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A proposed vocabulary for liquid scintillation cocktail preparations

R. Collé

National Institute of Standards and Technology

A vocabulary of descriptive terms to specify liquid scintillation (LS) cocktail preparations and their components is proposed. Adoption and use of the proposed systematic nomenclature may result in more consistent usages and remove some of the vagaries and confusions that presently occur in the experimental LS literature.

Keywords: cocktail; liquid scintillation (LS); measurement; nomenclature; radioactivity; spectrometry; standard; terminology; vocabulary

an entropic state (i.e., in a state of some increasing chaos)

The terminology commonly employed to describe liquid scintillation (LS) cocktail components and preparations is in a state of some chaos. This situation has become increasing apparent and disconcerting to me in the past year or so. Having written about six or so papers (in this time interval) on LS spectrometry (with an emphasis on cocktail composition effects), I became increasing aware of the difficulty in finding a judicious selection of words to convey what was actually experimentally done, while at the same time using words that comport with past and current usages. Having reviewed about triple this number of papers (in the same time frame), it is clear that the respective authors of these papers were sometimes equally in a state of confusion. Finally, having read or cursorily examined perhaps about close to 50 or so archival papers, it ultimately occurred to me that there was a dire need for a "standardized" vocabulary, particularly on an international basis amongst laboratories from different countries. Extant "standards" on LS practice [1-3] offer scant guidance. Even more surprisingly, it is apparent that documentations from the commercial manufacturers of LS materials or spectrometers are also of no avail. Let's just consider a few of my (and perhaps others) confusions.

In the early days of LS spectrometry, one finds continual references: to the "solvent" or "primary solvent" (which may or may not consist of molecules that actually scintillate); to the "primary solute"

(e.g., the well-known and popular PPO (2,5-diphenyloxazole) which is always a "fluor" or "scintillator" or fluorescent molecule that scintillates); to "secondary solutes" (e.g., bis-MSB [*p*-bis(*o*-methylstyryl)benzene] or POPOP [1,4-bis-[2-(5-phenyloxazoly)]benzene] which are "wave-shifters" that act to shift the original fluorescent light (from the primary solute) to wavelengths that are more readily detected by photomultiplier tubes); and perhaps to "secondary solvents" (that accomplish some other intended function in the overall LS detection and measurement process).

Now, in reality, we presently deal with commercially-prepared, ready-to-use, fluids that generally consist of a largely unknown and horrendously complex mix of: "solvent"; primary "solute" scintillating molecules; "secondary solute", chemical "wave-shifter" molecules; and then some generally unspecified combinations of bizarre "stabilizers", "non-ionic surfactants", "emulsifiers", etc. (sometimes called the above noted "secondary solvents") that are incorporated into the mix for some particular need (e.g., to increase the capacity to load various kinds of solutions). This stuff that comes out of the jugs provided by their respective manufacturers has been called nearly everything, from a "cocktail", to a "scintillator", to an "LS solution", to a "scintillation fluid", to a "fluor", to a "scintillant". So, what logically and consistently should we call such fluids?

Please recognize that we haven't even addressed anything that we might choose to actually add to this "from-the-jug stuff" (to perform our intended experiments). The added entities are also referred to by an assortment of terms, ranging from the relatively technically-specific "aliquants" (of an added radionuclidic solution) to the more useful, but regrettably vague word "samples". But yet, "samples" also sometimes means the actual LS counting sources which consist of the "stuff-from-the-jug" fluid plus whatever we added to it and <u>as contained</u> in some type of LS counting vial. Now, with the advent and maturation of efficiency-tracing methods, e.g., the CIEMAT/NIST protocol, we oft impose controlled additions of chemical quenching agents (e.g., CCl_4 or CH_3NO_2) to a prepared series of cocktails to vary the detection efficiencies (and quenching) over some range. How might these additions be described with respect to characterizing the LS counting sources that we actually measure? And what do we then call the extra stuff (e.g., the blank carrier solution that may be added to match cocktail compositions between sources, or the extra water that may be added to improve cocktail stabilities) that we decide to put in? Lastly, after we finish adding whatever we wish to add to the "from-the-jug stuff", what should we call this artifact that we actually insert into the LS spectrometer for measurement? This conceptually simple entity has been referred to as a "cocktail", a "sample", and a "source"; and not necessarily consistently.

Pick up nearly any experimental paper on LS measurements. Encounter the word "scintillator". Do you know what it actually refers to? If you are lucky, you might figure it out from the context. If you are unlucky, you may discover that its usage is so vague that you are not certain as to what it actually

refers to, and then you'll have to guess. Any metrologist should abhor such guessing exercises. The same situations are equally true on encountering words like "fluor", "quencher", and "cocktail". The confusions are such that one can sometimes even find contradictory and duplicate descriptors within the same paper: such as by finding that the jug stuff is first called a "scintillator", and then later finding that the identical word "scintillator" is used to describe the molecules that scintillate in discussing the interactions of these fluors in the cocktail mix; or finding that the added radionuclidic solution is termed a "sample" in one place, and then finding that the entire counting source vial is referred to as a "sample" at another location; or finding that the word "cocktail" is used synonymously and interchangeably with two other words (like the counting source and the from-the-jug scintillation fluid). I have deliberately refrained from attaching specific citations to the any of the above quotations to avoid casting any unnecessary and unintended aspersions on the original authors' texts. Astute readers can easily scan the literature on their own and find any number of such confusions and inconsistencies. If anything, such examples should perhaps, more importantly, call to question the quality of the reviews given to such papers.

Given the above chaotic state of things, I, therefore, offer the following proposals for a more systematic basis for the terminology that may be employed for LS cocktail preparations. This proposed guidance is wholly intended to have an immediate and practical utility for pedestrian metrologists like myself, and is merely offered for your consideration. It is not meant to engender extensive semantic imbroglios, of unending duration, amongst the academician types and professional writers of "paper standards" within our discipline. The choice of terms and their definitions is largely experientially based in that I have tried to provide a logical sequence of nearly self-evident definitions for a set of words and terms that can be used in any number of specific contexts to uniquely describe actual experimental conditions. Each gloss largely describes a given experimental entity that might be encountered in experimental practice.

A Glossary of LS Cocktail Preparation Entities

(terms within a given definition that also appear in the glossary are underscored)

1.0 counting source

refers to the entire scintillating artifact that is actually placed in the LS spectrometer for the intended measurement. It generally consists of a suitable LS vial and its contained cocktail (i.e., a scintillant and whatever was added to the scintillant). The counting source may be a blank that does not contain any deliberately introduced radionuclides. The counting source would normally be specified in terms of the type and size of vial, and the nature (composition) and size (volume or mass) of the contained cocktail.

2.0 cocktail

refers to the mix of all chemical entities added to the LS vial to form the counting source. It generally consists of a scintillant, a radioactive sample (or sample blank) and perhaps other imposed composition alterants or imposed quenching agents. The cocktail composition would normally be specified in terms of both the specific chemical components used to form the mix and their respective concentrations.

Note: Although commercially-prepared scintillants which consist of a mix of various chemicals can, by their very nature, be considered to be a type of cocktail, use of the term "cocktail" for "scintillant" in this case is not recommended in order to maintain a clear distinction between the two entities.

3.0 scintillant

, a principal component of a cocktail, refers to the fluid (often a commercially-prepared, ready-to-use mix) in which a sample is added to form a counting source for measurement in a LS spectrometer.

Note: The following terms refer to the components of the scintillant should one need to more specifically identify these chemical components.

3.1 solvent refers to the primary fluid medium of the scintillant in which the fluor(s), other additives, and samples are dissolved or incorporated within a miscible mix.

3.2 primary fluor refers to the scintillating molecules in the scintillant which are responsible for absorbing the radioactive decay energy (as transferred from the solvent or additives) and for emitting fluorescent light photons in the LS measurement process.

3.3 secondary fluor(s) refers to any scintillating molecules present in the scintillant that act to absorb the emitted fluorescent light of the primary fluor and to re-emit the absorbed energy at longer, more readily detectable wavelengths (to improve LS detection efficiencies).

Note: Use of the term "**scintillator**" for a fluor (either primary or secondary) is deprecated unless its meaning is absolutely unambiguous in context.

3.4 additives refers to any other components (e.g., "**stabilizers**" "**emulsifiers**", "**surfactants**", etc.) which are employed in the scintillant for some specific purpose.

4.0 sample

refers to the specific radioactive solution (and its quantity) that is added as part of the cocktail to form the counting source.

5.0 blank

, a generic term, refers to the material(s) used to form cocktails and counting sources that do not

contain any deliberately added radioactivity.

Note: Several different types of blanks can de distinguished.

5.1 sample blank refers to a solution of near identical composition as a sample.

5.2 alterant blank refers to any solution or imposed composition alterant that is used to alter or adjust the composition of a cocktail in a counting source.

5.3 counting source blank, primarily used for LS background subtractions, refers to a counting source that is matched in composition and size to a counting source that contains a radioactive sample.

6.0 imposed composition alterant(s)

refers to any other chemical components (exclusive of the scintillant, sample, and imposed quenching agent) that are introduced to the cocktail to form the counting source. Generally, such components are blank solutions added to achieve matching of compositions amongst cocktails, or to satisfy a particular composition need such as obtain sufficiently high cocktail water fractions.

Note: The imposed composition alterants are, of necessity, also imposed quenching agents. The distinction, in terms of the objective for their addition (composition changes versus quenching), should be maintained for clarity.

7.0 imposed quenching agent

refers to the specific chemical or solution that is deliberately introduced (normally by a controlled addition) to the cocktail to vary the quenching (and hence LS detection efficiency) in the counting source.

The following example illustrates the use of a substantial fraction of the terms as might be employed for the experimental section of a hypothetical paper.

Example

Two matched sets of ^{3}H and ^{63}Ni LS counting sources were prepared. The sources (11 in each set) consisted of 9.8 g cocktails in nominal 20-mL glass LS vials (with polyethylene vee-cone liners on plastic caps). All cocktails were formed with "Scintajunk", a commercial scintillant supplied by Megacorp (Wash. DC), which consists of a mix of pseudocumene as a solvent, PPO and bis-MSB fluors, and unspecified non-ionic surfactants. Those for the ^{3}H sources typically were composed of gravimetrically-determined 50 mg aliquant samples of the tritiated-water standard; while those for ^{63}Ni consisted of about 20 mg samples of the solution (containing 1 $mol \cdot L^{-1}$ HCl and 80 μg Ni^{+2} per gram). Both sets of cocktails contained additional composition alterants, viz., about 0.5 g of blank H_2O (to increase the aqueous fractions to achieve greater cocktail stabilities) and about 0.02 mol HCl and 1.6 μg Ni^{+2} to the ^{3}H cocktails (to match the chemical composition to that for the ^{63}Ni cocktails). Efficiency variations in the two sets of sources (for the efficiency tracing) were achieved by use of controlled additions of variable quantities of a 10 % solution of CH_3NO_2 in ethanol as an imposed quenching agent (quencher). A series of matched counting source blanks of identical cocktail

composition and size were also prepared for background-subtraction corrections.

The level of detail given in the above example may often be unnecessary in many cases. It certainly could be substantially abbreviated while still maintaining the spirit of the proposed vocabulary and its clarity. Nevertheless, the example should adequately illustrate how the clear and consistent usage of terms results in the absence of possible textual ambiguities. Such clarity also simplifies the choice of terms that might be needed for any subsequent discussions, as in:

Each source was measured.....

The effect of cocktail composition on stability .....

The solvent used in this scintillant is not ....

The Ni^{+2} concentration in the aqueous portion of the ^{3}H cocktails, as adjusted by the imposed carrier solution alterant, was .....

In comparison to other commercial scintillants, Scintajunk was found .....

The efficiency range of the imposed quencher, and ~~its effect on~~.....

The sample radionuclides and fluor molecules, for any given cocktail composition, must be ....

From the above examples, it should by now be apparent that words chosen for use within a given text should become inviolably unique. For examples: one should not use the expression "sample" to refer to more than one kind of physical entity; nor should one use an expression like "scintillator" without implicit understanding or explicit clarification as to its meaning.

The most common and greatest faults that appear in the extant literature (in regard to the experimental aspects of LS cocktail preparations) occur as a result of just such vague and inconsistent use of simple terms. As noted, words such as "scintillator", "quencher", "fluor", "cocktail", "sample", and "source" can mean many things to many readers. Their seemingly near random deployment within some texts oft causes utter confusions. The above proposed vocabulary (and attendant examples) are not provided with the intent of necessarily or absolutely excluding (or recommending against) the use of any other equally logical, consistent, and unambiguous terminology. Rather, I merely plead for more consistent usages of terminology for LS cocktail preparations. Any employed terms should firstly be explicitly defined or implicitly self-evident within their textual context, and secondly be used in a consistent and unique manner. Hopefully, the proposed guidance, given herein, will be of some modest assistance to others in avoiding these problems.

Acknowledgements
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Biographies

Dr. **R. Collé** is a research chemist in the Radioactivity Group of the NIST Physics Laboratory (Ionizing Radiation Division), and presently specializes in radionuclidic metrology and standardizations including by LS spectrometry techniques.

R. Collé
Physics Laboratory
National Institute of Standards and Technology
Gaithersburg, MD 20899 U.S.A.
telephone: 301-975-5527
fax: 301-926-7416