

On Byproducts and Side Products

We at Scientific Update are a fussy lot. Following my colleague John Knight's editorial about the misuse of various terms, particularly the distinction between crystallisation and precipitation, my beef is about the use of "side products" and "byproducts".

These two terms are bandied about indiscriminately and concern materials other than the desired products that result from the reactions. However, there are two distinct types of materials that are formed during a chemical reaction, and if the terms are used correctly, these can be classified as either byproducts or side products.

When we carry out a chemical reaction and it follows the desired pathway, we obtain the product and, unless it is a unimolecular process or a cycloaddition type of reaction, some byproducts. Byproducts are materials that are produced as a direct result of the desired reaction, and so they will appear as part of the fully balanced chemical equation. Side products, on the other hand, are the result of side reactions. Let me explain a little further. If we carry out a decarboxylation reaction, we will expect a stoichiometric amount of CO₂ to be produced; if we carry out a Suzuki coupling, we will similarly produce a stoichiometric amount of borate byproducts and HX, with HX usually being neutralised by the base present in the reaction mixture. Similarly, any catalyst residues and ligands are also byproducts because they will appear in the fully balanced equation, albeit usually on the arrow, but they are really little different from the byproducts arising from stoichiometric reagents apart from being present in substoichiometric (catalytic) quantities.

Side products are impurities which appear during the reaction as a result of (1) side reactions that can be alternative reaction pathways or (2) further reaction/degradation of the desired product after it has formed. Once we isolate our product, it is likely to contain some impurities, and these can be either byproducts or side products. These can often be removed or reduced during work and purification; however, if we want to eliminate their formation in the first place, we have different options. To stop the formation of byproducts we would have to change the chemistry being carried out or the reagent(s) we are using. This may also reduce the side products being formed, but the formation of side products can often be eliminated simply by changing the reaction conditions.

If we look at a more complex case such as a multistep process where A is converted to B, and then to C, or even further on to D, the rules can be applied in the same way. Any unreacted B (and/or C) will count as byproducts, although in some respects they are like unreacted starting material.

Now, what about resolutions and kinetic resolutions? In both cases the unwanted enantiomer/diastereomer or component will appear as part of the balanced chemical equation and so will count as a byproduct using the definition described above.

So please, let us use the terms byproduct and side product correctly. "What about impurities that are carried through from a previous step?" you ask? Does it matter if they are byproducts or side products from the previous step? Are there any

suggestions? Should they be called preproducts, pre-impurities, or...?

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Notes

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