

Reporting Significant Digits: Guidelines

(1) In every experiment, there are "real quantities" or "realities" and "derived quantities". Suppose you add 0.056 g of something to a flask. This is a "real quantity" consisting of two significant digits. Molecular weights can be calculated to many significant digits. Therefore you know "derived quantities" such as #mmol to two significant digits. If you have added 1.55 mL of something to a flask, and know the density (or molarity) to 3 or more significant digits, then you know "derived quantities" such as mass or #mmol to three significant digits.

(2) FANTASY DIGITS ARE FORBIDDEN. 1.000 grams means you used a very good balance and carefully added/subtracted the sample from the balance to achieve exactly this amount. If you didn't do this, then the last two or three digits of 1.000 can be regarded as a fantasy.

(3) GIVE THE CUSTOMER ALL THE DIGITS THEY HAVE PAID FOR. If you carefully did #2 above, do not reduce 1.000 g to "1 g" in the experimental section. *There is no rule that the starting materials for all reactions in a paper should be given to the same number of significant digits*. Each individual experimental should reflect the quality and reality of that experiment.

(4) Experimental sections should give the mass (g or mg) and molar quantity (mol or mmol) of every educt and important product. The preferred units in the jag group are g and mmol. We avoid switching units on readers within a paper. Other comments:

(4.1) when a pure liquid is delivered volumetrically (preferred unit mL), also give the mass

(4.2) when a solution is delivered, give the volume, molarity of solution, and "how you knew the concentration". "I believed what Aldrich told me" etc., is not valid. Often you will need to standardize something via a literature procedure (give the reference). It is difficult to anticipate all situations in advance, so apply common sense.

(4.3) A molarity that is only known to two significant digits (1.5 M) limits the number of significant digits in all derived quantities. For example, one would say that a 2.15 mL aliquot contains 3.2 mmol of the solute, not 3.225 mmol as would be obtained by direct multiplication.

(4.4) don't forget to include the mass of any solvate in the molecular weight

(5) In general, we report yields to two significant digits, i.e., 75%, 22%, etc. However, we seek to "carry enough digits along" so that a third significant digit could be calculated.

(6) In general, "publication quality" experimentals should use high-quality balances that weigh to the nearest 0.1 mg (0.0001 g). Other comments:

(6.1) if an experimental procedure requires ca. 10 g of an educt, a more primitive balance (one that would read 10.2 g for example) is satisfactory.

(6.2) if an experimental procedure requires less than 100 mg of an educt, it is especially important to use the highest quality balance, otherwise there are only 1-2 significant digits. Such small scale reactions are more "environmentally friendly" and are encouraged.

(7) From time to time, it may seem like a good idea to give mol/mmol to one more

significant digit than is rigorously merited (example: 0.0974 g, 1.023 mmol). This is not a problem, but it should not be done routinely. Never give two digits more than are merited.

(8) When a liquid educt is delivered volumetrically, the number of significant digits depends upon the quality of the syringe. Other comments:

(8.1) if you are not certain, just "bring jag the syringe" and he can help

(8.2) An alternative is to weigh an empty syringe, and weigh it again after it has been filled with educt. Be sure to deliver the dead volume of the needle with a back-fill of the reaction medium.

(9) General issues of errors in weighing, volumes, etc. are discussed in paper #184: Dewey, M. A.; Gladysz, J. A. *Organometallics* **1993**, *12*, 2390.

(10) Calculators give lots of digits. Suppose your calculator says that 0.446 g of something corresponds to 0.55551 mmol. You will have to round the latter quantity down to three significant digits. Normally jag rounds 0.55551 up to 0.556 and 0.55549 down to 0.555. However, some texts suggest more involved treatments. We do not obsess about rounding protocols in the Gladysz group, but the use of more involved methods is acceptable

(11) Other wisdoms, or similar things said differently:

(11.1) non-zero digits are always significant;

(11.2) any zeros between non-zero digits are significant

(11.3) "trailing zeros" are not addressed in the above treatment. For example, 3.20 g would usually be regarded by jag as having three significant digits. However, a molar extinction coefficient ϵ of 32,000 $\text{M}^{-1}\text{cm}^{-1}$ might be read as having two significant digits, three significant digits (one case out of 10), or four (one case of 100). One way to "guess" would be to look at the other ϵ values in the Table and see if there are any given with three digits, e.g., 42,400 $\text{M}^{-1}\text{cm}^{-1}$.

(11.4) A common way of removing this ambiguity is to use exponents: 3.2×10^4 for two significant digits, 3.20×10^4 for three significant digits, 3.200×10^4 for four significant digits. In general, jag tries to avoid exponents in papers where numbers are being compared.

(12) "Exact numbers", such as the number of students in a classroom, have an infinite number of significant digits. Exact numbers are made by counting up how many of something is present. They are not derived from instrumental measurements.