What is our best measurand when measuring “something” in “something”?

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The specified entity embedded in the matrix material

In the previous Editorial we addressed the task of measuring a suitable measurand related to the matrix material.

We now turn to the task of finding a suitable measurand related to the specified entity contained in a sample of the complex matrix material. The mass of it evidently contributes to the mass of the sample of the complex material. But we cannot compare the mass of the entity we are interested in to the mass of our mass standard as described above, because the specified entity is buried in—or carried by—the complex material. We must look for a process, or processes, enabling us to distinguish the entity we are interested in, from the sample of the complex material. Because of this recurrent need, we have developed a large array of detection equipment using a unique characteristic property of the specified entity to base our measurement on. That can be, e.g., the possibility to ionize, which we can use to convert neutral atoms or molecules into charged particles which we can separate in an electromagnetic field where ions correspond to specified entities. Or we can choose the absorption by these entities we are interested in, of a selected frequency from the radiation we have used to irradiate our sample. We can also make use of the radiation of a given frequency which is emitted by the entity and which we can then measure selectively on the basis of that frequency. Mostly we end up with charged particles (ions) or photons, through which we can measure the selected measurand via the measurement of an electric current $I(E^+)$, where E stands for entity, hence E^+ stands for one charged entity (element or molecule). That gives us access

to the panoply of electrical measurement equipment, which we have developed in a very large variety and to a high degree of sophistication. We can measure electric currents very well and the measured results can be processed easily by computers to produce an indication which is proportional to the number of entities $N(E)$.

We should see clearly that we hereby use a basic property of matter in nature known as “numerosity” [1] or “countability”. It enables us to think in terms of numbers of things and it provides us with a basis on which we can conceive a quantity “number of entities” (some, including this author, claim that this should be a formal *base quantity* in the SI; now it is only “regarded” as a base quantity [2]). It makes one think about the very start of measuring thousands of years ago: counting a number of cattle, or horses, or other “things” in trading. An accepted base unit for “number of entities” (in any system of units, not only in the SI), is exceedingly simple: it is one entity. “For number of entities, the number one, symbol 1, can be regarded as a base unit in any system of units” [3]. For all its simplicity, one entity has a disadvantage in chemistry: using it as a unit would force us to report measurement results in very large numbers (approaching 10^{23}). The remedy for that: we work with a fixed, constant multiple of one entity: 1 mole (about 6.022×10^{23} entities) and call that our unit for amount measurement. We have consistently used “entity” in the measurement task described here. In many cases in chemistry, the entity is related to a “substance” [and any number of entities is a natural multiple of that unit].

When we convert neutral entities into charged particles or entities, we note that the number of ions per second in an electric current $I(E^+)$ is proportional to the number of specified entities $N(E) = K(E) \cdot I(E^+)$ where K is a proportionality factor. The measurement of $I(E^+)$ and its conversion to $N(E)$ constitutes the measurement. It needs to

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be calibrated. That can be done by using an appropriate “calibrator” [4] (appropriate measurement standard) delivered by a calibrator producer (usually called a reference material producer). The producer delivers a value (with uncertainty) for $N_{\text{cal}}(E)$ for a given sample size of that calibrator. When the user measures this calibrator, an $I_{\text{cal}}(E^+)$ is produced. From the relation $N_{\text{cal}}(E) = K_{\text{cal}}(E) \cdot I_{\text{cal}}(E^+)$, a value for $K_{\text{cal}}(E)$ can be obtained which is specific for the user’s measuring system. It can now be used in the first equation which stands as measurement function for the measurement of the unknown $N(E)$ in the sample of the complex matrix material by the user’s measuring system, since, within an evaluated measurement uncertainty, $K(E) = K_{\text{cal}}(E)$.

Under “an appropriate measurement standard” we understand a material with the same complex matrix structure (or as similar as possible), containing the same specified entity as our unknown in the same concentration range. To a first approximation $K(E) = K_{\text{cal}}(E)$ applies and any possible difference because of systematic effects caused by the matrix has to be evaluated for inclusion in the measurement uncertainty of K_{cal} . Also, the more the value of the calibrator’s value for $I_{\text{cal}}(E^+)$ is different from $I(E^+)$, the larger the uncertainty of $K(E)$ will be. It is a matter of applicability or commutability of the chosen calibrator for the measurement case the user is handling.

Hence, the influence of the matrix on the measurement of the element embodied in the matrix material, is a matter

of the measurement uncertainty of the calibration of the measurement of the content of that entity.

At the end of these two Editorials, the answer to the question asked in their titles is: measuring amount (of substance) per mass of material.

The correct name for that quantity is “content”.

Its associated unit is mol/kg.

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