresponding true atomic-weight **(**$\boldsymbol{A_{Cl}}$ **[**cf. Eq.(2)**]**, however for considering the true isotopic-masses as**:** $\boldsymbol{[M_1 \equiv M_{35}]}$ **= 34.968852682**, and**:** $\boldsymbol{[M_2 \equiv M_{37}]}$ **= 36.965902602)** to be**:** $\boldsymbol{A_{Cl}}$**=** **35.45293763**. Thus, as clarified above (cf. section 2.2.1 and/or Appendix **3**), the output-variable (as either: $\boldsymbol{Y_{35}}$, or: $\boldsymbol{Y_{37}}$, or: $\boldsymbol{A_{Cl}}$) specific input-*to*-output *variation*-parameters can also be readily evaluated (cf. **Appendix 5**).

Here, we are dealing with an input-output-system, which involves a single *measurement*-**[**input]-variable**:** ($\boldsymbol{X_m \equiv X_{37/35}}$). Yet, it may really be emphasized that the

output-*governing* parameters **(**as the relative-**rates**-of-variations, **[*MF*]*(s)*** [cf. Eq.**(4)**], of the different desired-variables $\boldsymbol{Y_{35}}$, $\boldsymbol{Y_{37}}$, and $\boldsymbol{A_{Cl}}$ as a function of their **common** input-variable $\boldsymbol{X_{37/35}}$; and/ or the corresponding uncertainty-*factors* (**[*UF*]*(s)***, cf. Eq.**(7))** and thus (cf. Eq.**(6)**) the uncertainties $\boldsymbol{\epsilon_{35}^{Y}}$, $\boldsymbol{\epsilon_{37}^{Y}}$, and $\boldsymbol{\epsilon_{Cl}^{A}}$ (i.e. those for determining the **^{35}Cl** and **^{37}Cl** *natural-abundances* and the *atomic-weight*, respectively) are predicted to be different from one another and, most importantly, from the *input*-ratio-uncertainty**:** $\boldsymbol{u_m \equiv u_{37/35} \equiv {}^{G}u}$ (i.e. [cf. **Appendix 5**]**:** $\boldsymbol{\epsilon_{35}^{Y} \neq \epsilon_{37}^{Y} \neq \epsilon_{Cl}^{A} \neq u_{37/35}}$). However, the interesting point is that any desired-estimate ($\boldsymbol{y_{35}}$ or, $\boldsymbol{y_{37}}$ or, $\boldsymbol{a_{Cl}}$) is predicted to be ***less*** *erroneous* than even the input-(ratio)-estimate ($\boldsymbol{x_m \equiv x_{37/35}}$) itself**:** $\boldsymbol{\epsilon_{35}^{Y} < u_{37/35}}$; $\boldsymbol{\epsilon_{37}^{Y} < u_{37/35}}$ and: $\boldsymbol{\epsilon_{Cl}^{A} < u_{37/35}}$.

Moreover, the predicted facts (cf. Appendix **5**, and Eq.**(6a/ 6b):** $\boldsymbol{\epsilon = ([UF] \times u_m)}$) are further highlighted in **Fig. 1**, which depicts the different desired-*output*-variables ($\boldsymbol{Y_{35}}$, $\boldsymbol{Y_{37}}$ and, $\boldsymbol{A_{Cl}}$) specific *plots* of **"output-**uncertainty ($\boldsymbol{\epsilon}$) **vs. input-**uncertainty ($\boldsymbol{u_m \equiv u_{37/35}}$)**".** Thus, perhaps the unusual prediction ($\boldsymbol{\epsilon < u_m}$, cf. Appendix **5**, i.e.) that the **SSR** as either Eq.**(1)** or Eq.**(2)** should, in the overall process of the *indirect*-measurement, act as the concerned-*variable*-specific ***sink*** of input-[experimental]-*error* is better revealed in **Fig. 1**, which reflects the ***slopes*** of all the *three* variables-*specific* "$\boldsymbol{\epsilon}$ vs. $\boldsymbol{u_m}$" variation-lines being**: (i)** *different* from one another, and**: (ii) "<1".**

Here, it may also be pointed out (cf. **Appendix 5**) that the uncertainty-factor, $\boldsymbol{[UF]_d}$, and thus the uncertainty, $\boldsymbol{\epsilon_d^Y}$, of determining the isotopic-abundance ($\boldsymbol{Y_d}$) are predicted to be inversely proportional to (the magnitude of) "$\boldsymbol{Y_d}$". And the **"**$\boldsymbol{[UF]_d}$**"** should, for any ***bi-****isotopic* (***d* = 1** and **2**) case as here, take the value as**:** $\boldsymbol{[UF]_1 = \left|[MF]_m^1\right| = 0.2424 = Y_2}$ (i.e. here**:** $\boldsymbol{[UF]_{35} = Y_{37}}$) and/ or**:** $\boldsymbol{[UF]_2 = \left|[MF]_m^2\right| = 0.7576 = Y_1}$ (here: $\boldsymbol{[UF]_{37} = Y_{35}}$).

Moreover, it should be significant to note (cf. Appendix **5**) that any **SSR** rather output-variable ($\boldsymbol{Y_d}$, or $\boldsymbol{A_{Cl}}$) specific *input*-**to**-*output*-variation-*rate* (**[*MF*]**) and, in turn, the

uncertainty-factor (**[UF]**) and/ or the uncertainty (ϵ) is shown to be *decided* by the measurement-(*input*)-variable ($X_m \equiv X_{37/35}$) itself, e.g.**:** $[MF]_m^{35} = f_{35}(X_m)$. That is, **firstly**, the uncertainty (ϵ) of determining an isotopic-abundance (Y_d) or the atomic-weight (A_{Cl}) should be *varying* as a function of even (the magnitude of) the isotopic-ratio: X_m.

Thus, let's consider (in the place of the *natural* chlorine ($X_m \equiv X_{37/35}$) **= 0.3199578**) a ***non-****natural* chlorine (**Cl**$^{/}$), e.g.**:**($X_m^{/} \equiv X_{37/35}^{/}$) **= 0.6**. Then one can, like the natural case (Appendix **5**), verify that the uncertainties ($\epsilon^{/}(s)$) of determining any such (a kind of) *non-natural* chlorine isotopic abundances ($\{Y_d^{/}\}_{d=1}^{2}$) and the atomic weight ($A_{Cl}^{/}$) should get (*varied* from the natural case) as**:** $\epsilon_{35}^{Y/} = (0.375 \times u_m)$, $\epsilon_{37}^{Y/} = (0.625 \times u_m)$, and**:** $\epsilon_{Cl}^{A/} = (0.0131044 \times u_m)$.

Secondly, both of the kinds of isotopic-**SSRs** (**Eq.(1)** and **Eq.(2)**, here) should, *like* the **IRMS-**measurement-model**:** f_δ (cf. Appendix **4**), belong to the "**F.2**" *family* [14,16] of **SSRs-**cum-mathematical-**models**. Yet, it should be worth pointing out that any present-isotopic-**SSR** and the **IRMS-**model are *opposite* by their intrinsic *input*-**to**-*output* variation features, namely, while either the function**:** f_d (cf. Eq. (1) or the function**:** f_E (cf. Eq. (2) should act as an intrinsic *sink* of experimental-*error*, the **IRMS-**model (function**:** f_δ) has been shown [14,16,19,20] to act as an extraneous *error-source* (in the respective cases of indirect measurements). These should clarify why an 'a priori' study of *intrinsic* input-**to**-output variation behaviour of any **SSR**/ **model**, representing an *indirect*-measurement to be carried out, should help to properly pre-plan and/ or to pre-assess the outcome of the ***proposed*** measurement.

Moreover, it should be important noting that **neither** the process of evaluating the input-**to**-output variation governing-parameters **(**cf. **Eqs**. (4-7)**) nor** their implications (cf.

Appendix **5**, and **Fig. 1**) did require to take into consideration the fact that the isotopic abundances "$(Y_1 \equiv Y_{35})$ and $(Y_2 \equiv Y_{37})$" are *interdependent*.

3.1.1.1 *Multi-measurement-feature of the bi-isotopic system as atomic weight*

Above, we have discussed how the uncertainty ($u_m \equiv u_{37/35}$) of the single possible measurable variable ($X_m \equiv X_{37/35}$) be transformed into, even, the uncertainty (ϵ_{Cl}^{A}) of determining the atomic-weight (A_{Cl}). However the isotopic masses, though being used as recommended Table-data, are subject to certain uncertainties**:** ($\{M_d = [m_d \pm u_d^M]\}_{d=1}^{N=2}$). Thus, it should here be of interest to find out how much the *mass*-errors ($\{u_d^M\}_{d=1}^{N}$) be causing the desired-result (a_{Cl}) and therefore, the resultant-error **(ϵ_{Cl}^{A})**, to be varied.

Nevertheless, like the above case ($u_m \rightarrow \epsilon_{Cl}^{A}$), one can verify that the **multi**-inputs (isotopic ratio and masses) based uncertainty-transformation, here**: ($[u_m, u_{35}^M, u_{37}^M] \rightarrow \epsilon_{Cl}^{A}$),** be dictated, ***collectively***, by the isotopic ratio-X_m-*specific* and each of the two different isotopic masses-*specific* inputs-**to**-output variation-parameters **(**of the atomic-weigh, A_{Cl}, defining **SSR: Eq.2**) shown in the **Appendices 5 and 6**, respectively.

The present (multi-measurement) consideration, it may be pointed out, should also explain *why***: (i)** the relative-**rate**-of-variation, **[*MF*]** (cf. Eq.(4), is being referred to here as, also, the *individual*-error-multiplication-factor, and**: (ii)** the uncertainty-factor, **[*UF*]** (cf. Eq.(7)/ (7a), as either the *collective* **(**i.e. **SSR/** desired-**output**-variable specific**)** error-magnification-factor, or even the *collective***-**rate-of-variation.

Moreover, it should be of interest to note (cf. Appendix **6**) that the d^{th}-isotopic-mass (M_d, cf. Eq.(2)) dependent error-multiplication-factor ($[MF]_{M_d}^{A_{Cl}}$) has turned out to represent (by its formulation and/ or magnitude) the d^{th}-isotopic-*mass-**fraction***. And, which is why, the *sum* of the individual mass-(M_d)-dependent rates-of-variations equals to unity **($\sum_{d=1}^{2} \left|[MF]_{M_d}^{A_{Cl}}\right| = 1.0$**; cf. Appendix **6 (**for the *uncertainty-factor*, $[UF]_{A_{Cl}}$**))**. However the

important point here is that, as any "$[\boldsymbol{MF}]_{\boldsymbol{M_d}}^{\boldsymbol{A_{Cl}}}$" is a fraction, the **SSR** (Eq.(2)) should **(**with reference to, *either* any individual mass-specific error ($\boldsymbol{u_d^M}$), *or* all three inputs specific collective-error) act as the desired-output (here**:** $\boldsymbol{A_{Cl}}$) specific ***sink***-of-*error* in the corresponding-case of indirect-measurement.

Here, it may be repeated that mass-error cannot cause the desired-estimate ($\boldsymbol{a_{Cl}}$) to vary between measurements and/or labs. Yet (cf. Appendix **6**), it could be noted that **(**the *input*-to-*output* variation-*rate***:** $\left|[\boldsymbol{MF}]_{\boldsymbol{M_d}}^{\boldsymbol{A_{Cl}}}\right| \gg \left|[\boldsymbol{MF}]_{\boldsymbol{X_m}}^{\boldsymbol{A_{Cl}}}\right|$, i.e.**)** the desired-estimate ($\boldsymbol{a_{Cl}}$) is predicted to be **more** vulnerable towards a given variation ($^{G}\boldsymbol{u}$) in any isotopic-mass ($\boldsymbol{M_d}$) than that in the isotopic-ratio ($\boldsymbol{X_m}$). This should in turn explain why the mass ($\boldsymbol{M_d}$) specific *uncertainty-factor* has turned out to be so much higher as **≈100** times of the *ratio* ($\boldsymbol{X_m}$) specific *uncertainty-factor* **(**i.e. while [cf. Appendix **6** and even no. **5]** the **ratio-**based-uncertainty**:** $^{(Ratio)}\boldsymbol{\epsilon_{Cl}^{A}} = (^{(Ratio)}[\boldsymbol{UF}]_{\boldsymbol{A_{Cl}}} \times {}^{G}\boldsymbol{u}) = (\boldsymbol{0.0103445} \times {}^{G}\boldsymbol{u})$, the ***mass***-specific uncertainty**:** $^{(Mass)}\boldsymbol{\epsilon_{Cl}^{A}} = (^{(Mass)}[\boldsymbol{UF}]_{\boldsymbol{A_{Cl}}} \times {}^{G}\boldsymbol{u}) = (\boldsymbol{1.0} \times {}^{G}\boldsymbol{u})$**)**.

3.1.2 *Should the above predictions be true?: exemplification of facts*

Let the **(**preset/ pre-established ^{37}**Cl**/^{35}**Cl** ratio-*measurement* and detected-*biases*-corrected**)** input-uncertainty, ($[^{Max.}|\Delta_{\boldsymbol{m}}| \equiv \boldsymbol{u_m}] = {}^{G}\boldsymbol{u}$), be **0.01**%. Then the correspondingly *estimated* natural ^{35}**Cl** and ^{37}**Cl** abundances **(**$\boldsymbol{y_{35}}$ and $\boldsymbol{y_{37}}$, cf. Eq.(1a)**)** and atomic weight **(**$\boldsymbol{a_{Cl}}$, cf. Eq.(2a)**)** are predicted (cf. **Appendix 5**) to turn out to be as accurate (uncertain) as**:** $(^{\text{Pred.}}\boldsymbol{\epsilon_{35}^{Y}} = [^{\text{Pred.}}[\boldsymbol{UF}]_{\boldsymbol{35}} \times {}^{G}\boldsymbol{u}] = [0.2424 \times \boldsymbol{0.01}\%] =)$ 0.002424%, $(^{\text{Pred.}}\epsilon_{37}^{Y} = [0.7576 \times \boldsymbol{u_m}] =)$ 0.007576%, and**:** $(^{\text{Pred.}}\epsilon_{Cl}^{A} = [0.0103445 \times \boldsymbol{u_m}] =)$ 0.000103445%, respectively.

Now, let us suppose that two different real world measurements of the chlorine standard, ($\boldsymbol{X_m} \equiv \boldsymbol{X_{37/35}}$) = **0.3199578**, have yielded the possible bias corrected *ratio-estimates* (i.e. inputs) as**: (i)** $\boldsymbol{x_m}$= **[**(X_m+ u_m) = ($\boldsymbol{X_m}$+ **0.01**%) = ($\boldsymbol{X_m}$+ **[**0.0001 × $\boldsymbol{X_m}$**]**)] = **0.3199898**; and**: (ii)** $\boldsymbol{x_m}$= **[**($\boldsymbol{X_m} - \boldsymbol{u_m}$) = ($\boldsymbol{X_m}$ − [0.0001 × $\boldsymbol{X_m}$])] = **0.31992580**.

Then it could be verified that the output-*estimates* by all of the three chlorine-**SSRs** (**Y_{35}**-specific-Eq.**(1)**, **Y_{37}**-specific-Eq.**(1)** and **A_{Cl}**-specific-Eq.**(2)**) turn out to really be as accurate as predicted. That is, for**:** x_m= **0.3199898** (cf. input no. **(i)**), one should obtain**:**

y_{35} = 0.75758164 **(**= [$Y_{35} - (0.00002424 \times Y_{35})$] = [**0.7576** − $^{\text{Pred.}}\epsilon^{Y}_{35}$]**)**;

y_{37} = 0.242418386 **(**= [$Y_{37} + (0.00007576 \times Y_{37})$] = [**0.2424** + $^{\text{Pred.}}\epsilon^{Y}_{37}$]**)**; and:

a_{Cl} = 35.45297430 **(**= [A_{Cl} + (0.00000103445 × A_{Cl})] = (**35.45293763** + $^{\text{Pred.}}\epsilon^{A}_{Cl}$).

And, the "input no. **(ii)**: x_m = **0.31992580**" should in turn yield**:**

y_{35} = 0.75761834 = **(**Y_{35} + $^{\text{Pred.}}\epsilon^{Y}_{35}$**)**;

y_{37} = 0.24238166 = **(**Y_{37} − $^{\text{Pred.}}\epsilon^{Y}_{37}$**)**; and**:**

a_{Cl} = 35.45290095 = (A_{Cl} − $^{\text{Pred.}}\epsilon^{A}_{Cl}$).

3.1.2.1 *Consideration of even mass-uncertainty (*u^{M}_{d}*): Verification of "*$^{\text{Pred.}}\epsilon^{A}_{Cl}$*"*

Let the *input*-ratio-uncertainty (u_m) as well as the -mass-uncertainty (u^{M}_{d}) to be 0.01%**:** ^{G}u **(**$u_m = u^{M}_{35} = u^{M}_{37}$ **=)** $^{\text{Max.}}|\Delta|$ = **0.01**%. Then the correspondingly estimated atomic weight (a_{Cl}) should turn out **(**[cf. Appendix **6**]: $^{\text{Pred.}}\epsilon^{A}_{Cl}$ = [1.0103445 × ^{G}u] **=)** 0.010103445% accurate. Thus, it should be of interest to note that the mod-**sum** of input-errors, corresponding to any possible case where *each* of the three different input-estimates (*ratio***:** x_m, and *masses***:** m_{35} and m_{37}) be subject to exactly **±0.01%** error, becomes**:** $3^{G}u$ = **0.03**%. However the corresponding output-error ($|\Delta^{A}_{Cl}|$) is predicted to, firstly, be ***less*** than "$3^{G}u$ **= 0.03%**" and, secondly, be so *restricted* as**:** $|\Delta^{A}_{Cl}| \leq (\text{Pred.}\,\epsilon^{A}_{Cl} = \mathbf{0.010103}\%)$.

Let now, for examining the veracity of our above prediction, consider certain sets (viz. those as the example nos. **(1)-(5)** in the **Appendix 7**) of the three *input*-(ratio and mass)**-**estimates having subject to exactly **±0.01%** errors, and evaluate the corresponding results of the atomic-weight (A_{Cl}). It may thus be noted (cf. Appendix 7) that the true-*output***-**error "$|\Delta^{A}_{Cl}|$" has either *equalled* the predicted *highest-possible-error* ($^{\text{Pred.}}\epsilon^{A}_{Cl}$ = 0.010103%, cf.

Example no. **(1)** and no. **(2)**), *or* turned out to be *less* than "$^{\text{Pred.}}\epsilon_{Cl}^{A}$ (cf. Example nos. **(3)-(5)**)"; but in ***no*** *case* exceeded "$^{\text{Pred.}}\epsilon_{Cl}^{A}$". Above all the prediction that the **SSR** as the "Eq.(2)" should act as a sink-of-error is verified by the fact that "$\left|\Delta_{Cl}^{A}\right|$" has in every case turned out to be *much* ***less*** than the mod-**sum** (0.03%) of input-errors.

Thus, it should be clear that (cf. Appendices (5-7)) any output (variable-specific-uncertainty-factor "**[*UF*]**" and hence the) uncertainty "$\boldsymbol{\epsilon}$" be unquestionably decided by the **(***input(s)*-**to**-*output* **variation-***characteristics* of the**)** exactly corresponding **SSR**, which should in any of our isotopic cases act as the output**-**variable *specific* ***sink*** of experimental (input) error in the overall process of the desired-*indirect*-measurement.

Yet, it may be enquired: should the *nature* of the above discussed facts be **different** for cases of *isotopic-multiplicity* (***N***) "**> 2**"?

3.2 Tri-isotopic systems

The variation of *isotopic-multiplicity* (***N***) from "(***N*** **= 2**)" should essentially cause the **number** of, significantly, the *measurable-*$\boldsymbol{X_m}$**-**variables being involved in the evaluation-process (**SSR**) as either Eq.(1) or Eq.(2) to be varied from only one as above to "**>1**". Therefore, for "(***N*** **> 2**)", the inputs-**to**-output uncertainty-transformation process should basically be no different from that discussed above, particularly, under the "*multi-measurement-feature* of **bi-isotopic**-systems" (cf. section **3.1.1.1**).

However, the isotopic-mass "$\boldsymbol{M_d}$, cf. Eq.(2)" is never being a lab-measurable variable. Thus any possible *tri-isotopic* element, for which the determination of isotopic abundances ($\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{3}}$ **(**cf. Eq.(1)**)**) and/ or atomic weight ($\boldsymbol{A_E}$ **(**Eq.(2)**)**) requires the measurement of two different isotopic-abundance-ratios "$\{\boldsymbol{X_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{3}}$", should stand for the simplest possible real world *multi*-measurement system. It is therefore considered here worth to re-affirm the features of (and/ or to point out the difference if any in) the output-

uncertainty evaluation process (cf. **Eq.(6/ 6b)**) in the light of a tri-isotopic element, viz. Oxygen.

Actually, recollecting the facts discussed above, it may at this outset be pointed out that the input-ratio-($\boldsymbol{X_m}$)-dependent *individual* and *collective* **rates** of output-variations (**[*MF*]** and **[*UF*]**, respectively) cannot, i.e. unlike ***bi-isotopic***-cases, be (by magnitude) the same for systems of "($\boldsymbol{N > 2}$)". Anyway, we will now exemplify the facts by choosing the *natural* oxygen [21] as the required isotopic-**standard**.

3.2.1 ***Predictive consideration***

The oxygen isotopes, their masses (true $\boldsymbol{M_d}$-values), *relative*-abundances (i.e. true values of the measurable- $\boldsymbol{X_m}$ -variables), atom fractions (true $\boldsymbol{Y_d}$ -values) and the corresponding (**Eq.(1)**, i.e. the *output-variable*) $\boldsymbol{Y_d}$ specific predicted input-**to**-output *variation*-governing-parameters **(**as**:** $[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}$, $[\boldsymbol{UF}]_{\boldsymbol{d}}$ and $\boldsymbol{\epsilon_d^Y}$**)** are furnished in Table 1. Similarly, the true atomic weight of oxygen ($\boldsymbol{A_O}$) and the corresponding **(**Eq.**(2)**, i.e. the *variable***:** $\boldsymbol{A_O}$, specific**)** input-**to**-output variation-parameters are tabulated in Table 2. However it may here be re-noted, i.e. like the ***bi-****isotopic* case, that the prediction of any *output-uncertainty* "$\boldsymbol{\epsilon}$" (cf. Table 1 and Table 2) did in no way require to take into account that the isotopic-abundances ($\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{3}}$) and/ or their ratios ($\{\boldsymbol{X_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{3}}$) are correlated.

Further, the predictions (cf. Table 1 and Table 2) are, as pointed out below, no different, by their basic-features, from those for the *bi-isotopic*-systems discussed above:

i) **(**Irrespective of whether the *measurement*-accuracy, $\boldsymbol{u_m}$, should be the ratio-$\boldsymbol{X_m}$-specific**)**, the achievable accuracy ($\boldsymbol{\epsilon_d^Y}$) of determining any isotopic-abundance, $\boldsymbol{Y_d}$, should be the *isotope* "***d***" specific (*comparison between* 2nd, 3rd and 4th *rows in* Table 1).

ii) The "$\boldsymbol{Y_d}$ vs. $\boldsymbol{X_m}$" variation-rate ($[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}$, cf. the Cols. 6 and 7 in Table 1 for specified**:** ***d*** and ***m*****)** and thus the achievable accuracy, $\boldsymbol{\epsilon_d^Y}$ (cf. Col. 8), of determining any atom fraction ($\boldsymbol{Y_d}$) are, again like *bi-isotopic*-systems, shown to be *governed* by the

measurable variables ($\boldsymbol{X_2}$ and $\boldsymbol{X_3}$); thereby re-ascertaining that the **"Eq.(1)**" should, for its intrinsic input(s)-to-out variation feature(s), belong to the **F.2** family of **SSRs**.

iii) The uncertainty-factor ($[\boldsymbol{UF}]_{\boldsymbol{d}}$) and/ or the uncertainty ($\boldsymbol{\epsilon_d^Y}$, cf. Col. 8 in Table 1**)** of determining an isotopic abundance ($\boldsymbol{Y_d}$) is also here predicted to bear inverse relation with the "$\boldsymbol{Y_d}$" to be estimated.

iv) The **SSRs,** *isotopic*-Eq.(1) and *element*-specific-Eq.(2), are also here asserted to act, in the overall processes of the corresponding indirect measurements, as the respective isotope-***d***- and element-***E***-specific ***sinks*** of net-input-*error* (i.e. *any*, corresponding, input-**to**-output variation-*rate*)**:** $|[\boldsymbol{MF}]| < 1$ (cf. Table 1 and Table 2).

v) The atomic weight $\boldsymbol{A_O}$ is (also like the above discussed "$\boldsymbol{A_{Cl}}$") predicted to be more susceptible towards a given variation ($^{G}\boldsymbol{u}$) in any isotopic-*mass* ($\boldsymbol{M_d}$) than that in any isotopic-*ratio* ($\boldsymbol{X_m}$). And, the reason is also the same as that for "$\boldsymbol{A_{Cl}}$".

That is, though the *uncertainty-factor* ($[\boldsymbol{UF}]_{\boldsymbol{A_O}}$, and/ or the *uncertainty* $\boldsymbol{\epsilon_O^A}$) of determining the atomic weigh ($\boldsymbol{A_O}$) is predicted to be significant (cf. col. 7 in Table 2)**:** $[\boldsymbol{UF}]_{\boldsymbol{A_O}} = \mathbf{1.00028}$ (and thus**:** $\boldsymbol{\epsilon_O^A} = (\mathbf{1.00028} \times {}^{G}\boldsymbol{u})$), the *ratio*-based uncertainty-factor is insignificant**:** $^{(Ratio)}[\boldsymbol{UF}]_{\boldsymbol{A_O}} = \sum_{m=2}^{3}\left|[\boldsymbol{MF}]_{X_m}^{A_O}\right| = \mathbf{0.00028}$, and the *mass*-dependent-part (which can here also be verified to represent the sum of mass fractions, and thus) is relatively so high as unity**:** $^{(Mass)}[\boldsymbol{UF}]_{\boldsymbol{A_O}} = \sum_{d=1}^{3}[\boldsymbol{MF}]_{M_d}^{A_O} = \mathbf{1}$.

However, the *isotopic masses* should remain ***invariable*** from one experiment/ lab to another. Therefore, even for an unexpectedly higher ratio-measurement uncertainty as "$^{G}\boldsymbol{u} = \mathbf{1\%}$", the *uncertainty* ($\boldsymbol{\epsilon_O^A}$) of determining the atomic weigh ($\boldsymbol{A_O}$, involving, say for simplicity, equally uncertain input-ratios $\boldsymbol{x_2}$ and $\boldsymbol{x_3}$) should rather be insignificant:

$\epsilon_O^A = ([UF]_{A_O} \times {}^{G}u) = \mathbf{0.00028\%}$.

However, should the predictions be true?

3.2.2 Verification of the predictions

Let the input-ratio-uncertainty be: $(\boldsymbol{u_2} \equiv {}^{\text{Max.}}|\Delta_2|) = (\boldsymbol{u_3} \equiv {}^{\text{Max.}}|\Delta_3| = {}^{G}\boldsymbol{u} = \pm\mathbf{0.01}\%$.

Then, for our predictions (cf. *Col.* 8 in Table 1) to be correct, the true-*error* ($\Delta_{\boldsymbol{d}}^{\boldsymbol{Y}}$) in the correspondingly estimated $^{16}\mathbf{O}$, $^{17}\mathbf{O}$, and $^{18}\mathbf{O}$ *abundances* ($\boldsymbol{y_1}$, $\boldsymbol{y_2}$and $\boldsymbol{y_3}$, respectively) should be restricted as**:** $\left|\Delta_{\mathbf{16}}^{\boldsymbol{Y}}\right| \leq (\boldsymbol{\epsilon}_{\mathbf{16}}^{\boldsymbol{Y}} = \mathbf{0.0000243}\%)$; $\left|\Delta_{\mathbf{17}}^{\boldsymbol{Y}}\right| \leq (\boldsymbol{\epsilon}_{\mathbf{17}}^{\boldsymbol{Y}} = \mathbf{0.0100167}\%)$; and**:** $\left|\Delta_{\mathbf{18}}^{\boldsymbol{Y}}\right| \leq (\boldsymbol{\epsilon}_{\mathbf{18}}^{\boldsymbol{Y}} = \mathbf{0.0099833}\%)$.

And, if all the isotopic *masses* are also considered, here for verifying the related prediction (cf. Col. 7 in Table 2), to be subject to 0.01% uncertainty **(**i.e. if: ${}^{\text{Max.}}\left|\Delta_{\boldsymbol{d}}^{\boldsymbol{M}}\right| = \pm\, 0.01\%$, with:*d* = 1, 2 and 3**)**; then the true-*error* ($\Delta_{\boldsymbol{O}}^{\boldsymbol{A}}$) of the *estimated* atomic-weight ($\boldsymbol{a_O}$) should turn out to be**:** $\left|\Delta_{\boldsymbol{O}}^{\boldsymbol{A}}\right| \leq (\boldsymbol{\epsilon}_{\boldsymbol{O}}^{\boldsymbol{A}} = \mathbf{0.0100028}\%)$.

However, do the said-output-errors follow the said-dictums?

Here, we are dealing with a case of known (true values of) $\boldsymbol{X_m}$ and, $\boldsymbol{Y_d}$**,** and $\boldsymbol{M_d}$ (cf. Table 1). Therefore, as shown for the bi-isotopic case, the predictions here can also be verified in terms of *generated*-input-estimates (of the *known-error* "$\pm\mathbf{0.01}\%$") as:

$$x_m = (X_m \pm u_m) = (X_m \pm {}^{\text{Max.}}|\Delta_m|) = (X_m \pm\ 0.01\%) \qquad (8)$$

And:

$$m_d = (M_d \pm {}^{\text{Max.}}|\Delta_d^M|) = (M_d \pm\ 0.01\%) \qquad (8a)$$

Such an endeavour is made in Table 3. However it may be noted that, in Table 3, we have considered the input**-***estimates* **(**for both of the Eq.(1) and Eq.(2), *cf. Cols*. 2 and 6**)** having subject to not only "$\pm\mathbf{0.01}\%$ errors (*cf. Example nos.* 1 and 2)" but also as high as "$\pm\mathbf{1.0}\%$ errors (*cf. Examples* 3 *and* 4); and presented the correspondingly derived estimates of $^{16}\mathbf{O}$, $^{17}\mathbf{O}$, and $^{18}\mathbf{O}$ abundances (*cf. Cols*. 3, 4 and 5) and atomic-weight **(**$\boldsymbol{A_O}$**,** [*cf. Col.* 7]**)**, and their *observed*-true-errors **(**$\Delta_{\boldsymbol{d}}^{\boldsymbol{Y}}$ and $\Delta_{\boldsymbol{O}}^{\boldsymbol{A}}$-values**)** and also, for immediate comparison, their ***predicted***-true-errors (${}^{\text{Pred.}}\Delta_{\boldsymbol{d}}^{\boldsymbol{Y}}$ and ${}^{\text{Pred.}}\Delta_{\boldsymbol{O}}^{\boldsymbol{A}}$, cf. Eq.(**5**)) and -uncertainties ($\boldsymbol{\epsilon}_{\boldsymbol{d}}^{\boldsymbol{Y}}$and $\boldsymbol{\epsilon}_{\boldsymbol{O}}^{\boldsymbol{A}}$).

However, it should be noted that the *example no*. 4 in Table 3 considers the isotopic *masses* as **constants**, thereby offering the opportunity to verify the predicted *accuracies* for determining the atomic weight against the ***variable***, and ***invariable***, isotopic-masses (*comparison between example no.* 3 *and no.*4).

At this stage, it might be kept in mind that Eq. (1) and Eq. (2) are *non-linear*. Yet, as Table 3 verifies, the predictions above (and/ or as of Tables 1 and 2) are correct for the ***highest*** *possible* (individual) input-*error* of not only $\pm 0.01\%$ (**cf.** example nos. 1 and 2) but also $\pm 1.0\%$ (**cf.** example nos. 3 and 4). Thus it may, for clarity, be pointed out that the **mod-sum** of input-*ratio*-errors is 0.02% (cf. either example no. 1 or no. 2) or as high as 2.0% (cf. example nos. 3 and 4). However, the output**-**(*abundance*)-errors are, firstly, *different* for different isotopes **(***comparison*, for a given example, between column nos. 3, 4 and 5**)**; secondly, *less* (by the magnitude) than the corresponding-input-error-**sum**; and thirdly, in *agreement* with their predicted values **(**e.g.: $(\Delta_{16}^{Y} = {}^{\mathbf{Pred.}}\boldsymbol{\Delta_{16}^{Y}}) \leq {}^{\mathbf{Pred.}}\boldsymbol{\epsilon_{16}^{Y}}$ [cf. any of the example nos. 1-4; and/ or [see, specifically, the *example no.* 2]: $(\Delta_{16}^{Y} = {}^{\mathbf{Pred.}}\boldsymbol{\Delta_{16}^{Y}}) < {}^{\mathbf{Pred.}}\boldsymbol{\epsilon_{16}^{Y}}$**)**. Over and above, the output error has in **no** case, numerically, exceeded the corresponding predicted uncertainty. Thus, simply for making the foresaid fact somewhat vivid, the *output error* in Table 3 has been *emboldened*, however, **only** in those cases where it has acquired its *highest* predicted value (cf. e.g. [example no. 1 and column 3]**:** $|\Delta_{16}^{Y}| = {}^{\text{Pred.}}|\Delta_{16}^{Y}| = {}^{\mathbf{Pred.}}\boldsymbol{\epsilon_{16}^{Y}}$; or [example 2 and column 4]**:** $|\Delta_{17}^{Y}| = {}^{\text{Pred.}}|\Delta_{17}^{Y}| = {}^{\mathbf{Pred.}}\boldsymbol{\epsilon_{17}^{Y}}$).

It should also be pointed out here that, for evaluating the atomic weight ($\boldsymbol{A_O}$, [*cf. Col.* 7 in Table 3), the mod**-sum** of *input*-errors (*cf. Cols.* 2 and 6 in Table 3) is as high as either **0.05%** (cf. example no. 1 or 2) or 2**.0%** (cf. example no. 4) or **5.0%** (cf. example no. 3). However, as predicted, the error (Δ_O^A) of the evaluated estimate ($\boldsymbol{a_O}$) is much *less* than the corresponding-input-error-**sum**, and is in *agreement* with its predicted value **(**i.e.: ($\Delta_O^A =$

$^{\text{Pred.}}\Delta_O^A) < {}^{\text{Pred.}}\epsilon_O^A$ [cf. Col. 7 for example no. 2], and/ or: $(\Delta_O^A = {}^{\text{Pred.}}\Delta_O^A) \leq {}^{\text{Pred.}}\epsilon_O^A$ [cf. any of the example nos. 1-4]**)**.

Furthermore, the example no. **4 (**which considers the *isotopic masses* as certain ***constants***, and thus their *invariability* between experiments/ labs**)** confirms that the computational step as Eq. **(2)** should, in the overall process of the corresponding-indirect-measurement, play the role of really a ***sink*** of input-(*experimental*)-*error* (viz. the mod-sum input-error of "**2%**" is caused to be reduced to "**0.00028%**" as the output error). This fact is, moreover, elaborated in Fig. **2**, which depicts the variation of the *output-error* (Δ_O^A) as a function of the *mod-**sum**-of-input-errors* as $2\boldsymbol{u_m}$ (i.e. mod-sum-errors of the [known] *equally* erroneous *two* different input-ratios $\boldsymbol{x_2}$ and $\boldsymbol{x_3}$). It may thus be noted that **(**irrespective of any possible value of the input-ratio-error "$\boldsymbol{u_m}$"**):** $\Delta_O^A \ll (2\boldsymbol{u_m})$**.**

The present considerations should thus assert that **(***irrespective* of the isotopic-multiplicity (***N***), interdependence of isotopic-abundances/ -ratios and so**)** the output-uncertainty "$\boldsymbol{\epsilon}$" be the corresponding input-output **SSR** governed systematic parameter.

However how should the output-uncertainty "$\boldsymbol{\epsilon}$" be, in any *unknown* case, evaluated?

3.3 An unknown case and the output-uncertainty "ϵ"

Let us consider *an abundance spectrum from the literature* for discussion.

The measured [4] estimates ($\boldsymbol{x_m}$-values) of the isotopic-abundance-ratios of xenon and the corresponding reported [4] uncertainties, the correspondingly reported atom-fractions ($\boldsymbol{y_d}$-values) and their probable errors ($\boldsymbol{\rho_d}$-values), and the atomic weight ($\boldsymbol{a_{Xe}}$) and its probable error ($\boldsymbol{\rho_{Xe}}$), are reproduced in Table 4 (*cf. Cols.*4 and 5, and *the bottom leftmost box*, respectively). However it should be noted (cf. Col. 4 in Table 4) that "$^{\text{Max.}}|\Delta \boldsymbol{X_m}|$" refers to the reported [4] *absolute* value of the $\boldsymbol{m^{th}}$-ratio-*uncertainty* and, "$\boldsymbol{u_m}$" to the (correspondingly computed) *relative* value. Similarly, "$^{\text{Max.}}|\Delta \boldsymbol{M_d}|$" and "$\boldsymbol{u_d^M}$" (cf. Col. 2) represent the

reported [4] *absolute* and the (correspondingly computed) *relative* uncertainties in the isotopic-mass ($\boldsymbol{m_d}$).

3.3.1 *Prediction of the output-uncertainties* ($\{\epsilon_d^Y\}_{d=1}^{9}$ *and,* ϵ_{Xe}^A)

We have here also evaluated, corresponding to the reported [4] *inputs* (cols. 2 and 4 in Table 4), the desired *results* (outputs). This was so done for examining whether our computations cause the results to vary from the reported [4] ones. Our evaluated atom fractions ($\boldsymbol{y_d}$-values) and atomic weight ($\boldsymbol{a_{Xe}}$-value), along with their respective probable errors ($\boldsymbol{\rho_d}$- and $\boldsymbol{\rho_{Xe}}$-values, but which were computed using the Eq. 3 above) and the *predicted* (cf. Eq.6/ 6b) uncertainties ($^{\mathbf{Pred.}}\boldsymbol{\epsilon_d^Y}$ and $^{\mathbf{Pred.}}\boldsymbol{\epsilon_{Xe}^A}$ values), are also furnished in the Table 4 (cf. Col. 6 and the bottom side middle box, respectively). The discrepancy, if there is at all any between the reported [4] and our computed atom-fractions (*comparison* of $\boldsymbol{y_d}$-values between *cols.* 5 and 6) and/ or between the estimates of atomic weight (*comparison* of $\boldsymbol{a_{Xe}}$-values between the bottom side *left* and *middle* blocks), should mostly be due to the truncation of data.

However, it should be noted that the output-uncertainties, $^{\mathbf{Pred.}}\boldsymbol{\epsilon_d^Y}$ and $^{\mathbf{Pred.}}\boldsymbol{\epsilon_{Xe}^A}$, are here predicted (cf. Eq. 6/ 6b) by considering the corresponding input-uncertainties (as the $\boldsymbol{u_m}$-values and also, for the case of atomic weight, the $\boldsymbol{u_d^M}$-values) to be exactly as those reported [4] and/ or tabulated in cols. 4 and 2, respectively, of Table 4.

Moreover, it may be important mentioning here that the *method* whatsoever, employed for evaluating the uncertainty on any (unknown) output-estimate, should demand to consider (at least in the back of the mind) the *estimate* itself as its ***true-****value*. Thus, irrespective of whether the foregoing statement should be a fact or not, we have here considered **(**either for *predicting* (cf. Eq. 6/ 6b) the uncertainties on the reported [4] estimates of xenon-isotopic-abundances and atomic weight "$\{\boldsymbol{y_d}\}_{d=1}^{9}$ and $\boldsymbol{a_{Xe}}$, respectively"; **or** for *verifying* subsequently whether our predictions are correct or not**)** the measured cum reported [4] isotopic-

abundance-ratios ($\boldsymbol{x_m}$-*values*, cf. Col.4 in Table 4) as their true-values. That is, we have here evaluated the ($\boldsymbol{Y_d}$ vs. $\boldsymbol{X_m}$), ($\boldsymbol{A_{Xe}}$ vs. $\boldsymbol{X_m}$) and even ($\boldsymbol{A_{Xe}}$ vs. $\boldsymbol{[X_m, M_d]}$) specific variation-parameters (as $\boldsymbol{[MF]}$- and $\boldsymbol{[UF]}$-values, cf. Eq.4 and Eq. 7, respectively) by assuming that: $\{\boldsymbol{X_m = x_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{9}}$ and hence: $\{\boldsymbol{Y_d = y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{9}}$, and: $(\boldsymbol{A_{Xe} = a_{Xe}})$.

The determination of xenon isotopic abundances ($\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{9}}$) involves eight ($\boldsymbol{m}$ = 2-9, cf. Eq.(1)) different ratio-$\boldsymbol{X_m}$-measurements. Therefore, any $\boldsymbol{Y_d}$-specific uncertainty ($\boldsymbol{\epsilon_d^Y}$, cf. Eq.6/ 6b) should also be decided by eight individual ratio-$\boldsymbol{X_m}$-dependent *input*-**to**-*output* variation-*rates*: $\{[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}\}_{\boldsymbol{m=2}}^{\boldsymbol{9}}$. However it should be noted that, for simplicity, only the $\boldsymbol{Y_d}$-specific *highest*-[$\boldsymbol{MF}$]-*value* ($^{\mathbf{Max.}}\left|[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}\right|$) and, of course, the corresponding *collective*-variation-*rate* (uncertainty-factor: $\boldsymbol{[UF]_d}$, cf. Eq.(7)) are tabulated in Table 4 (cf. Cols. 7 and 8, respectively). Moreover, the determination of atomic weight ($\boldsymbol{A_{Xe}}$, cf. Eq.(2)) should *additionally* be subject to so many as the nine different isotopic-mass-uncertainties ($\left\{\boldsymbol{u_d^M}\right\}_{\boldsymbol{d=1}}^{\boldsymbol{9}}$), and hence so many mass-$\boldsymbol{M_d}$-specific *input*-**to**-*output* variation-*rates* ($\left\{[\boldsymbol{MF}]_{\boldsymbol{M_d}}^{\boldsymbol{A_{Xe}}}\right\}_{\boldsymbol{d=1}}^{\boldsymbol{9}}$).

Here, it may also be re-noted that the determination of xenon isotopic abundances requires ***eight*** ($\boldsymbol{m}$ = 2-9, cf. Eq.(1)) different ratio-$\boldsymbol{X_m}$-measurements. Therefore, the (*true-**error*** and, hence the) *uncertainty* of each of the **nine** *estimated*-isotopic-abundances ($\{\boldsymbol{y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{9}}$) should be decided by the ***collective*** contribution of the **eight** different ***input***-*isotopic-ratios* "$\{\boldsymbol{x_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{9}}$" specific (*true-**errors*** and, thus the) *uncertainties* "$\{\boldsymbol{u_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{9}}$" (respectively). And, the determination of atomic weight ($\boldsymbol{A_{Xe}}$, cf. Eq.(2)) should **additionally** be subject to so many as the **nine** different isotopic-mass-uncertainties ($\left\{\boldsymbol{u_d^M}\right\}_{\boldsymbol{d=1}}^{\boldsymbol{9}}$). However, *only* the corresponding-*collective* "$\boldsymbol{A_{Xe}}$ **vs.** $\boldsymbol{(X_m, M_d)}$" variation-rate (*uncertainty-factor*: $\boldsymbol{[UF]_{A_{Xe}}}$) is furnished in Table 4 (cf. the bottommost row/ box).

Yet, the content as the Table 4 should be self-explicable that, *by nature*, its implications are no different from those for either ***bi-*** or ***tri-****isotopic* cases above, viz.**:** (i) the uncertainty $\boldsymbol{\epsilon_d^Y}$ should be the isotope (***d***) specific, (ii) the computational-step**,** Eq. (1), should act as an *error-sink* **(**and is because that, even, the "$^{\textbf{Max.}}\left|[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}\right|$" is, irrespective of the isotope ***d***, "**<1**"**)**; and**:** (iii) Eq. (2) should behave as the isotopic-abundance-*pattern*- and/ or *element*-sensitive error-***sink*** **(**as**:** $^{\textit{Ratio}}[\boldsymbol{UF}]_{\boldsymbol{A_{Xe}}} = \sum_{m=2}^{9}\left|[MF]_{X_m}^{A_{Xe}}\right| = \mathbf{0.0116323}$ [cf. the bottommost row in Table 4**)**. Thus say that all the eight estimated-ratios ($\{\boldsymbol{x_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{9}}$) are *equally* erroneous, viz.**:** $^{G}\boldsymbol{u} = |\Delta_{\boldsymbol{m}}| = \mathbf{1.0\%}$. Then, though the net-input-error ($\sum_{m=2}^{9}|\Delta_m|$) becomes as high as **8**%, the *highest*-possible-output-*error* ($^{\textbf{Max.}}\left|\Delta_{\boldsymbol{Xe}}^{\boldsymbol{A}}\right| = {}^{\textit{Ratio}}\boldsymbol{\epsilon_{Xe}^{A}}$) should turn out to be **(**[cf. Eq.(6a)]**:** $^{\textit{Ratio}}\boldsymbol{\epsilon_{Xe}^{A}} = (^{\textit{Ratio}}[\boldsymbol{UF}]_{\boldsymbol{A_{Xe}}} \times {}^{G}\boldsymbol{u}) = (0.0116323 \times {}^{G}u) =$**) 0.0116323**% only.

Moreover, the present predictive implications are further clarified in **Fig. 3**, where it is (for simplicity) assumed that all the required ratio-estimates ($\{\boldsymbol{x_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{9}}$) to be *equally* uncertain as "$\boldsymbol{u_m}$" and offered the *input*-**to**-*output* uncertainty-*variations* as "$\boldsymbol{\epsilon_d^Y}$ **v**s. $\boldsymbol{u_m}$" **(**however, for only three typical isotopes [namely, "***d***" as the highest, middle and lowest abundant ^{132}**Xe**, ^{134}**Xe** and ^{126}**Xe,** respectively]**),** and also "$\boldsymbol{\epsilon_{Xe}^{A}}$vs. $\boldsymbol{u_m}$". Thus, it may be noted that the *slope* **(**[***UF***], cf. Eq.**(6a))** of any isotope "***d***" e.g. ^{132}**Xe**-specific "$\boldsymbol{\epsilon_d^Y}$ **v**s. $\boldsymbol{u_m}$" line is *different* from the *slope* of any other isotope or even ($\boldsymbol{\epsilon_{Xe}^{A}}$vs. $\boldsymbol{u_m}$; i.e.) atomic-weight-$\boldsymbol{A_{Xe}}$ specific line. Above all that the computational-step, **SSR** as either Eq.(1) or Eq.(2), should characteristically act as a kind of (input/ experimental) error-*sink* is reflected by the fact that **(**any variable-specific output-uncertainty**):** $\boldsymbol{\epsilon < 8u_m}$ (rather, $\boldsymbol{\epsilon \ll 8u_m}$).

Moreover the isotopic mass ($\boldsymbol{M_d}$) dependent *rate of variation* of atomic weight (i.e.**:** $\left|[\boldsymbol{MF}]_{\boldsymbol{M_d}}^{\boldsymbol{A_{Xe}}}\right|$) could, like the chlorine or the oxygen case above, be shown to equal the corresponding ($\boldsymbol{d^{th}}$) isotopic mass *fraction* (e.g.: $[\boldsymbol{MF}]_{\boldsymbol{M_{124}}}^{\boldsymbol{A_{Xe}}} = 0.00089796$; or: $[\boldsymbol{MF}]_{\boldsymbol{M_{129}}}^{\boldsymbol{A_{Xe}}} = 0.25920437$; and of course, it could be shown that**:** $\sum_{d=1}^{9}\left|[\boldsymbol{MF}]_{\boldsymbol{M_d}}^{\boldsymbol{A_{Xe}}}\right| = \mathbf{1.0}$). That is, any

individual *mass*-uncertainty ($\boldsymbol{u_d^M}$), which is though generally insignificant, should in the process of defining (cf. Eq.(2a) the output-estimate ($\boldsymbol{a_{Xe}}$) and hence, the output-uncertainty ($\boldsymbol{\epsilon_{Xe}^A}$), be further *reduced* by a factor equalling the corresponding isotopic mass-fraction.

It should over and above be noted that our considerations on the *unknown* isotopic-abundance-pattern [4] here did in **no** way, i.e. like those above on the known ***bi-*** or ***tri-*** isotopic case, require to take the interdependence of isotopic abundances ($\{\boldsymbol{Y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{9}}$) and/ or ratios ($\{\boldsymbol{x_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{9}}$) into account.

However, it should also be pointed out (cf. Table **4**) that the uncertainty ($\boldsymbol{\epsilon}$) of determining any Xe-atom-fraction "$\boldsymbol{Y_d}$" (*Col.* 6) or even the atomic weight "$\boldsymbol{A_{Xe}}$" (*cf. the bottom side middle block*) is predicted to be higher than the corresponding reported [4] combined standard uncertainty **(**or than that evaluated using the Eq. (3) here**)**: $^{\textbf{Pred.}}\boldsymbol{\epsilon_d^Y} > \boldsymbol{\rho_d}$, and even: $^{\textbf{Pred.}}\boldsymbol{\epsilon_{Xe}^A} > \boldsymbol{\rho_{Xe}}$.

However, should there be any way for examining the veracity of our predictions on the present *unknown* case [4]?

3.3.2 *Validation of predictions: experimental view-point*

We have, for our predictions above, considered the reported [4] *estimates* (cf. col. 4 in Table 4) of isotopic-ratios as their *true-values*, i.e.**:** $\{\boldsymbol{X_m} = \boldsymbol{x_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{9}}$ and hence: $\{\boldsymbol{Y_d} = \boldsymbol{y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{9}}$, and**:** $\boldsymbol{A_{Xe}} = \boldsymbol{a_{Xe}}$. Therefore, exactly like the *known* bi- or tri-isotopic case, the predictions here can be verified in terms of *generated* input-estimates of *known* errors **(** $\boldsymbol{x_m} = (\boldsymbol{X_m} \pm \boldsymbol{u_m}) = (\boldsymbol{X_m} \pm {}^{\textbf{Max.}}|\Delta_{\boldsymbol{m}}|)$, with: *m* = 2-9**)** and: ($\boldsymbol{m_d} = (\boldsymbol{M_d} \pm \boldsymbol{u_d^M}) = (\boldsymbol{M_d} \pm {}^{\textbf{Max.}}|\Delta_{\boldsymbol{d}}^{\boldsymbol{M}}|)$, with: *d* = 1-9**)**. Such an opportunity is offered in Table 5.

However, it should be noted (cf. Table **5**) that**:** (i) Ex. Nos. 1 and 2 refer to the input ratio- and mass-errors ($\Delta_{\boldsymbol{m}}$ and $\Delta_{\boldsymbol{d}}^{\boldsymbol{M}}$) as *exactly* the reported [4] ratio- and mass-uncertainties ($\pm\boldsymbol{u_m}$ and $\pm\boldsymbol{u_d^M}$; tabulated in Cols.4 and 2 of Table **4**), respectively; (ii) Ex. Nos. 2a and 3

correspond to**:** $\{\Delta_{\boldsymbol{m}} = \pm \boldsymbol{u_m}\}_{m=2}^{9}$, but $\left\{\Delta_{\boldsymbol{d}}^{\boldsymbol{M}} = \boldsymbol{0.0}\right\}_{d=1}^{9}$; (iii) Ex. No. 4 gives the results for**:** $\{\Delta_{\boldsymbol{m}} = \pm \boldsymbol{1.0}\%_m\}_{m=2}^{9}$, and $\left\{\Delta_{\boldsymbol{d}}^{\boldsymbol{M}} = \boldsymbol{0.0}\right\}_{d=1}^{9}$"; and**:** (iv) Ex. No. 5 refers to all the different ratio- and mass-errors as $\pm \boldsymbol{1.0}\%$. However the results of *abundance* (i.e. "$\boldsymbol{Y_d}$ vs. $\boldsymbol{X_m}$") *variations*, corresponding to any foresaid case, are in Table 5 shown for, only, three typical isotopes, namely, the somewhat *lower*-, *highest*- and *middle*-abundant ^{124}Xe, ^{132}Xe and ^{136}Xe (cf. Cols. 3, 4 and 5), respectively. This is so done for simplifying the presentation.

However the point to be noted (cf. Table 5) is that, irrespective of whether the input-*errors* are **small** as the reported [4] input-*uncertainties* (cf. Example Nos. 1-3) or so **high** as $\pm \boldsymbol{1.0}\%$ (cf. Example Nos. 4 and 5), the results of all of the above said-*inputs*-**to-***output* variations (cf. cols. 3, 4, 5 and 7) supplement the *predictions*; e.g. any output-error is**:** (i) by magnitude, ***less*** than the corresponding input-error-**sum**, (ii) in *agreement* with its predicted (cf. Eq.**5**) value; **viz.:** $\Delta_{\boldsymbol{124}}^{\boldsymbol{Y}} = {}^{\textbf{Pred.}}\Delta_{\boldsymbol{124}}^{\boldsymbol{Y}}$, and even: $\Delta_{\boldsymbol{Xe}}^{\boldsymbol{A}} = {}^{\textbf{Pred.}}\Delta_{\boldsymbol{Xe}}^{\boldsymbol{A}}$ (cf. Cols. 3 and 7, respectively, for *any of the examples* 1-5), and/ or**:** (iii) "$\leq^{\textbf{Pred.}}\boldsymbol{\epsilon}$ (predicted-uncertainty)" e.g. : $\left(\left|\Delta_{\boldsymbol{124}}^{\boldsymbol{Y}}\right| = {}^{\text{Pred.}}\left|\Delta_{\boldsymbol{124}}^{\boldsymbol{Y}}\right|\right) < {}^{\textbf{Pred.}}\boldsymbol{\epsilon}_{\boldsymbol{124}}^{\boldsymbol{Y}}$ (*cf. Ex. Nos.* 2-5), and**:** $(|\Delta_{Xe}^{A}| = {}^{\text{Pred.}}|\Delta_{Xe}^{A}|) < {}^{\textbf{Pred.}}\boldsymbol{\epsilon}_{\boldsymbol{Xe}}^{\boldsymbol{A}}$ (*cf. Ex. Nos.* 1, 3 and 5).

Should the above shown agreement between the theory of indirect measurement uncertainty (Eq. 6/ 6b) and the observations on correlated quantities be accidental?

Actually, it had already been clarified elsewhere [14-16,19,20] that the method of evaluating the indirect measurement uncertainty "Eq.(6/ 6b)" should *not* be dependent on the (*nature* of the *variables* of the *derived*) *system* to be applied. Yet, we may here examine our considerations in terms of some other isotopic data from the literature.

3.4 Considerations for certain [6] isotopic estimates of Nd

As indicated in Table 6, we have assumed the TIMS-measured [6] **Nd**-isotopic abundance ratios ($\{\boldsymbol{x_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{7}}$, cf. col. 4), the correspondingly estimated [6] isotopic abundances ($\{\boldsymbol{y_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{7}}$, cf. col. 5) and atomic-weight ($\boldsymbol{a_{Nd}}$, cf. the bottom side 1stblock) as

their respective true values**:** $\{\boldsymbol{X_m} = \boldsymbol{x_m}\}_{m=2}^{7}$, $\{\boldsymbol{Y_d} = \boldsymbol{y_d}\}_{d=1}^{7}$, and**:** $\boldsymbol{A_{Nd}} = \boldsymbol{a_{Nd}}$. And, in terms of the reported [6] input-ratio-uncertainties ($\{\boldsymbol{u_m}\}_{m=2}^{7}$, cf. col.4), we have evaluated the *uncertainties* **(**$\boldsymbol{\epsilon(s)}$, cf. Eq. (6/ 6b)**)** and the *probable errors* **(**$\boldsymbol{\rho(s)}$, cf. Eq. (3)**)** to be expected (i.e. as per our consideration) on the reported [6] *results* as **(**$\{\boldsymbol{y_d}\}_{d=1}^{7}$, cf. col. 5**)** and **(**$\boldsymbol{a_{Nd}}$, cf. the bottom side 1st block**)**; and furnished the same, however for comparison, along with our computed output-estimates ($\{\boldsymbol{y_d}\}_{d=1}^{7}$, and $\boldsymbol{a_{Nd}}$) in the Table 6 itself **(**cf. col. 6 and the bottom side **2nd** block, respectively**)**. Thus, it may be pointed out (cf. Table 6) that our computed output-estimates are not really different from the respective reported ones (*comparison between* the cols. 5 and 6; and *between* the bottom side 1st and 2nd boxes). Moreover, the prediction of any output-uncertainty "$\boldsymbol{\epsilon}$", here again, did in no way require to take into consideration the fact that the isotopic abundances ($\{\boldsymbol{Y_d}\}_{d=1}^{7}$) are correlated.

However, should the predictions be correct?

For verifying the predicted uncertainties (${}^{\textbf{Pred.}}\boldsymbol{\epsilon_d^Y}$ and ${}^{\textbf{Pred.}}\boldsymbol{\epsilon_{Nd}^A}$), we have offered in the Table 6 itself (cf. example nos. 1, 2 and 3) the results of "$\boldsymbol{Y_d}$ **vs.** $\boldsymbol{X_m}$" and "$\boldsymbol{A_{Nd}}$ **vs.** $\boldsymbol{X_m}$" variations based on (like the above cases) the generated input-ratios ($\{\boldsymbol{x_m}\}_{m=2}^{7}$) of *known*-errors **(**as (cf. Eq. (8)/ (8a))**:** $\boldsymbol{x_m} = [\boldsymbol{X_m} \pm {}^{\textbf{Max.}}|\Delta_m|] = [\boldsymbol{X_m} \pm \boldsymbol{u_m}]$**,** with $\boldsymbol{u_m}$-*values* being the **reported** [6] ratio-uncertainties shown in col. 4 of the Table **6)**.

Thus, it should be noted that even the present results of *input*-**to**-*output* variations **(**cf. **Col.** No. 8 or 10 or 12 [for: $\boldsymbol{Y_d}$]; and the bottom side **block** corresponding to the **Ex. No.** 1 or 2 or 3 [for: $\boldsymbol{A_{Nd}}$]**)** are in corroboration with the theory **(**Eq. **(5)** and/ or Eq. **(6/ 6b)):** (i) ($\Delta_d^Y = {}^{\textbf{Pred.}}\Delta_d^Y$), or ($\left|\Delta_d^Y\right| = {}^{\textbf{Pred.}}\left|\Delta_d^Y\right|$) ≤ (${}^{\textbf{Pred.}}\boldsymbol{\epsilon_d^Y}$ [see the col. 6]); and**:** (ii) ($\Delta_{Nd}^A = {}^{\textbf{Pred.}}\Delta_{Nd}^A$), or**:** ($\left|\Delta_{Nd}^A\right| = {}^{\textbf{Pred.}}\left|\Delta_{Nd}^A\right|$) ≤ (${}^{\textbf{Pred.}}\boldsymbol{\epsilon_{Nd}^A}$= 0.0005437% [see the bottom **2nd** leftmost block]).

Moreover the **SSRs**-dependent aspects **(**corresponding to at least the assumable case where all the six input-ratios be *equally* uncertain as "$\boldsymbol{u_m}$" [cf. Eq.(6a) and also Eq.(7)]**)** are further elucidated in **Fig. (4a)**, which depicts certain typical variables specific **(**namely, for

the *highest* abundant **^{142}Nd**, the 2nd-highest abundant cum *reference* [6] isotope **^{144}Nd**, the *lowest* abundant **^{150}Nd;** and also: $\boldsymbol{A_{Nd}}$**)** "$\boldsymbol{\epsilon}$ vs. $\boldsymbol{u_m}$" *variations*. The figure shows that the *slopes* of the four different "$\boldsymbol{\epsilon}$ vs. $\boldsymbol{u_m}$" *lines* are different, i.e. **(**like the ***bi-isotopic*** system specific Fig.**1** or the **Xe** system representative Fig.**3)** asserts that, for any non-zero input-uncertainty ($\boldsymbol{u_m} \neq 0$), the output-uncertainty ($\boldsymbol{\epsilon}$) should be decided by the *exactly*-corresponding input-output **SSR)**.

Here, it may also be pointed out that the *isotopic-masses* (cf. Eq.**(2)**) are, for depicting the "$\boldsymbol{A_{Nd}}$ **vs.** $\boldsymbol{X_m}$" variation **(**cf. Fig.(4a)**)**, considered as *invariants*. That is, all the four different plots in Fig. **(4a)** refer to the cases of employing the *one* and the *same set* of measurable-[input]-variables. However, the figure shows that**: "**slope **(**$[\boldsymbol{UF}]_{\mathbf{A_{Nd}}}$**)** $<$ **"**slope **(**$[\boldsymbol{UF}]_{\boldsymbol{d}}$, with "***d***" as either **^{150}Nd** or **^{142}Nd** or even **^{144}Nd)**". That is, any possible input-[***ratio***]-error should cause the *estimated* atomic-weight ($\boldsymbol{a_{Nd}}$) to be much ***less*** erroneous than the *estimated* atom-fraction ($\boldsymbol{y_d}$).

Again, as shown in Table 6, the observed/ predicted mod-error **(** $|\boldsymbol{\Delta}|$, or the predicted uncertainty: $^{\mathbf{Pred.}}\boldsymbol{\epsilon}$**)** of any output-estimate ($\boldsymbol{y_d}$, or $\boldsymbol{a_{Nd}}$) is, irrespective of example, ***less*** than the mod-sum of the input-errors ($\sum_{m=2}^{7}|\boldsymbol{u_m}|$ **= 0.311346**). That is, even the present case underlines the fact that the **SSR** as either Eq.**(1)** or Eq.**(2)** should in the process of translating the input-*estimate(s)* into the desired *result* act as a kind of (experimental)-*error*-sink. The reason is, it can here again be shown, that any **SSR** specific inputs-to-output variation-*rates* ([***MF***]***(s)***) should (*by magnitude*) be "**<1**"; e.g. the "$\boldsymbol{A_{Nd}}$" specific Eq.**(2)** is characterized by**:** $[\boldsymbol{MF}]_{\boldsymbol{X_2}}^{\boldsymbol{A_{Nd}}}$=−0.004393, $[\boldsymbol{MF}]_{\boldsymbol{X_3}}^{\boldsymbol{A_{Nd}}} = -0.001124$, $[\boldsymbol{MF}]_{\boldsymbol{X_4}}^{\boldsymbol{A_{Nd}}} = 0.0003858$, $[\boldsymbol{MF}]_{\boldsymbol{X_5}}^{\boldsymbol{A_{Nd}}} = 0.001992$, $[\boldsymbol{MF}]_{\boldsymbol{X_6}}^{\boldsymbol{A_{Nd}}} = 0.0014666$ and, $[\boldsymbol{MF}]_{\boldsymbol{X_7}}^{\boldsymbol{A_{Nd}}} = 0.002220$. Furthermore, that the true-*error* ($\Delta_{\boldsymbol{Nd}}^{\boldsymbol{A}}$) of determining the atomic weight ($\boldsymbol{A_{Nd}}$) should really never exceed the corresponding predicted *uncertainty* ($^{\mathbf{Pred.}}\boldsymbol{\epsilon}_{\boldsymbol{Nd}}^{\boldsymbol{A}}$) is clarified in **Fig. (4b)**, which depicts the *variation* of the "observed-

output-error (Δ^{A}_{Nd})" as a function of the "mod-sum of (certain typical "±" combinations of the known equally-*erroneous* six) *input*-ratio-errors ($\sum_{m=2}^{7}|\pm\Delta_m| = \sum_{m=2}^{7}|\pm u_m| = 6u_m$)".

4. Conclusions

We have above chosen the determination of the *correlated* quantities, isotopic abundances ($\{Y_d\}_{d=1}^{N}$) and thus also the atomic weight (A_E) of any possible multi (N) isotopic element (E), as the *indirect* measurement (input-output) systems for discussion on the uncertainties ($\epsilon_d^Y(s)$ and ϵ_E^A) of the correspondingly derived estimates ($y_d(s)$ and, a_E, respectively). However it is, in contrary to the usual conception, clarified that the *inter-dependence* of the desired output-variables ($\{Y_d\}_{d=1}^{N}$) and hence, of the measurable input-variables (isotopic-abundance-ratios**:** $\{X_m\}_{m=2}^{N}$), should *in no way* govern the output-uncertainty (ϵ_d^Y or ϵ_E^A).

The output-estimates (y_d and a_E) and their uncertainties (ϵ_d^Y and ϵ_E^A) are, like any other kind of indirect-measurement (e.g. **non-**correlated) variable-specific-estimate(s) and uncertainty(s) [14-16], shown above to really be the exactly corresponding isotope-d and element-E specific input-output **SSRs** (i.e. respective functions **"**f_d[cf. Eq.(1)]**"** and **"**f_E [cf. Eq.(2)]**"**) governed systematic parameters (*irrespective* of whether the possible cause of the real-world-measurement cum input-[ratio]-uncertainty(s) "$u_m(s)$" be purely statistical or systematic or both), and therefore the output-uncertainties (ϵ_d^Y and ϵ_E^A) be 'a priori' *predictable*. It is above exemplified how any **SSR**-characterizing *input(s)*-**to**-*output* **variation**-parameters should be ascertained, and/ or the uncertainties "ϵ_d^Y**"** and "ϵ_E^A", corresponding to any possible case of even *unknown* isotopic-abundance-pattern of the element (E), could be 'a priori' predicted and be validated.

However, the uncertainty ϵ_d^Y **(**of determining the atom-fraction: Y_d) and, even ϵ_E^A **(**of determining the atom-weight: A_E), are shown above to vary as a function of the measurable (input ratio) variable X_m itself. Thus, both the isotopic-abundance (Y_d**)** and the atomic-

weight ($\boldsymbol{A_E}$) defining **SSRs (**Eq. (1) and Eq. (2), respectively**)** should, like the well-known **IRMS**-measurement-model: $\boldsymbol{Y_\delta} = \left(\frac{X_S}{X_W} - \mathbf{1}\right)$, belong to the **F.2**-family [14] of all conceivable input-output **SSRs** and mathematical-**models**. However, while the *delta*-model "$\boldsymbol{Y_\delta} = \left(\frac{X_S}{X_W} - \mathbf{1}\right)$" have been shown elsewhere [16,19,20] to act as a kind of error-*source* in the overall process of the "$\boldsymbol{Y_\delta}$" measurement; the present **F.2**-members "Eq.(1): $\boldsymbol{Y_d} = \boldsymbol{f_d}(\{\boldsymbol{X_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}})$" and: "Eq.(2): $\boldsymbol{Y_d} = \boldsymbol{f_d}(\{\boldsymbol{X_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}})$" are, in contrast, shown above to behave as the "$\boldsymbol{f_d}$" and "$\boldsymbol{f_E}$" specific *sinks* of experimental-errors in determining "$\boldsymbol{Y_d}$" and "$\boldsymbol{A_E}$", respectively. These signify that, in the case of any *proposed* indirect measurement, an 'a priori' study of the concerned-**SSR** specific input-to-output *variation*-behaviour should help to ascertain beforehand**: (i)** the *achievable*-output-accuracy, i.e. *whether* the corresponding (real world) measurement to be carried out would serve its purpose and/ or**: (ii)** in the case where the input-output **SSR** might stand for a proposed-mathematical-**model**, whether the "proposed-*model*" is purpose-suiting.

REFERENCES

1. ISO, *Guide to the Expression of Uncertainty in Measuremen*t, 1995**(**ISO/IEC Guide 98-3:2008).
2. Qi-Lu and Akimasa Masuda; The isotopic composition and atomic weight of molybdenum, Int. J. Mass Spectrom. and Ion Processes, 130 (1994) 65.
3. F. Schaefer, P. D. P. Taylor, S. Valkiers and P. De Bievre; Computational procedures for the treatment of measured or published isotopic abundance data, Int. J. Mass Spectrom. and Ion Processes, 133 (1994) 65.
4. S. Valkiers, Y. Aregbe, P. D. P. Taylor and P. De Bievre; A primary xenon isotopic gas standard with SI traceable values for isotopic composition and molar mass, Int. J. Mass Spectrom. and Ion Processes, 173 (1998) 55.

5. J. R. de Laeter, J. K. Bohlke, P. De Bievre, H. Hidaka, H. S. Pieser, K. J. R. Rosman and P. D. P. Taylor; Atomic weights of elements: review 2000, Pure Appl. Chem. 75 (2003) 683.
6. M. Zhao, T. Zhou, J. Wang. H. Lu and F. Xiang; Absolute measurements of neodymium isotopic abundances and atomic weight by MC-ICPMS, Int. J. Mass Spectrom., 245 (2005) 36.
7. W. Pritzkow, S. Wunderli, J. Vogl and G. Fortunato; The isotopic abundances and the atomic weight of cadmium by a metrological approach; Int. J. Mass Spectrom., 261 (2007) 74.
8. S. Burger, R. M. Essex, K. J. Mathew, S. Richter and R. B. Thomas; Implementation of Guide to the expression of Uncertainty in Measurement (GUM) to multi-collector TIMS uranium isotope ratio metrology, Int. J. Mass Spectrom. 294 (2010) 65.
9. Shuoyun Tong, Juris Meija, Lian Zhou, Brad Methven, Zoltán Mester, and Lu Yang; High-Precision Measurements of the Isotopic Composition of Common Lead Using MC-ICPMS: Comparison of Calibration Strategies Based on Full Gravimetric Isotope Mixture and Regression Models, Anal. Chem. 91 (2019) 4164 (https://doi.org/10.1021/acs.analchem.9b00020).
10. Kristýna Kantnerová, Nils Kuhlbusch, Dieter Juchelka, Andreas Hilkert, Sebastian Kopf, Cajetan Neubauer; A guide to precise measurements of isotope abundance by ESI-Orbitrap MS. Nat Protoc 19 (2024) 2435, **(**https://www.nature.com/articles/s41596-024-00981-5**)**.
11. Manfred Gröning; Some pitfalls in the uncertainty evaluation of isotope delta reference materials, *Accreditation and Quality Assurance* 28 (2023) 101.
12. M. Ángeles Herrador, Agustín G. Asuero, A. Gustavo González; Estimation of the uncertainty of indirect measurements from the propagation of distributions by using the Monte-Carlo method: An overview, *Chemometrics and Intelligent Laboratory Systems* 79 (2005) 115.

13. J. B. Scarborough, *Numerical Mathematical Analysis*, Oxford & IBH Publishing Co., Kolkata, 1966.

14. B. P. Datta, The theory of uncertainty for derived results: properties of equations representing physicochemical evaluation systems. *arXiv*: 0712:1732 [*physics.data-an*], 2007.

15. B. P. Datta, Uncertainty factors for stage-specific and cumulative results of indirect measurements. *arXiv*: 0909:1651 [*physics.data-an*], 2009.

16. B. P. Datta, Prospects of ratio and differential (δ) ratio based measurement-models: a case study for IRMS evaluation. *arXiv*: 1511.01057 [*physics.data-an*], 2015**.**

17. B. P. Datta, P. S. Khodade, A. R. Parab, A. H. Goyal, S. A. Chitambar and H. C. Jain; Thermal Ionization Mass Spectrometry of $Li_2BO_2^+$ Ions: Determination of Isotopic Abundance Ratio of Lithium, *Int. J. Mass Spectrom. Ion. Processes* 116 (1992) 87 (and Erratum 121 (1992) 247).

18. B. P. Datta, P. S. Khodade, A. R. Parab, A. H. Goyal, S. A. Chitambar and H. C. Jain; Molecular Ion Beam Method of Isotopic Analysis: Effects of Error Propagation, a Case Study with $Li_2BO_2^+$, *Rapid Commun. Mass Spectrom.*7 (1993) 581.

19. B. P. Datta, Pros and cons of the technique of processing IRMS data as desired-δ values: a case study for determining carbon and oxygen isotopic abundance ratios as CO_2^+.*arXiv*:1101.0973 [*physics.data-an*], 2011.

20. B. P. Datta, Study of variations as desired-relative (δ), rather than absolute, differences: falsification of the purpose of achieving source-representative and closely comparable lab-results,*arXiv*:1401.1094 [*physics.data-an*], 2014.

21. Karlsruhe Nuclide Chart, 2006 **(**Zsolt Sóti, Joseph Magill, Raymond Dreher, Karlsruhe Nuclide Chart–New 10th edition 2018 , EPJ Nuclear Sci. Technol. 5, 6 (2019)**)**.

——— ——— ———

Appendix 1: Notations and Clarifications

1) The index "***d***" refers to the term "***derived***/ *desired*" and thus the "d^{th}" *output* (Variable/ estimate/ error or so).

2) The *index* "***m***" signifies "***measured/ measurable***" and therefore the "m^{th}" ***input*** (Variable/ estimate/ uncertainty or so).

3) "$\boldsymbol{Y_d}$"**:** The **UPPER** CASE letter/ symbol as "$\boldsymbol{Y_d}$" is, by the usual convention [cf. section 4.1.1 in ref.**1**], referred to here as — the (**TRUE**-value of the *derived*/ desired

[and therefore of the]) "d^{th} [*output* ***VARIABLE*** as the] *Isotopic* ***abundance***/ *Atom* ***fraction***"; and — the ***LOWER*** case symbol "$\boldsymbol{y_d}$" represents the ***corresponding*** (desired/ *derived* [d^{th} output]) "***estimate***".

4) "$\boldsymbol{X_m}$" represents the (**TRU**E-value of the ***measurement***/ *measurable* [and therefore of the]) "m^{th}" [*input* VARIABLE as the] ***Isotopic-****abundance-****ratio***"; and "$\boldsymbol{x_m}$" stands for the ***corresponding*** (*m^{th} input*) "***estimate***".
5) "$\boldsymbol{M_d}$" stands for the **TRU**E-value of the "***Variable*****:** (d^{th}) *Isotopic* ***mass***"; and "$\boldsymbol{m_d}$" for the *corresponding* "***estimate***".
6) "$\boldsymbol{A_E}$"**:** the (**TRU**E-value of the *derived*/ desired) *output-****variable*** "*Atomic weight* (of the element ***E***)" — [which is, however for uniquely distinguishing *from* the ***output*** variable as "$\boldsymbol{Y_d}$", represented as "$\boldsymbol{A_E}$"]; and the *corresponding* "***estimate***" as "$\boldsymbol{a_E}$".
7) "$\boldsymbol{u_m}$" represents the "***uncertainty***" in (i.e. the ***accuracy*** of) the ***estimate*** "x_m" — (of the $\boldsymbol{m^{th}}$ measurable [*input*] ***Variable*** as the *Isotopic-abundance-ratio* "$\boldsymbol{X_m}$").
8) "$\boldsymbol{u_d^M}$" is referred to as the "***uncertainty***" in (i.e. the ***accuracy*** of) the ***estimate*** "m_d" — (of the $\boldsymbol{d^{th}}$ *Isotopic-mass* "$\boldsymbol{M_d}$").
9) "$\boldsymbol{\epsilon}$"**:** the **Output** *uncertainty*/ ***accuracy*** — (which is, for uniquely distinguishing ***from*** the input-uncertainty "$\boldsymbol{u}$", referred to here by the symbol "$\boldsymbol{\epsilon}$").
10) "$\boldsymbol{\epsilon_d^Y}$" stands for the "***uncertainty***" of the ***estimate*** "$\boldsymbol{y_d}$" — (of the desired $\boldsymbol{d^{th}}$- output-variable as the *Atom fraction* "$\boldsymbol{Y_d}$").
11) "$\boldsymbol{\epsilon_E^A}$" is referred to as the "***uncertainty***" in the output-***estimate*** "$\boldsymbol{a_E}$" — (of the atomic weight variable "$\boldsymbol{A_E}$").
12) "$\boldsymbol{\rho_d}$" stands for combined standard [1] or probable [11] uncertainty in the output-estimate "$\boldsymbol{y_d}$".
13) "$\boldsymbol{\rho_E}$" refers to the combined standard/ probable uncertainty in the output-estimate "$\boldsymbol{a_E}$".
14) $\boldsymbol{\Delta_m}$**:** (True) error in the ($\boldsymbol{m^{th}}$ *measured/* **input**) *estimate* "x_m" — (of [the $\boldsymbol{m^{th}}$ *Isotopic-abundance-ratio*] "$\boldsymbol{X_m}$").
15) $\boldsymbol{\Delta_d^Y}$**:** (True) error in the ($\boldsymbol{d^{th}}$ Output) ***estimate*** "$\boldsymbol{y_d}$" — (of [the $\boldsymbol{d^{th}}$ desired *Isotopic* ***abundance***/ *Atom* ***fraction***] "$\boldsymbol{Y_d}$").
16) $\boldsymbol{\Delta_d^M}$**:** (True) error in the (input) ***estimate*** "$\boldsymbol{m_d}$" — (of [the $\boldsymbol{d^{th}}$ Isotopic mass] "$\boldsymbol{M_d}$").
17) $\boldsymbol{\Delta_E^A}$**:** (True) error in the [OUTPUT] ***estimate*** "$\boldsymbol{a_E}$" — (of [the desired *Atomic weight* of the element ***E***] "$\boldsymbol{A_E}$").
18) $\boldsymbol{[MF]_m^d}$ **:** the $\boldsymbol{d^{th}}$-desired **SSR**/ *model/ function* "$\boldsymbol{f_d}$" specific (relative) **rate of variation**, i.e. the *relative-rate of variation* of the $\boldsymbol{d^{th}}$ output [desired-isotopic-abundance] variable "$\boldsymbol{Y_d}$" as a function of the $\boldsymbol{m^{th}}$ input [measurable] variable "$\boldsymbol{X_m}$". The "$\boldsymbol{[MF]_m^d}$" is also called as the $\boldsymbol{m^{th}}$ *individual* (input-[measurable]-ratio "$\boldsymbol{X_m}$" specific) ***error-***multiplication-[*magnification*]***-factor*** of determining the $\boldsymbol{d^{th}}$ output [desired-isotopic-abundance] variable "$\boldsymbol{Y_d}$".
19) "$\boldsymbol{[UF]_d}$"**:** the desired-output [isotopic-abundance] variable "$\boldsymbol{Y_d}$" (i.e. the exactly corresponding **SSR**/ model/ function "$\boldsymbol{f_d}$") specific ***uncertainty-factor***, representing the ***collective*** *rate of variation of* "$\boldsymbol{Y_d}$" as a function *of* **all** the measurable variables

"$\{\boldsymbol{X_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$" (together). The "$[\boldsymbol{UF}]_{\boldsymbol{d}}$" is also referred to as the ***collective-****error-magnification-****factor*** of determining [the isotopic-abundance] "$\boldsymbol{Y_d}$".

20) $[\boldsymbol{MF}]_{\boldsymbol{X_m}}^{\boldsymbol{A_E}}$ **:** *Individual*-isotopic-ratio ($\boldsymbol{X_m}$) specific ***error-****magnification-****factor*** of determining [the element ***E*** specific *Atomic weight*] "$\boldsymbol{A_E}$".

21) $[\boldsymbol{MF}]_{\boldsymbol{M_d}}^{\boldsymbol{A_E}}$ **:** *Individual*-isotopic-mass ($\boldsymbol{M_d}$) specific ***error-****magnification-****factor*** of determining [the *Atomic weight*] "$\boldsymbol{A_E}$".

22) $[\boldsymbol{UF}]_{\boldsymbol{A_E}}$ **:** the **SSR**/ model/ function "$\boldsymbol{f_E}$ (cf. Eq. 2)" specific ***uncertainty-factor***, representing the ***collective*** *rate of variation of* "$\boldsymbol{A_E}$" as a function *of* **all** the corresponding input-[measurable]-variables (together), i.e. the ***collective-****error-magnification-****factor*** of determining "$\boldsymbol{A_E}$".

——— ——— ———

Appendix 2: On the aim, uncertainty (*inaccuracy*) and accuracy of any measurement

The *minimization* of possible-error (specifically, the elimination of detected sources of systematic-errors) is well-known to be the motto behind *developing* the method of a required-measurement whatever. Therefore, by any measurement, it should mean the *bracketing* of the corresponding-estimate with its (probable) true-value.

The above-said statement should stand as a fact, though**:** (i) any *true*-value always refers to a ***relative***-truth (i.e. a value with reference to *corresponding-something* as the *attributed*-standard), and/ or**:** (ii) any true-value is, **otherwise**, indeterminate. Therefore, the precision ($\boldsymbol{\sigma_m}$) of a required set of bias-free-measurements of any quantity should be the measure of either the corresponding (***least*** *possible*) uncertainty or its (***best*** *achievable*) accuracy.

However**: (i)** a small measurement-bias might even get undetected (i.e. the variation due to certain *bias* can really get shadowed by the *random*-variation); **(ii)** the process of correcting a detected-bias might itself stand for an indirect-measurement, i.e. should cause the *direct*-measurement-uncertainty to be systematically altered and thus, the corresponding-(input)-uncertainty ($\boldsymbol{u_m}$) be essentially systematic in nature. That is to say that the *standard deviation* [1], $\boldsymbol{\sigma_m}$, of a required set of, here, ratio-($\boldsymbol{X_m}$)-measurements may not always turn out to be a measure of purely statistical variation.

Furthermore, neither any desired *derived*-result itself, (and therefore) nor its (unknown) *true*-error, nor even its *possible*-error (uncertainty), can get varied depending on whether the cause of the (unknown) true-error and/ or possible-error in any corresponding given *input*-estimate is purely statistical or not. Therefore, for rather presuming the cause of a (real world) *measurement*-variation to be either random or systematic or both in nature, the idea of accordingly referring to the *possible*-variation of any corresponding (directly-measured/ input/ output/ reported) estimate as either the *uncertainty*, or the *accuracy*, or *so*, should **not** in practice be useful. Thus, in order to avoid the confusion in terms of terminologies their-selves, the ***possible-****error* of any (kind of directly or indirectly) measured *estimate* is referred to [14,15] , even here, as either *uncertainty* or *inaccuracy* or *accuracy*.

——— ——— ———

Appendix 3: Fundamentals underlining the evaluation of output-uncertainty "ϵ"

- ERROR (Δ and $\boldsymbol{\epsilon}$)**:** Different relevant-*relative*-errors, only, should be *inter-comparable*. Therefore, any (variable specific) *true* as well as *possible* errors (Δ and $\boldsymbol{\epsilon}$, respectively) have been considered by us [14] to be *relative*. Thus, by any ratio-[*input*]-uncertainty $\boldsymbol{u_m}$ and, any [*output*]-uncertainty e.g. $\boldsymbol{\epsilon_d^Y}$ **(**of determining the isotopic-abundance **[**$\boldsymbol{Y_d}$, cf. Eq. (1)]**)**, it should be meant that**:** $\boldsymbol{u_m} = {}^{\text{Max.}}|\Delta_m| = {}^{\text{Max.}}\left|\frac{\Delta X_m}{X_m}\right| = {}^{\text{Max.}}\left|\frac{x_m - X_m}{X_m}\right|$; and**:** $\boldsymbol{\epsilon_d^Y} = {}^{\text{Max.}}\left|\Delta_d^Y\right| = {}^{\text{Max.}}\left|\frac{\Delta Y_d}{Y_d}\right| = {}^{\text{Max.}}\left|\frac{y_d - Y_d}{Y_d}\right|$; (with Δ_m and Δ_d^Y as the corresponding [generally unknown] true-errors), respectively.
- INDIVIDUAL-input specific RATE of output-VARIATION ($[\boldsymbol{MF}]_m^d$)**:** Let an input-output **SSR (**in fact, irrespective of what exactly the indirect-measurement-system being represented by it**)** e.g. the Eq. (1) is given. Then, the corresponding function "$\boldsymbol{f_d}$" dictated *relative-**rate-**of-variation* ($[\boldsymbol{MF}]_m^d$) of the desired [$\boldsymbol{d^{th}}$-isotopic-abundance] variable, $\boldsymbol{Y_d}$, as a function of any of its measurable-cum-input variable [$\boldsymbol{m^{th}}$-abundance-ratio], $\boldsymbol{X_m}$, should naturally be given [14-16]:

$$[MF]_m^d = \left(\frac{\partial Y_d}{\partial X_m}\right)\left(\frac{X_m}{Y_d}\right) = \left(\frac{\partial Y_d/Y_d}{\partial X_m/X_m}\right), \quad (m = 2, 3 \ldots N) \tag{4}$$

Therefore, the (true) output-error ($\Delta_{\boldsymbol{d}}^{\boldsymbol{Y}}$) should be accountable as:

$$\Delta_d^Y = \sum_{m=2}^{N} ([MF]_m^d \times \Delta_m) \tag{5}$$

And, the output-uncertainty ($\boldsymbol{\epsilon}_{\boldsymbol{d}}^{\boldsymbol{Y}}$) should get decided [14-16] as:

$$\epsilon_d^Y = \sum_{m=2}^{N} (|[MF]_m^d| \times u_m) \tag{6}$$

It may be pointed out (cf. Eq.**(4)**) that the **individual**-input specific variation-rate ($[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}$) numerically equals to the *relative-error-magnification-factor* [17,18] of determining the desired-($\boldsymbol{d^{th}}$)-variable, $\boldsymbol{Y_d}$, with respect to its $\boldsymbol{m^{th}}$-measurable-variable $\boldsymbol{X_m}$. Thus, "$[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}$" is also referred to here as the **(SSR**/ function "$\boldsymbol{f_d}$" governed**) individual**-error-magnification-factor.

- **SSR** specific COLLECTIVE-rate of output-variation (**[*UF*]:** Let's consider a special case where all the measurable-[input: $\boldsymbol{X_m}$]-variables be subject to a *given*-variation ($\boldsymbol{u_m}$= $^{G}\boldsymbol{u}$ [$\boldsymbol{m}$ = 2, 3, ...*N*], with "$^{G}\boldsymbol{u}$**"** as the measurement-accuracy, say, preset to be achieved before developing the required experimental-methodology). Then, a *measure* of the [concerned-**SSR**/ -model, e.g. the] Eq.(1) specific ***collective***-rate-of-variation ($[\boldsymbol{UF}]_{\boldsymbol{d}}$) should be obtained (see also Eq.(4)) as:

  $$[UF]_d = \sum_{m=2}^{N} |[MF]_m^d| \tag{7}$$

The "$[\boldsymbol{UF}]_{\boldsymbol{d}}$" as the Eq.**(5)**, which gives a measure of the relative-rate-of-variation of the desired-**[**$\boldsymbol{d^{th}}$-output]-variable ($\boldsymbol{Y_d}$) as a function of ***all*** *equally varied* measurable-variables ($\{\boldsymbol{X_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$) *together*, may also be called as the *collective*-error-magnification-factor or ***uncertainty****-factor* [15] of determining the $\boldsymbol{d^{th}}$-isotopic-abundance ($\boldsymbol{Y_d}$). Thus, a tentative measure of the output-uncertainty ($\boldsymbol{\epsilon}_{\boldsymbol{d}}^{\boldsymbol{Y}}$) should 'a priori' be obtainable (cf. Eq.(6)) as:

$$\epsilon_d^Y = \sum_{m=2}^{N} (|[MF]_m^d| \times u_m) = (\sum_{m=2}^{N} |[MF]_m^d|) \times u_m = ([UF]_d \times {}^{G}u) \tag{6a}$$

However, if the input ($\boldsymbol{X_m}$) specific uncertainties ($\{\boldsymbol{u_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{N}}$) should be pre-established, then defining a factor "$\boldsymbol{F_m}$" as "$\boldsymbol{F_m = (u_m/^G u)}$, with $^{\boldsymbol{G}}\boldsymbol{u}$ as any (preset or, say, lowest-established) $\boldsymbol{u_m}$-value", the corresponding **SSR**/ model e.g. the Eq.(1) specific uncertainty-factor "$[\boldsymbol{UF}]_{\boldsymbol{d}}$" and/ or *uncertainty* ($\boldsymbol{\epsilon_d^Y}$) should be best (in fact, in any possible case of *linear* **SSR**/ model, *exactly*) accountable/ predictable [14-16] as:

$$\epsilon_d^Y = \sum_{m=2}^{N} (|[MF]_m^d| \times u_m) = ([\sum_{m=2}^{N} (|[MF]_m^d| \times F_m)] \times {}^G u) = ([UF]_d \times {}^G u) \quad (6b)$$

Where:

$$[UF]_d = \sum_{m=2}^{N} (|[MF]_m^d| \times F_m) \quad (7a)$$

——— ——— ———

Appendix 4: Family characteristics of SSRs/ Models

Any conceivable **SSR**/ model/ function **(**e.g. "$\boldsymbol{f_d}$, (cf. **Eq.(1)**)]"**)** has been shown [14,16] to belong, depending on whether (any of) its characteristic *input(s)*-**to**-*output* variation-*rate(s)* "$[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}(\boldsymbol{s})$" being decided or not by the corresponding *measurable*-variable(s), to one of the **two** possible, namely, the *measurable*-variable-*independent* (**F.1**) and **-***dependent* (**F.2**), families.

- An **F.1** Family member is characterized by**:** $\{\left|[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}\right| = \boldsymbol{1}\}_{\boldsymbol{m=1}}^{\boldsymbol{N}}$**.**
- An **F.2** Family member should be bracketed with**:** $\left|[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}\right| \neq \boldsymbol{1}$ **(**for, at least, any *single* "$\boldsymbol{m}$ (i.e. input-variable)"**)**.

Thus, for any **F.1** family-member, the output-uncertainty ($\boldsymbol{\epsilon_d^Y}$,- cf. **Eq. (6b)**) should be governed by ***solely*** the measurement-[input]-uncertainties as:

$$\epsilon_d^Y = \sum_{m=1}^{N} (|[MF]_m^d| \times u_m) = \sum_{m=1}^{N} u_m = ([\sum_{m=1}^{N} F_m] \times {}^G u) = ([UF]_d \times {}^G u) \quad (6b.F.1)$$

where the uncertainty-factor, $[\boldsymbol{UF}]_{\boldsymbol{d}}$ (cf. also **Eq.(7a)**), should get decided as:

$$[UF]_d = (\epsilon_d / {}^G u) = \sum_{m=1}^{N} F_m = \sum_{m=1}^{N} (u_m / {}^G u) \quad (7a.F.1)$$

Further, if the input-uncertainty "$\boldsymbol{u_m}$" should be *independent* of the measurable-[input] variable "$\boldsymbol{X_m}$" (viz. $\boldsymbol{u_m = {}^{G}u}$, i.e. if**:** $\boldsymbol{F_m = 1}$, with**:** $\boldsymbol{m = 1, 2 \ldots N}$), then the uncertainty-($\boldsymbol{\epsilon_d^Y}$)-expression "Eq. (**6b.F.1**)" could be re-written as **(**see also **Eq. (6b)** and Eq. **(6a))**:

$$\epsilon_d^Y = \sum_{m=1}^{N} (|[MF]_m^d| \times u_m) = (N \times u_m) = (N \times {}^{G}u) = ([UF]_d \times {}^{G}u) \qquad \text{(6a.F.1)}$$

And, thus, the "$\boldsymbol{[UF]_d}$"-expression **(**Eq. (**7a.F.1**)**)** reduces as **(**see also Eq. **(7a.F.1)** and **Eq.7)**:

$$[UF]_d = (\epsilon_d / {}^{G}u) = \sum_{m=1}^{N} (u_m / {}^{G}u) = N \qquad \text{(7.F.1)}$$

It should however be noted that the isotopic-abundance-variable "$\boldsymbol{Y_d}$, (cf. **Eq.(1)**]" is been treated, here above, as any ***general*** output-variable, which is determined from "***N***" different measurable-[input**:** $\boldsymbol{X_m}$]-variables. And, for our real world **isotopic** cases, "***N***" should get replaced by the number "($\boldsymbol{N - 1}$)" of the different possible isotopic-ratios, i.e.**:** ($\boldsymbol{m}$ = **2, 3 ... *N***).

Thus, if truly the isotopic-**SSR** "**Eq. (1)**" be an **F.1** family member, then the uncertainty ($\boldsymbol{\epsilon_d^Y}$) of determining the corresponding atom-fraction ($\boldsymbol{Y_d}$) should be decided by simply the **(**"($\boldsymbol{N - 1}$)"**)** ratio-*measurement*-[input]-uncertainties **(**cf. Eq. (**6a.F.1**) or (**6bF.1**)**)**. That is, the desired-result ($\boldsymbol{y_d}$) should**: (i)** turn out, however, only in the case of any *bi-isotopic* element, as accurate as the corresponding single possible ratio-estimate ($\boldsymbol{x_m}$, as: $\boldsymbol{\epsilon_d^Y = \sum_{m=2}^{N} u_m = u_m}$); but can ***never*** be better accurate than the estimated-ratio "$\boldsymbol{x_m}$"; and**: (ii)** for any case of "$\boldsymbol{N \geq 3}$" and e.g. equally varied inputs ($\boldsymbol{u_m = {}^{G}u}$, [$\boldsymbol{m = 2, 3 \ldots N}$), be subject to the uncertainty as high as "**([**$\boldsymbol{(N - 1)u_m}$**] ≡ [**$\boldsymbol{(N - 1)\,{}^{G}u}$**])**".

Alternatively, let **Eq. (1)** to be belonging to the "**F.2**" family. Then, there should *on the one* be the possibility that "$\boldsymbol{[MF]_m^d(s) < 1}$" or even "$\boldsymbol{[MF]_m^d(s) \ll 1}$", thereby enabling to achieve**:** $\boldsymbol{[UF]_d < 1}$, and hence "**(**output-uncertainty**:** $\boldsymbol{\epsilon_d^Y}$**)** < (input-uncertainty**:** $\boldsymbol{u_m}$; cf. Eq.(6b)**)**". **(**Here, it may be pointed out that, if the function "$\boldsymbol{f_d}$" should have stood for a proposed **F.2-model**, then a *careful* modelling/ remodelling of the function "$\boldsymbol{f_d}$" might also offer the opportunity of achieving "$\boldsymbol{[MF]_m^d(s) \ll 1}$" and/ or "$\boldsymbol{\epsilon_d^Y < u_m}$".**)** And, ***on the other***,

Eq. (1) may turn out to be characterized by "$[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}\boldsymbol{(s)} > \mathbf{1}$", thereby causing "$[\boldsymbol{UF}]_{\boldsymbol{d}} > \mathbf{1}$" (or even "$[\boldsymbol{UF}]_{\boldsymbol{d}} \gg \mathbf{1}$"), and hence**:** "$\boldsymbol{\epsilon_d^Y > u_m}$".

Perhaps, it will be worth illustrating the family-features a little further. Thus, e.g. while the **SSR** "$\boldsymbol{Y_R = f_R(X_S, X_W)} = \frac{\boldsymbol{X_S}}{\boldsymbol{X_W}}$" should belong to the **F.1-**family [14], the apparently similar **SSR** "$\boldsymbol{Y_\delta = f_\delta(X_S, X_W)} = \left(\frac{\boldsymbol{X_S}}{\boldsymbol{X_W}} - \mathbf{1}\right)$" is a member of the **F.2**-family [16]. And, it could be verified [14,16,19,20] that the uncertainty ($\boldsymbol{\epsilon_R^Y}$) of determining the ***simple-ratio*** "$\boldsymbol{Y_R}$" should solely be governed as**:** $\boldsymbol{\epsilon_R^Y = [u_S + u_W]}$; but the uncertainty ($\boldsymbol{\epsilon_\delta^Y}$) in a corresponding-***differential***-*estimate* ($\boldsymbol{y_\delta}$) be decided as**:** $\boldsymbol{\epsilon_\delta^Y} = \left(\left|\frac{\boldsymbol{X_S}}{\boldsymbol{X_S - X_W}}\right| \times [\boldsymbol{u_S + u_W}]\right) = \left(\left|\frac{\boldsymbol{X_S}}{\boldsymbol{X_S - X_W}}\right| \times \boldsymbol{\epsilon_R^Y}\right)$. Clearly, for "$\boldsymbol{|X_S - X_W| \to 0}$", the (*measurement*-accuracy "$\boldsymbol{u}$" might improve, but the) desired *differential*-estimate ($\boldsymbol{y_\delta}$) should itself be increasingly ***erroneous***. These should explain why in any possible case of the isotope-ratio-mass-spectrometry (**IRMS)**, where "$\boldsymbol{|X_S - X_W| \to 0}$" is rather a requirement, the modelling of "**IRMS-***measurement* (data-*evaluation*) as "$\boldsymbol{f_\delta}$" rather than as "$\boldsymbol{f_R}$" is illogical [16,20], and/ or why there should be confusion [7] in dealing with the **IRMS** data. Truly, such a fact has led us to study here the input(s)-**to**-output variation**-**features of the isotopic-**SSRs** "Eqs. (1) and (2)".

——— ——— ———

<u>Appendix 5: Measurable</u> [*Input*] **<u>Variable</u>**-($[\boldsymbol{X_m \equiv X_{37/35}}] = \mathbf{0.3199578}$)-**<u>based</u>** *<u>Outputs</u>*, **<u>and</u>** *Input*-**to**-*Output* **<u>Variation</u>**-<u>parameters, for the **SSRs** as **Eq.(1)** and **Eq.(2)**</u>

<u>Outputs of **Eq.(1)**</u>**:**

- $(\boldsymbol{Y_{(d=1)} \equiv Y_{35}}) = \left(\frac{X_d}{\sum_{m=1}^{2} X_m} = \frac{X_1}{X_1 + X_2} = \frac{\mathbf{1}}{\mathbf{1} + \boldsymbol{X_m}}\right) = \mathbf{0.7576}$.
- $(\boldsymbol{Y_2 \equiv Y_{37}}) = \left(\frac{X_2}{X_1 + X_2} = \frac{\boldsymbol{X_m}}{\mathbf{1}+\boldsymbol{X_m}}\right) = \mathbf{0.2424}$.

<u>Output of **Eq.(2)**</u>, <u>using</u> $(\boldsymbol{[M_1 \equiv M_{35}]} = \mathbf{34.968852682}$ <u>and</u>**,** $\boldsymbol{[M_2 \equiv M_{37}]} = \mathbf{36.965902602})$:

- $\boldsymbol{A_{\mathrm{Cl}}} = \sum_{d=1}^{N}(\boldsymbol{M_d} \times \boldsymbol{Y_d}) = \sum_{d=1}^{2}\left(\boldsymbol{M_d} \times \frac{\boldsymbol{X_d}}{\boldsymbol{1+X_m}}\right) = \mathbf{35.45293763}$.

Eq.(1) specific *Input*-**to**-*Output* **Variation**-parameters**:**

- $\boldsymbol{Y_1}$ **-*specific*** **[***variation-rate*: $\left([\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{1}} \equiv [MF]_{37/35}^{35}\right) = \left(-\frac{\boldsymbol{X_m}}{\boldsymbol{1+X_m}}\right) = \boldsymbol{-0.2424}$, *uncertainty-factor*: $\left([\boldsymbol{UF}]_{\boldsymbol{1}} \equiv [UF]_{35}\right) = \sum_{\boldsymbol{m=2}}^{\boldsymbol{2}}\left|[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}\right| = \left|[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{1}}\right| = \boldsymbol{0.2424}$; and**]** ***uncertainty***: $(\boldsymbol{\epsilon_1^Y} \equiv \epsilon_{35}^{Y}) = \sum_{\boldsymbol{m=2}}^{\boldsymbol{2}}\left(\left|[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{1}}\right| \times \boldsymbol{u_m}\right) = \left(\left|[MF]_m^1\right| \times u_m\right) = \left([\boldsymbol{UF}]_{\boldsymbol{1}} \times \boldsymbol{u_m}\right) = \left(\frac{\boldsymbol{X_m}}{\boldsymbol{1+X_m}} \times \boldsymbol{u_m}\right) = \boldsymbol{(0.2424 \times u_m)}$.
- $\boldsymbol{Y_2}$**-*specific*** **[***variation-rate*: $\boldsymbol{([MF]_m^2 \equiv [MF]_{37/35}^{37}) = \left(\frac{1}{1+X_m}\right) = 0.7576}$; *uncertainty-factor*:$\boldsymbol{([UF]_2 \equiv [UF]_{37}) = \left|[MF]_m^2\right| = 0.7576}$; and**]** ***uncertainty***: $(\boldsymbol{\epsilon_2^Y} \equiv \epsilon_{37}^{Y}) = \left(\left|[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{2}}\right| \times \boldsymbol{u_m}\right) = \left([\boldsymbol{UF}]_{\boldsymbol{2}} \times \boldsymbol{u_m}\right) = \left(\frac{\boldsymbol{1}}{\boldsymbol{1+X_m}} \times \boldsymbol{u_m}\right) = \boldsymbol{(0.7576 \times u_m)}$.

Eq.(2) specific *Input*-**to**-*Output* **Variation**-parameters**:**

- $\boldsymbol{A_{\mathrm{Cl}}}$ **-*specific*** **[***variation-rate*: $\left([\boldsymbol{MF}]_{\boldsymbol{X_m}}^{\boldsymbol{A_{Cl}}} \equiv [MF]_{X_{37/35}}^{A_{Cl}}\right) = \left(\frac{\boldsymbol{X_m(M_2 - M_1)}}{\boldsymbol{(1+X_m)(M_1 + [M_2 X_m])}}\right) = \boldsymbol{0.010344}$; *uncertainty-factor*: $[\boldsymbol{UF}]_{\boldsymbol{A_{Cl}}} = \sum_{m=2}^{2}\left|[MF]_{X_m}^{A_{Cl}}\right| = \left|[\boldsymbol{MF}]_{\boldsymbol{X_m}}^{\boldsymbol{A_{Cl}}}\right| = \boldsymbol{0.0103445}$; and**]** ***uncertainty***: $\boldsymbol{\epsilon_{Cl}^A} = \sum_{m=2}^{2}\left(\left|[\boldsymbol{MF}]_{\boldsymbol{X_m}}^{\boldsymbol{A_{Cl}}}\right| \times \boldsymbol{u_m}\right) = \left(\left|[MF]_{X_m}^{A_{Cl}}\right| \times u_m\right) = \boldsymbol{\left([UF]_{A_{Cl}} \times u_m\right)} = \left(\frac{X_m(M_2 - M_1)}{(1+X_m)(M_1 + [M_2 X_m])} \times u_m\right) = \boldsymbol{(0.0103445 \times u_m)}$.

——— ——— ———

Appendix 6: Isotopic-**mass** based *input*-**to**-*output* **variation**-parameters of the **Cl** *atomic-weight* ($\boldsymbol{A_{\mathrm{Cl}}}$) specific-**SSR as Eq.(2)**

- Mass "$\boldsymbol{M_{35}}$" dependent *rate of variation of* "$\boldsymbol{A_{\mathrm{Cl}}}$": $\boldsymbol{\left([MF]_{M_1}^{A_{Cl}} \equiv [MF]_{M_{35}}^{A_{Cl}}\right) = \left(\frac{M_1}{(M_1 + [M_2 X_m])} \equiv \frac{M_{35}}{(M_{37} + [M_{37} X_{37/35}])}\right) = 0.7472555}$.
- Mass "$\boldsymbol{M_{37}}$" dependent-*rate*: $\boldsymbol{\left([MF]_{M_2}^{A_{Cl}} \equiv [MF]_{M_{37}}^{A_{Cl}}\right) = \left(\frac{M_2 X_m}{(M_1 + [M_2 X_m])}\right) = 0.2527445}$.

- *Uncertainty-factor* (for: $\boldsymbol{u_m = u_1^M = u_2^M}$; cf. Eq.7) : $[\boldsymbol{UF}]_{\boldsymbol{A_{Cl}}} = (^{(Ratio)}[\boldsymbol{UF}]_{\boldsymbol{A_{Cl}}} + {}^{(Mass)}[\boldsymbol{UF}]_{\boldsymbol{A_{Cl}}}) = (\sum_{m=2}^{2}\left|[\boldsymbol{MF}]_{X_m}^{A_{Cl}}\right| + \sum_{d=1}^{2}\left|[\boldsymbol{MF}]_{M_d}^{A_{Cl}}\right|) = (\left|[MF]_{X_m}^{A_{Cl}}\right| + [\left|[\boldsymbol{MF}]_{\boldsymbol{M_1}}^{\boldsymbol{A_{Cl}}}\right| + \left|[\boldsymbol{MF}]_{M_2}^{A_{Cl}}\right|]) = (\mathbf{0.0103445} + [\mathbf{0.7472555} + \mathbf{0.2527445}]) = (0.0103445 + \mathbf{1.0}) = \mathbf{1.0103445}$.

- ***Uncertainty***: $\boldsymbol{\epsilon_{Cl}^{A}} = (\sum_{m=2}^{2}[\left|[MF]_{X_m}^{A_{Cl}}\right| \times u_m] + \sum_{d=1}^{2}[\left|[\boldsymbol{MF}]_{M_d}^{A_{Cl}}\right| \times \boldsymbol{u_d^M}]) = (\left[\left|[MF]_{X_m}^{A_{Cl}}\right| \times u_m\right] + \sum_{d=1}^{2}[\left|[\boldsymbol{MF}]_{M_d}^{A_{Cl}}\right| \times \boldsymbol{u_d^M}]) = (([0.0103445 \times u_m] + [\mathbf{0.7472555} \times \boldsymbol{u_1^M}] + [\mathbf{0.2527445} \times \boldsymbol{u_2^M}])$.

- Or ($\boldsymbol{u_m = u_1^M = u_2^M = {}^{G}u}$)-based-u***ncertainty***: $\boldsymbol{\epsilon_{Cl}^{A}} = ([\boldsymbol{UF}]_{\boldsymbol{A_{Cl}}} \times {}^{G}\boldsymbol{u}) = (((^{(Ratio)}[\boldsymbol{UF}]_{\boldsymbol{A_{Cl}}} + {}^{(Mass)}[\boldsymbol{UF}]_{\boldsymbol{A_{Cl}}}) \times {}^{G}\boldsymbol{u}) = ((\mathbf{0.0103445} + \mathbf{1.0}) \times {}^{G}\boldsymbol{u}) = (\mathbf{1.0103445} \times {}^{G}\boldsymbol{u})$.

——— ——— ———

Appendix 7: Evaluated ***output****-errors* for cases where *each* of the three inputs ($\boldsymbol{x_m}$, $\boldsymbol{m_{35}}$, **and** $\boldsymbol{m_{37}}$) of the "$\boldsymbol{A_{Cl}}$" specific-**Eq.(2)** being subject to *exactly* **±0.01%** *error*

1) **Input**-estimates as: "$\boldsymbol{x_m}$= $[(\boldsymbol{X_m} + \boldsymbol{u_m}) = (X_m + [0.0001 \times X_m])]$ = 0.3199898, $\boldsymbol{m_{35}}$ = $[(\boldsymbol{M_{35}} + \boldsymbol{u_{35}^M}) = (M_{35} + [0.0001 \times M_{35}])]$ = 34.972349567, and: $\boldsymbol{m_{37}}$= $[(\boldsymbol{M_{37}} + \boldsymbol{u_{37}^M}) = (M_{37} + [0.0001 \times M_{37}])]$ = 36.969599192" ***yield*** the output as: $\boldsymbol{a_{Cl}}$ = 35.45651960 **(**= $[\boldsymbol{A_{Cl}} + (0.00010103 \times \boldsymbol{A_{Cl}})]$ = **[35.45293763 +** (*Error*: "$\left|\Delta_{Cl}^{A}\right|$ = $\mathbf{0.010103}$% = $^{\textbf{Pred.}}\boldsymbol{\epsilon_{Cl}^{A}}$")**]**).

2) **Input**-estimates as: "$\boldsymbol{x_m}$= $[(\boldsymbol{X_m} - \boldsymbol{u_m}) = (X_m - [0.0001 \times X_m])]$ = 0.31992580, $\boldsymbol{m_{35}}$= $[(\boldsymbol{M_{35}} - \boldsymbol{u_{35}^M}) = (M_{35} - [0.0001 \times M_{35}])]$ = 34.965355797, and:$\boldsymbol{m_{37}}$= $[(\boldsymbol{M_{37}} - \boldsymbol{u_{37}^M}) = (M_{37} - [0.0001 \times M_{37}])]$ = 36.962206012." ***give*** the **output** as: $\boldsymbol{a_{Cl}}$ = 35.44935566 **(**= $[\boldsymbol{A_{Cl}} - (0.00010103 \times \boldsymbol{A_{Cl}})]$ = **[35.45293763 −** (*Error*: "$\left|\Delta_{Cl}^{A}\right|$ = $\mathbf{0.010103}$% = $^{\textbf{Pred.}}\boldsymbol{\epsilon_{Cl}^{A}}$")**]**).

3) **Input**-estimates as: "**(**$\boldsymbol{x_m}$= $[(\boldsymbol{X_m} + \boldsymbol{u_m})$ = 0.3199898, $\boldsymbol{m_{35}}$= $[(\boldsymbol{M_{35}} - \boldsymbol{u_{35}^M})$ = 34.965355797, and: $\boldsymbol{m_{37}}$= $[(\boldsymbol{M_{37}} + \boldsymbol{u_{37}^M})$ = 36.962206012**)"** ***yield*** the **output** as: $\boldsymbol{a_{Cl}}$ = **35.45122125** = **(**$\boldsymbol{A_{Cl}} - [0.00004841 \times \boldsymbol{A_{Cl}}]$**)** = **(35.45293763 −** [*Error*: "($\left|\Delta_{Cl}^{A}\right|$ = **0.004841**%) < $^{\textbf{Pred.}}\boldsymbol{\epsilon_{Cl}^{A}}$"]**)**.

4) **Input**-estimates as: "**(**$\boldsymbol{x_m}$= $[(\boldsymbol{X_m} - \boldsymbol{u_m})$ = 0.31992580, $\boldsymbol{m_{35}}$= $[(\boldsymbol{M_{35}} + \boldsymbol{u_{35}^M})$ = 34.972349567, and: $\boldsymbol{m_{37}}$= $[(\boldsymbol{M_{37}} + \boldsymbol{u_{37}^M})$ = 36.969599192**)"** ***give*** the **output** as:

$\boldsymbol{a_{Cl}}$ = **35.45644624** = **(**$\boldsymbol{A_{Cl}}$ + [0.00009897 × $\boldsymbol{A_{Cl}}$]**)** = **(35.45293763** + [*Error*: "(|Δ_{Cl}^{A}| = **0.009897**%) < $^{\text{Pred.}}\boldsymbol{\epsilon_{Cl}^{A}}$"]**)**.

5) **Input**-estimates as**: "(**$\boldsymbol{x_m}$ = **[(**$\boldsymbol{X_m}$ + $\boldsymbol{u_m}$) = 0.3199898, $\boldsymbol{m_{35}}$ = **[(**$\boldsymbol{M_{35}}$ + $\boldsymbol{u_{35}^{M}}$) = 34.972349567, and**:** $\boldsymbol{m_{37}}$ = **[(**$\boldsymbol{M_{37}} - \boldsymbol{u_{37}^{M}}$) = 36.962206012**)"** ***yield*** the **output** as**:** $\boldsymbol{a_{Cl}}$ = **35.45472735** = **(**$\boldsymbol{A_{Cl}}$ + [0.00005048 × $\boldsymbol{A_{Cl}}$]**)** = **(35.45293763** + [*Error*: "(|Δ_{Cl}^{A}| = **0.005048**%) < $^{\text{Pred.}}\boldsymbol{\epsilon_{Cl}^{A}}$]**)**.

—— —— ——

Table 1

The natural oxygen isotopic details, and the correspondingly predicted individual error magnification factors ($\{[\boldsymbol{MF}]_{\boldsymbol{m}}^{\boldsymbol{d}}\}_{\boldsymbol{m=2}}^{\boldsymbol{3}}$), uncertainty-factor ($[\boldsymbol{UF}]_{\boldsymbol{d}}$) and the uncertainty ($\boldsymbol{\epsilon}_{\boldsymbol{d}}^{\boldsymbol{Y}}$) of determining any unknown but natural oxygen-isotope-fractions ($\{\boldsymbol{Y}_{\boldsymbol{d}}\}_{\boldsymbol{d=1}}^{\boldsymbol{3}}$, cf. Eq.(1))

Isotope (d)	Isotopic Mass (M_d)	Ratio no. (m)	Relative Abundance (i.e. the measurable ratio: X_m)	Atom/ Isotope Fraction (Y_d)	$[MF]_2^d$ (cf. Eq.(4))	$[MF]_3^d$ (cf. Eq.(4))	$[UF]_d$ [*1] ($\epsilon_d^Y = [[UF]_d \times {}^G u]$)
^{16}O	15.99491462	1	1.0	0.99757	$\frac{-X_2}{1+X_2+X_3} = -0.00038$	$\frac{-X_3}{1+X_2+X_3} = -0.00205$	0.00243 ($0.00243 \times {}^G u$)
^{17}O	16.99913150	2	38.092565×10^{-5}	0.00038	$\frac{1+X_3}{1+X_2+X_3} = 0.99962$	$\frac{-X_3}{1+X_2+X_3} = -0.00205$	1.00167 ($1.00167 \times {}^G u$)
^{18}O	17.99916040	3	20.549936×10^{-4}	0.00205	$\frac{-X_2}{1+X_2+X_3} = -0.00038$	$\frac{1+X_2}{1+X_2+X_3} = 0.99795$	0.99833 ($0.99833 \times {}^G u$)
Atomic weight (A_O) = 15.99940493					[*1]: (Assuming the estimates of "X_2 and X_3" to be equally accurate, i.e. for "$u_2 = u_3 = {}^G u$"; cf. Eq. (7): $[UF]_d = (\lvert[MF]_2^d\rvert + \lvert[MF]_3^d\rvert)$		

Table 2

The predicted relative-rates ($\left\{[\boldsymbol{MF}]_{\boldsymbol{M_d}}^{\boldsymbol{A_O}}\right\}_{\boldsymbol{d=1}}^{\boldsymbol{3}}$ and $\left\{[\boldsymbol{MF}]_{\boldsymbol{X_m}}^{\boldsymbol{A_O}}\right\}_{\boldsymbol{m=2}}^{\boldsymbol{3}}$) of variations (of $\boldsymbol{A_O}$ as a function of *individual* isotopic-*mass* and -*abundance-ratio*, $\boldsymbol{M_d}$ and $\boldsymbol{X_m}$, respectively); the *collective* rate of variation (i.e. the *uncertainty factor*: $[\boldsymbol{UF}]_{\boldsymbol{A_O}}$) and, the *uncertainty* ($\boldsymbol{\epsilon_O^A}$) of determining the natural oxygen atomic weight ($\boldsymbol{A_O}$)

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

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

[*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 "$u_1^M = u_2^M = u_3^M = u_2 = u_3 = {}^Gu$", cf. Eq. (7)):

$$[UF]_{A_O} = \left(\left|[MF]_{M_1}^{A_O}\right| + \left|[MF]_{M_2}^{A_O}\right| + \left|[MF]_{M_3}^{A_O}\right| + \left|[MF]_{X_2}^{A_O}\right| + \left|[MF]_{X_3}^{A_O}\right|\right) = 1.00028.$$

And (if "${}^Gu = 1\%$", then the uncertainty (cf. Eq. (6)):

$$\epsilon_O^A = ([UF]_{A_O} \times {}^Gu) = 1.00028\%.$$

Table 3

Output estimates **(**i.e. oxygen isotope-fractions: [$\{\boldsymbol{y_d} \pm \Delta_d^{\boldsymbol{Y}}\}_{\boldsymbol{d=1}}^{\boldsymbol{3}}$, cf. Eq.(1a)] and atomic weight [$(\boldsymbol{a_O} \pm \Delta_{\boldsymbol{O}}^{\boldsymbol{A}})$, cf. Eq.(2a)]**)** obtained against the relevant input estimates of **known** errors/ uncertainties ($\{\boldsymbol{x_m} = (\boldsymbol{X_m} \pm {}^{\textbf{Max.}}|\Delta_{\boldsymbol{m}}|)\}_{\boldsymbol{m=2}}^{\boldsymbol{3}}$, and $\{\boldsymbol{m_d} = (\boldsymbol{M_d} \pm {}^{\textbf{Max.}}|\Delta_{\boldsymbol{d}}^{\boldsymbol{M}}|)\}_{\boldsymbol{d=1}}^{\boldsymbol{3}}$; cf. Eq.8/ 8a)

Ex. No.	Input ratios: $\{x_m\}_{m=2}^3$ (for **given:** $^{G}\boldsymbol{u}$) i) x_2 $(\Delta_2 \times 10^2)$ ii) x_3 $(\Delta_3 \times 10^2)$	Output of Eq. (1a): y_d and its Observed & Predicted **True-errors**, and also the Predicted-**uncertainty**			Input masses: $\{m_d\}_{m=1}^3$ i) m_{16} $(\Delta_{16}^M \times 10^2)$ ii) m_{17} $(\Delta_{17}^M \times 10^2)$ iii) m_{18} $(\Delta_{18}^M \times 10^2)$	Output of Eq. (2a): a_O $(\Delta_O^A \times 10^2)$ [$^{\text{Pred.}}\Delta_O^A \times 10^2$; Eq. (4a)] $^{\textbf{Pred.}}\boldsymbol{\epsilon_O^A}$
		$y_{16} \times 10^2$ $(\Delta_{16}^Y \times 10^2)$ [$^{\text{Pred.}}\Delta_{16}^Y \times 10^2$, cf. Eq. 4a] $^{\textbf{Pred.}}\boldsymbol{\epsilon_{16}^Y}$	$y_{17} \times 10^2$ $(\Delta_{17}^Y \times 10^2)$ [$^{\text{Pred.}}\Delta_{17}^Y \times 10^2$, cf. Eq. 4a] $^{\textbf{Pred.}}\boldsymbol{\epsilon_{17}^Y}$	y_{18} $(\Delta_{18}^Y \times 10^2)$ [$^{\text{Pred.}}\Delta_{18}^Y \times 10^2$, cf. Eq. 4a] $^{\textbf{Pred.}}\boldsymbol{\epsilon_{18}^Y}$		
1	(for: $^{G}\boldsymbol{u}$ **= 0.01%)** i) 0.00038096 (0.01) ii) 0.00205520 (0.01)	99.756976 $(\boldsymbol{-24.30 \times 10^{-6}})$ $[-24.30 \times 10^{-6}]$ **0.0000243%**	0.038003791 (0.0099757) [0.0099757] **0.0100167%**	0.205020447 (0.0099757) [0.0099757] **0.0099833%**	i) 15.99651411 (0.01) ii) 17.00083141 (0.01) iii) 18.00096032 (0.01)	16.00100532 (**0.0100028**) [0.0100028] **0.0100028%**
2	(for: $^{G}\boldsymbol{u}$ **= 0.01%)** i) 0.00038089 (−0.01) ii) 0.00205520 (0.01)	99.756983 (−0.00001670) $[-16.70 \times 10^{-6}]$ **0.0000243%**	0.037996194 (**−0.0100167**) [−0.0100167] **0.0100167%**	0.205020462 (0.**0099833**) [0.0099833] **0.0099833%**	i) 15.99331513 (−0.01) ii) 16.99743159 (−0.01) iii) 18.00096032 (0.01)	15.9978127 (−0.0099515) [−0.0099516] **0.0100028%**
3	(for: $^{G}\boldsymbol{u}$ **= 1%)** i) 0.00038473 (1.0) ii) 0.00207554 (1.0)	99.754576 (**−0.002430**) [−0.002430] **0.00243%**	0.03837907 (0.997546) [0.997570] **1.00167%**	0.20704497 (0.997546) [0.997570] **0.99833%**	i) 16.15486377 (1.0) ii) 17.169122815 (1.0) iii) 18.179152004 (1.0)	16.15944422 (**1.00028**3) [1.000280] **1.000280%**
4	i) 0.00037712 (−1.0) ii) 0.00203444 (−1.0)	99.759424 (**0.002430**) [0.002430] **0.00243%**	0.03762091 (−0.997594) [−0.997570] **1.00167%**	0.20295493 (−0.997594) [−0.997570] **0.99833%**	i) 15.99491462 (**0.0**) ii) 16.99913150 (**0.0**) iii) 17.99916040 (**0.0**)	15.99936013 (**−0.000280**) [−0.000280] **0.000280%**

Table 4

Measured-cum-reported [4] isotopic-ratios ($\{\boldsymbol{x_m \pm u_m}\}_{\boldsymbol{m=2}}^{\boldsymbol{9}}$) and the thereby estimated [4] atom fractions ($\{\boldsymbol{y_d \pm \rho_d}\}_{\boldsymbol{d=1}}^{\boldsymbol{9}}$) and atomic weight ($\boldsymbol{a_{Xe} \pm \rho_{Xe}}$) of Xenon; and also, for comparison, our evaluated estimates ($\boldsymbol{y_d}$ and $\boldsymbol{a_{Xe}}$) and predicted uncertainties ($\boldsymbol{\epsilon_d^Y}$ and $\boldsymbol{\epsilon_{Xe}^A}$)

Iso-tope (d)	Isotopic Mass: m_d ($^{\text{Max.}}\lvert\Delta M_d\rvert$) [$u_d^M$ (%)]	m	Inputs and Outputs of Eq. (1/ 1a)			Predicted parameters	
			Reported: x_m ($^{\text{Max.}}\lvert\Delta X_m\rvert$) [$u_m$(%)]	Reported: $y_d \times 10^2$ ($^{\text{Max.}}\lvert\Delta Y_d\rvert$) [$\rho_d$(%)]	Our evaluated: $y_d \times 10^2$ [ρ_d(%)] $^{\text{Pred.}}\boldsymbol{\epsilon_d^Y}$**(%)** *2	$^{\text{Max.}}\lvert[MF]_m^d\rvert$ = (cf. Eq.(4))	$[UF]_d$ *1 (ϵ_d^Y = $[[UF]_d \times {}^G u$)
^{132}Xe	131.904154 (0.000001) [75.8×10^{-8}]	1	1.0	26.9086 (0.0033) [0.01226]	26.908653 [0.01235] **0.02207**	$\lvert[MF]_5^{132}\rvert$ = 0.26401	0.73091 (0.73091 $\times {}^G u$)
^{124}Xe	123.905896 (0.000002) [16.1×10^{-7}]	2	0.003536 (0.000012) [0.339367]	0.0952 (0.0003) [0.3152]	0.095149 [0.3393] **0.3608**	$\lvert[MF]_2^{124}\rvert$ = 0.99905	1.72901 (1.72901 $\times {}^G u$)
^{126}Xe	125.904269 (0.000007) [55.6×10^{-7}]	3	0.0033077 (0.0000072) [0.217674]	0.0890 (0.0002) [0.2247]	0.089006 [0.2178] **0.2394**	$\lvert[MF]_3^{126}\rvert$ = 0.99911	1.72913 (1.72913 $\times {}^G u$)
^{128}Xe	127.903530 (0.000002) [15.6×10^{-7}]	4	0.070989 (0.000029) [0.040851]	1.9102 (0.0008) [0.0419]	1.910218 [0.0419] **0.0614**	$\lvert[MF]_4^{128}\rvert$ = 0.98090	1.69271 (1.69271 $\times {}^G u$)
^{129}Xe	128.9047794 (0.0000009) [69.8×10^{-8}]	5	0.98112 0.00041 [0.041789]	26.4006 (0.0082) [0.0311]	26.400618 [0.03126] **0.0418**	$\lvert[MF]_5^{129}\rvert$ = 0.73599	1.20290 (1.2029 $\times {}^G u$)
^{130}Xe	129.903508 (0.000001) [77.0×10^{-8}]	6	0.151290 (0.000047) [0.031066]	4.0710 (0.0013) [0.0319]	4.071010 [0.03224] **0.0506-**	$\lvert[MF]_6^{130}\rvert$ = 0.95929	1.64949 (1.64949$\times$ $^G u$)
^{131}Xe	130.905082 (0.000001) [76.4×10^{-8}]	7	0.789055 (0.000076) [0.009632]	21.2324 (0.0030) [0.0141]	21.232407 [0.0144] **0.0276**	$\lvert[MF]_7^{131}\rvert$ = 0.78768	1.30627 (1.30627$\times$ $^G u$)
^{134}Xe	133.9053945 (0.0000009) [67.2×10^{-8}]	8	0.387819 (0.000069) [0.017792]	10.4357 (0.0021) [0.0201]	10.435687 [0.02008] **0.03615**	$\lvert[MF]_8^{134}\rvert$ = 0.89564	1.52220 (1.52220$\times$ $^G u$)
^{136}Xe	135.907220 (0.000008) [58.9×10^{-7}]	9	0.32916 (0.00017) [0.051647]	8.8573 (0.0044) [0.0497]	8.857252 [0.04845] **0.06457**	$\lvert[MF]_9^{136}\rvert$ = 0.91143	1.55377 (1.55377$\times$ $^G u$)

Reported [4] atomic weight (A_{Xe}) = 131.29275 $^{\text{Max.}}\lvert\Delta A\rvert$ = 0.00034 ρ_{Xe}(%) = 0.00026	(Our evaluated) $\boldsymbol{a_{Xe}}$ = 131.292761 ρ_{Xe}(%) = 0.0002617 $^{\text{Pred.}}\boldsymbol{\epsilon_{Xe}^A}$**(%) = 0.0004653** *2 *2: (cf. Eq. 6/ 6b) Valid only for the set of data & errors [4] used here.	*1: (cf. Eq. 7) Valid for "$\boldsymbol{u_m = {}^G u}$ (with: m = 2, 3,... 9)"; i.e. here: $[UF]_d = \sum_{m=2}^{9}\lvert[MF]_m^d\rvert$

For the estimates of "$\boldsymbol{M_d}$ and $\boldsymbol{X_m}$" to be **equally** accurate, i.e. for "$\boldsymbol{u_m = u_d^M = {}^G u}$ (with: m = 2, 3 ...9; and d = 1, 2 ... 9)", Eq. (7) predicts that:

$[UF]_{A_{Xe}} = \sum_{m=2}^{9}\left|[MF]_{X_m}^{A_{Xe}}\right| + \sum_{d=1}^{9}\left|[MF]_{M_d}^{A_{Xe}}\right|$ = 1.0116323; and: $\boldsymbol{\epsilon_{Xe}^A}$= (1.0116323$\times$ $^G u$).

But, if should the isotopic masses be treated as ***constants***, then: $^{\boldsymbol{Ratio}}[UF]_{A_{Xe}} = \sum_{m=2}^{9}\left|[MF]_{X_m}^{A_{Xe}}\right|$ = **0.0116323**; and: $^{\boldsymbol{Ratio}}\boldsymbol{\epsilon_{Xe}^A}$= (0.0116323$\times$ $^G u$).

Table 5: Typical *outputs* **(**atom fractions [$\{y_d \pm \Delta_d^Y\}$, with: "***d***" as **^{124}Xe**, **^{132}Xe** and **^{136}Xe**] by Eq. (1a); and atomic weight [$ao \pm \Delta_{Xe}^A$] by Eq.(2a)**)** corresponding to the relevant *input estimates* of known errors (as: $\{\pm\Delta_m\}_{m=2}^9$, and also, for Eq.(2a), $\{\pm\Delta_d^M]\}_{d=1}^9$)

Ex. No.	Input ratio-errors i) $\Delta_2 \times 10^2$ ii) $\Delta_3 \times 10^2$ iii) $\Delta_4 \times 10^2$ iv) $\Delta_5 \times 10^2$ v) $\Delta_6 \times 10^2$ vi) $\Delta_7 \times 10^2$ vii) $\Delta_8 \times 10^2$ viii) $\Delta_9 \times 10^2$	Output (cf. Eq, 1a): y_d and its Observed & Predicted **True-errors** and also its Predicted **uncertainty**			Input mass-errors i) $\Delta_{132}^M \times 10^2$ ii) $\Delta_{124}^M \times 10^2$ iii) $\Delta_{126}^M \times 10^2$ iv) $\Delta_{128}^M \times 10^2$ v) $\Delta_{129}^M \times 10^2$ vi) $\Delta_{130}^M \times 10^2$ vii) $\Delta_{131}^M \times 10^2$ viii) $\Delta_{134}^M \times 10^2$ ix) $\Delta_{136}^M \times 10^2$	Output of Eq. 2a: a_{Xe} ($\Delta_{Xe}^A \times 10^2$) [$^{\text{Pred.}}\Delta_{Xe}^A \times 10^2$; cf. Eq. (4a)] $^{\text{Pred.}}\boldsymbol{\epsilon_{Xe}^A}$
		$y_{124} \times 10^2$ ($\Delta_{124}^Y \times 10^2$) [$^{\text{Pred.}}\Delta_{124}^Y \times 10^2$, cf. Eq. 4a] $^{\text{Pred.}}\boldsymbol{\epsilon_{124}^Y}$	$y_{132} \times 10^2$ ($\Delta_{132}^Y \times 10^2$) [$^{\text{Pred.}}\Delta_{132}^Y \times 10^2$, cf. Eq. 4a] $^{\text{Pred.}}\boldsymbol{\epsilon_{132}^Y}$	$y_{136} \times 10^2$ ($\Delta_{136}^Y \times 10^2$) [$^{\text{Pred.}}\Delta_{136}^Y \times 10^2$, cf. Eq. 4a] $^{\text{Pred.}}\boldsymbol{\epsilon_{136}^Y}$		
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)	0.094806 ($-$**0.360**7) [-0.3608] **0.3608%**	26.902889 (-0.021420) [-0.021425] **0.022070%**	8.859928 (0.030215) [0.030222] **0.064568%**	i) -75.81×10^{-8} ii) -16.14×10^{-7} iii) -55.6×10^{-7} iv) -15.6×10^{-7} v) -69.8×10^{-8} vi) -77.0×10^{-8} vii) -76.4×10^{-8} Viii) -67.2×10^{-8} ix) -58.9×10^{-9}	131.292717 (-33.51×10^{-6}) [-33.51×10^{-6}] **0.0004653%**
2	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)	0.094835 (-0.3302) [-0.3302] **0.3608%**	26.911131 (0.009209) [0.009208] **0.022070%**	8.862643 (0.060860) [0.060855] **0.064568%**	i) 75.81×10^{-8} ii) 16.14×10^{-7} iii) 55.6×10^{-7} iv) 15.6×10^{-7} v) 69.8×10^{-8} vi) 77.0×10^{-8} vii) 76.4×10^{-8} Viii) 67.2×10^{-8} ix) 58.9×10^{-9}	131.293372 (**0.0004653**) [0.0004653] **0.0004653%**
(**Table 5** continued)						

Ex. No.	Input ratio-errors	Output (cf. Eq. 1a): y_d and its Observed & Predicted (True) Errors and **uncertainty**			Input mass-errors	Output of Eq. 2a: a_{Xe}
2a	Errors are exactly the **same** as shown for the Example No. 2	0.094835 (-0.3302) $[-0.3302]$ **0.3608%**	26.911131 (0.009209) [0.009208] **0.022070%**	8.862643 (0.060860) [0.060855] **0.064568%**	(i) to (ix): 0.0, i.e. $\{\Delta_d^M = \mathbf{0.0}\}_{d=1}^{9}$ (Isotopic masses are treated as **constants**)	131.293370 $(-\mathbf{0.0004641})$ $[-0.0004641]$ **0.0004641%**
3	**i)** 0.339367 **(ii)** to **(viii)**: Errors are exactly the **same** as shown for the Example No. 1	0.095451 (0.31723) [0.31730] **0.3608%**	26.902715 $(-\mathbf{0.022}66)$ $[-0.022070]$ **0.022070%**	8.859871 (0.029570) [0.029576] **0.064568%**	Isotopic masses are treated as **constants**	131.29267065 (-68.61×10^{-6}) $[-68.62 \times 10^{-6}]$ **0.0004641%**
4	(for: $^{G}\boldsymbol{u}$ **= 1%)** (i) to (vi): +1.0, i.e. $\{(\Delta_m = 1\%\}_{m=2}^{7}$ vii) $\Delta_8 = -1.0\%$ viii) $\Delta_9 = -1.0\%$	0.095770 (0.6527) [0.6549] **1.7290%**	26.816123 (-0.3439) $[-0.3451]$ **0.7309%**	8.738527 (-1.3404) $[-1.3451]$ **1.5538%**	See the Example No. 2a (Isotopic masses are treated as **constants**)	131.27754086 $(-\mathbf{0.011}592)$ $[-0.011632]$ **0.011632%**
5	(for: $^{G}\boldsymbol{u}$ **= 1%)** (i) to (vii): +1.0, i.e. $\{(\Delta_m = 1\%\}_{m=2}^{8}$ viii) -1.0%	0.095571 (0.4438) [0.4462] **1.7290%**	26.760462 (-0.5507) $[-0.5538]$ **0.7309%**	8.720389 $(-\mathbf{1.54}52)$ $[-1.5538]$ **1.5538%**	(i) to (ix): -1.0, i.e. $\{\Delta_d^M = -\mathbf{1.0}\%\}_{d=1}^{9}$	129.97016539 (-1.007363) $[-1.007479]$ **1.011632%**

Table 6

"$\boldsymbol{Y_d}$ **vs.** $\boldsymbol{X_m}$" and "$\boldsymbol{A_{Nd}}$ **vs.** $\boldsymbol{X_m}$" variations for **known** variations in TIMS-measured [6] isotopic abundance ratios ($\{x_m\}_{m=2}^{7}$) of Neodymium

Isotope (d)	Isotopic Mass: M_d	m	Let: $\{\boldsymbol{X_m} = x_m\}_{m=2}^{7} \& \{\boldsymbol{Y_d} = y_d\}_{d=1}^{7}$			Example No. 1		Example No. 2		Example No. 3	
			Reported: x_m ($^{\text{Max.}}\lvert\Delta X_m\rvert$) $[u_m(\%)]$	Reported: $y_d \times 10^2$	Our evaluated: $y_d \times 10^2$ $[\rho_d(\%)]$ $^{\textbf{Pred.}}\boldsymbol{\epsilon_d^Y(\%)}$	$x_m = (\boldsymbol{X_m} + u_m)$ $[u_m(\%)]$	$y_d \times 10^2$ $(\Delta_d^Y \times 10^2)$ $[^{\text{Pred.}}\Delta_d^Y \times 10^2$, cf. Eq. 5]	$x_m = (\boldsymbol{X_m} \pm u_m)$ $[u_m(\%)]$	$y_d \times 10^2$ $(\Delta_d^Y \times 10^2)$ $[^{\text{Pred.}}\Delta_d^Y \times 10^2$, cf. Eq. 5]	$x_m = (\boldsymbol{X_m} \pm u_m)$ $[u_m(\%)]$	$y_d \times 10^2$ $(\Delta_d^Y \times 10^2)$ $[^{\text{Pred.}}\Delta_d^Y \times 10^2$, cf. Eq. 5]
^{144}Nd	143.910083	1	1.0	23.798(12)	23.797738 [0.01458] **0.03332**	1.0	23.789812 (−**0.033**306) [−0.033317]	1.0	23.798418 (0.002856) [0.002856]	1.0	23.791850 (−0.024744) [−0.024750]
^{142}Nd	141.907719	2	1.14101 (0.00027) [0.023663]	27.153(19)	27.153457 [0.02164] **0.4413**	1.14128 [0.023663]	27.150837 (−0.009650) [−0.009654]	1.14128 [0.023663]	27.160658 (0.026520) [0.026519]	1.14128 [0.023663]	27.153162 (−0.001086) [−0.001086]
^{143}Nd	142.90981	3	0.51154 (0.00037) [0.072331]	12.173(18)	12.173495 [0.06458] **0.08804**	0.51191 [0.072331]	12.178243 (0.039001) [0.039014]	0.51191 [0.072331]	12.182648 (0.075188) [0.075186]	0.51191 [0.072331]	12.179286 (0.04757) [0.04758]
^{145}Nd	144.912569	4	0.34848 (0.00012) [0.034435]	8.293(7)	8.293036 [0.03466] **0.06204**	0.34860 [0.034435]	8.293129 (0.001118) [0.001118]	0.34836 [−0.034435]	8.290417 (−0.031580) [−0.031580]	0.34860 [0.034435]	8.293839 (0.009683) [0.009686]
^{146}Nd	145.913112	5	0.72228 0.00031 [0.042920]	17.189(17)	17.188630 [0.03770] **0.06148**	0.72259 [0.042920]	17.190280 (0.009600) [0.009603]	0.72197 [−0.042920]	17.181744 (−0.040065) [−0.040064]	0.72259 [0.042920]	17.191753 (0.018165) [0.018170]
^{148}Nd	147.916889	6	0.24186 (0.00015) [0.062019]	5.756(8)	5.755721 [0.06013] **0.08820**	0.24201 [0.062019]	5.757372 (0.028693) [0.028703]	0.24171 [−0.062019]	5.752316 (−0.059165) [−0.059164]	0.24201 [0.062019]	5.757866 (0.03726) [0.03727]
^{150}Nd	149.920887	7	0.23691 (0.00018) [0.075978]	5.638(9)	5.637922 [0.07304] **0.10073**	0.23709 [0.075978]	5.640327 (0.042647) [0.042661]	0.23673 [−0.075978]	5.633799 (−0.073125) [−0.073122]	0.236730 [−0.075978]	5.632245 (−**0.1007**0) [−0.10073]
Reported [6] atomic weight (A_{Nd}) = 144.2415			(Our evaluated) A_{Xe} = 144.241539 $\rho_{Xe}(\%)$ = 0.0002482 $^{\textbf{Pred.}}\boldsymbol{\epsilon_{Nd}^A(\%) = 0.0005437}$			a_{Xe} = 144.241788 (Δ_{Nd}^A= 0.00017308%) [$^{\text{Pred.}}\Delta_{Nd}^A$ = 0.00017314; Eq. 5]		a_{Xe} = 144.240754 (Δ_{Nd}^A= −**0.0005436**7%) [$^{\text{Pred.}}\Delta_{Nd}^A$ = −0.00054365; Eq. 5]		a_{Xe} = 144.241302 (Δ_{Nd}^A= −0.00016414%) [$^{\text{Pred.}}\Delta_{Nd}^A$ = −0.00016418;Eq. (5)]	

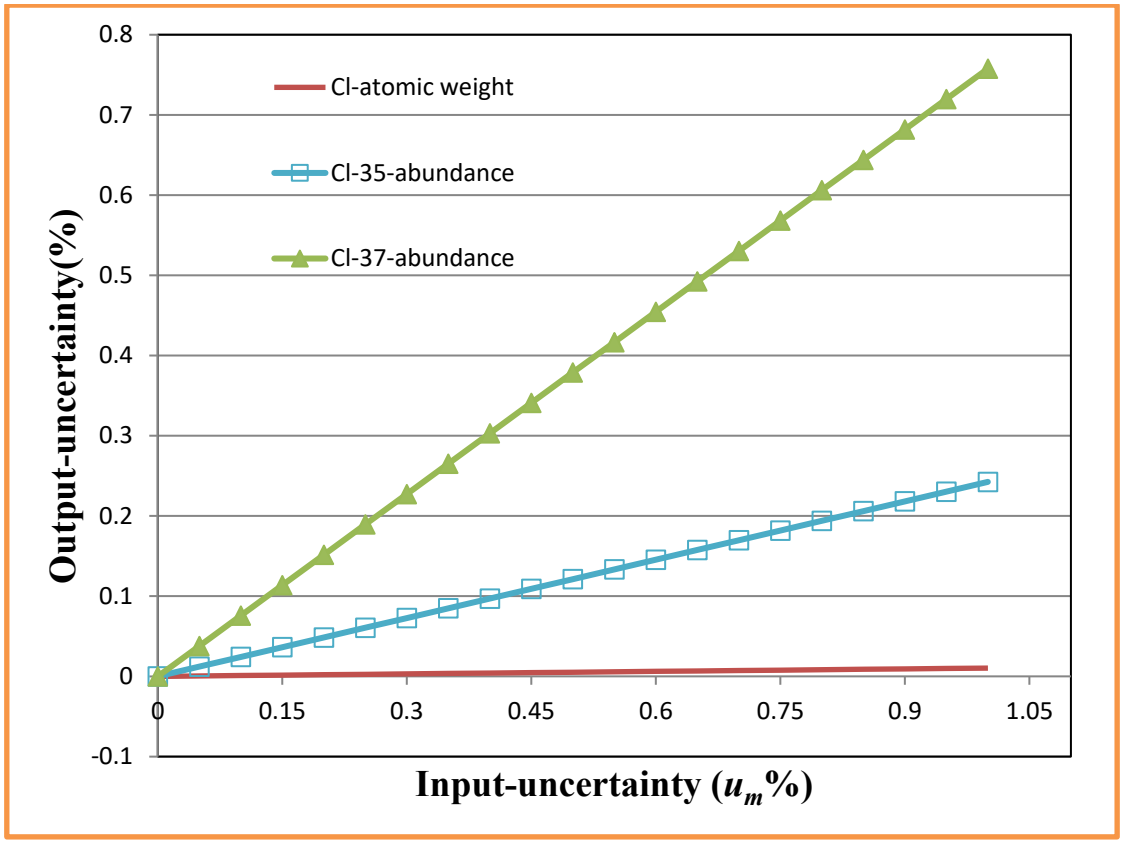


Fig. 1: Variation of ***uncertainties*** *of determining* the natural ^{35}**Cl-**abundance, ^{37}**Cl-**abundance and the atomic weight **(i.e. of the output-uncertainties ϵ_{35}^{Y}, ϵ_{37}^{Y} and ϵ_{Cl}^{A},** respectively**)** as a function of the ***input-ratio-uncertainty*** **($u_m \equiv u_{37/35}$)**

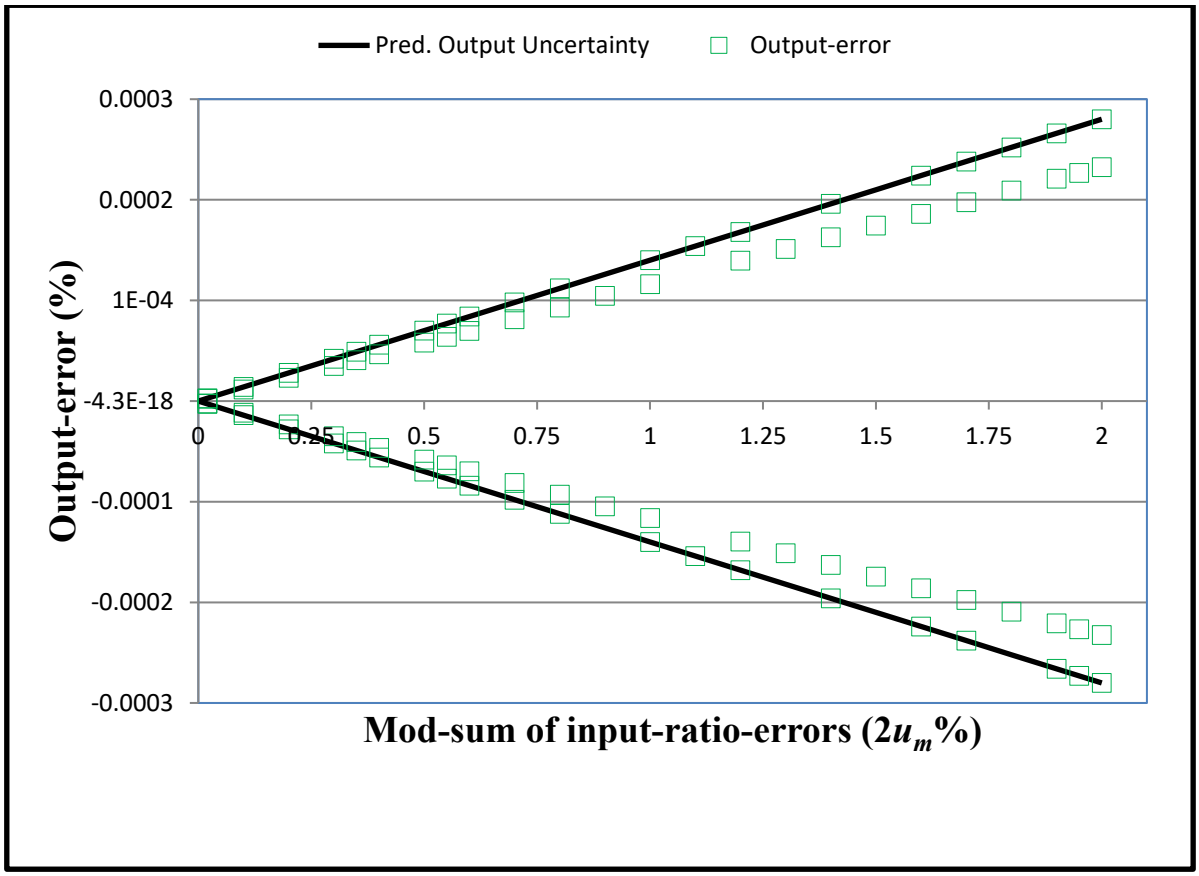


Fig. 2: *Variation* of the observed **true** *error* (Δ_O^A) of determining the atomic weight of oxygen as a function of the ***mod-sum*** of (the possible **"±"** ***combinations*** of the ***two***) *input-ratio-errors* ($\sum_{m=2}^{3}|\pm\Delta_m| = \sum_{m=2}^{3}|\pm u_m| = 2u_m$)

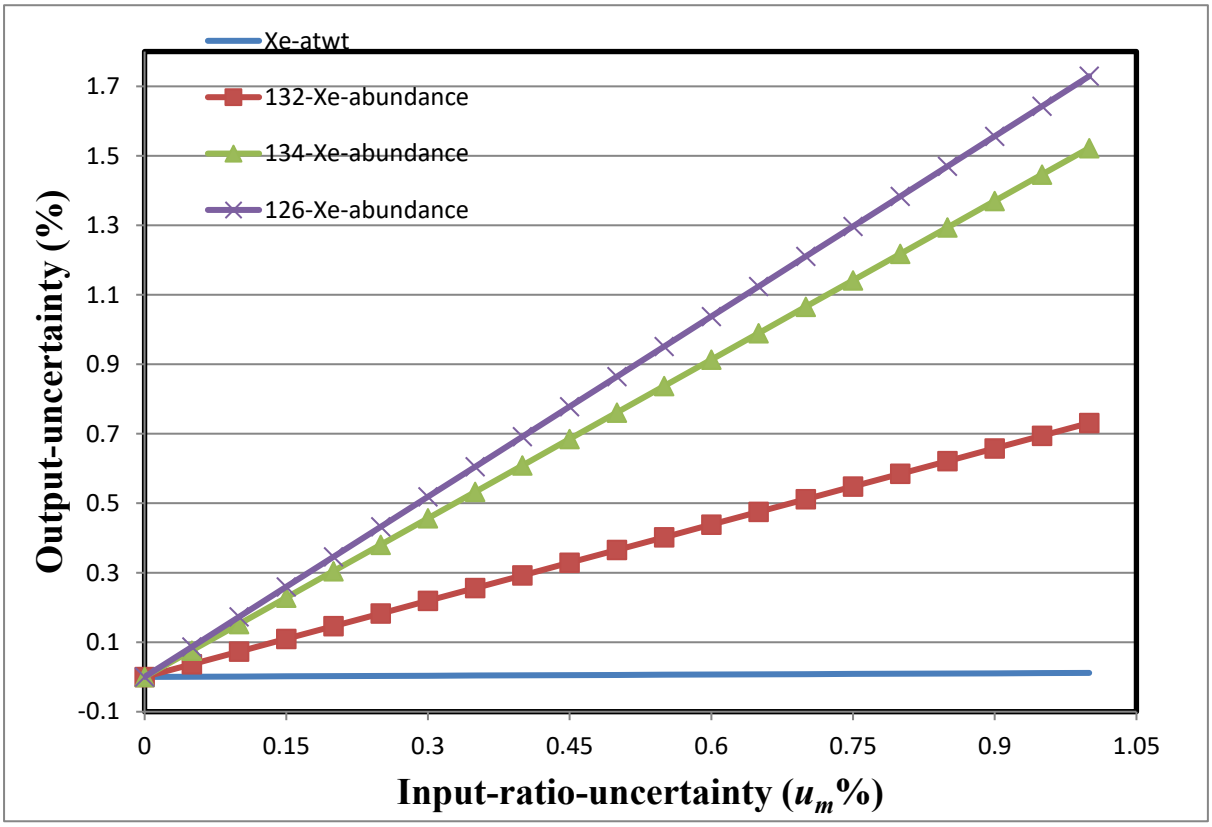


Fig. 3: Variation of the *output*-uncertainties (of determining the ^{126}Xe, ^{132}Xe and ^{134}Xe abundances and also the Xe atomic weight, i.e. of) ϵ^{Y}_{126}, ϵ^{Y}_{132} and ϵ^{Y}_{134} and also ϵ^{A}_{Xe} (respectively) as a function of the *uncertainty*, u_m, of all the eight *equally* uncertain *input-ratios*.

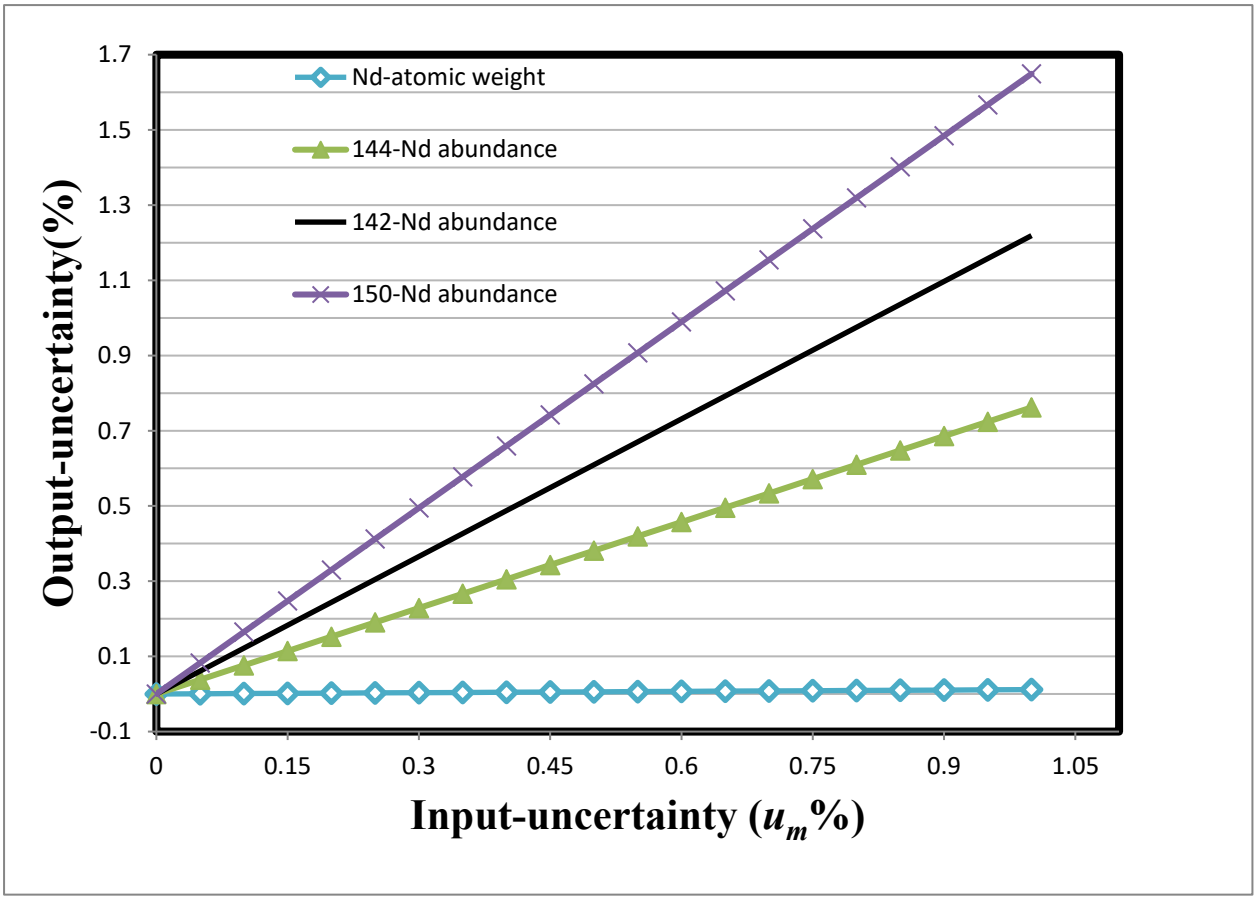


Fig. (4a): Variation of ***output****-uncertainty* (ϵ, for determining one or the other typical isotopic abundance or the atomic weight of **Nd**) as a function of (isotopic ratio measurement)-*uncertainty* **"u_m** (however for the specific case where all the *six* ***input-****ratios* to be ***equally*** uncertain as "u_m")**"**

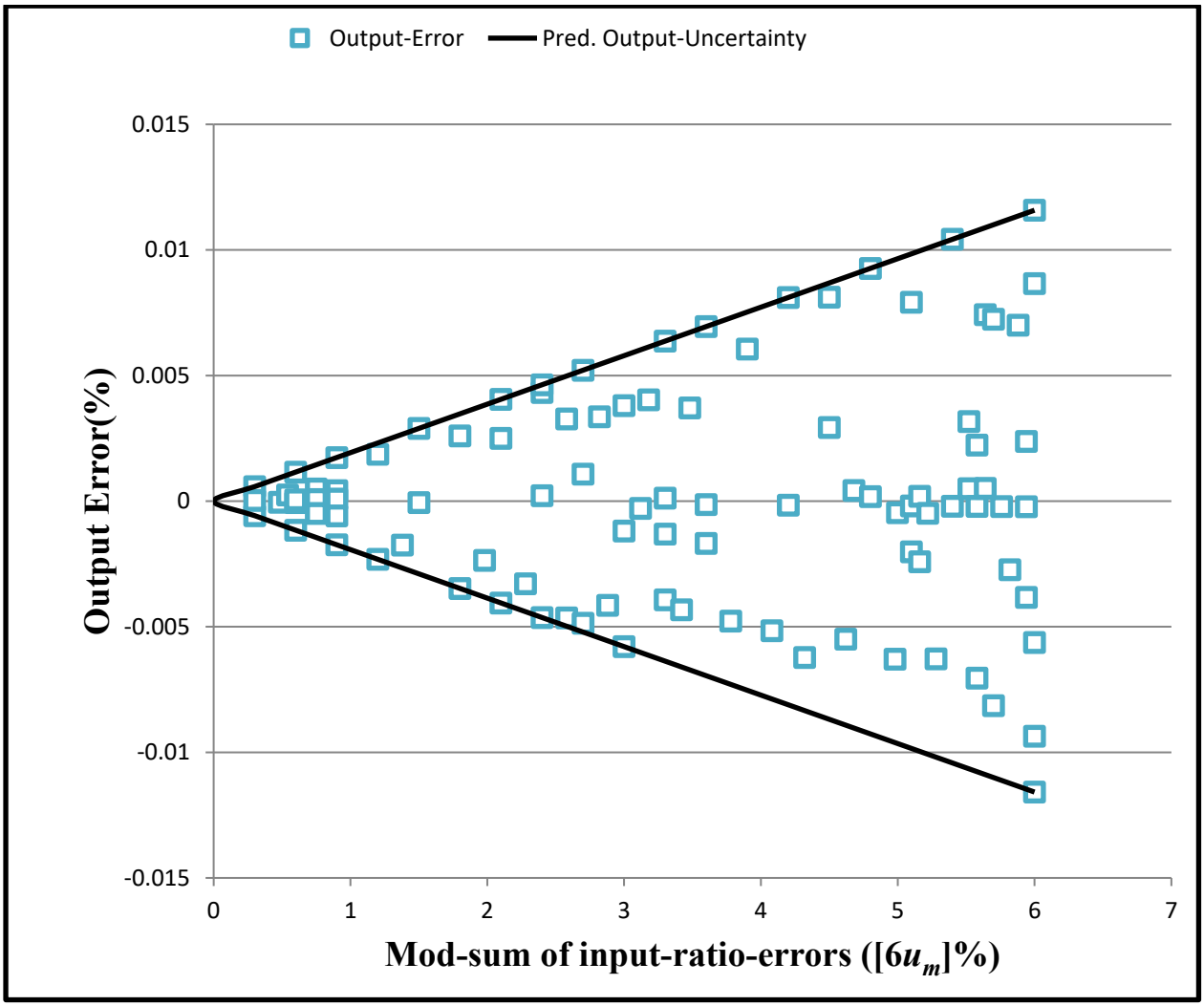


Fig. (4b): *Variation* of (observed **true** *error* of determining the atomic weight of Nd, i.e. of) the *output error* "Δ_{Nd}^{A}" as a function of the ***mod-sum*** of (certain typical "±"***combinations*** of the known ***equally****-erroneous* six) *input-ratio-errors* ($\sum_{m=2}^{7}|\pm\Delta_m| = \sum_{m=2}^{7}|\pm u_m| = 6u_m$)

Graphical Abstract

$$Y_d = f_d(\{X_m\}_{m=2}^{N}) \; ; with \; d = 1, 2 \ldots N$$

Thus: $(y_d \pm \epsilon_d^Y) = f_d(\{x_m \pm u_m\}_{m=2}^{N}) \; ; with \; d = 1, 2 \ldots N$

How: ($u_m(s)$ → ϵ_d^Y)? ➔ Answer: ($\epsilon_d^Y = f_d(\{u_m\}_{m=2}^{N})$)