

The Answer to: Are these organic molecules the same?

Egon Willighagen 

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Ten days ago I asked my readers if two molecules were the same or not. I guessed they were not, when I was asked [Are these organic molecules the same?](#) The people who replied to my post were quite convinced they were, and [Peter](#) gave the context of the pub quiz: assumptions may not be correct.

Indeed, I assumed there were hydrogens missing (implicit), and that line corners indicate places where carbons are. But the key to this problem was that I also assumed that the E/Z stereochemistry for the two double bonds were properly defined. Or, more accurately, I assumed that because I was comparing the two molecules, the E/Z stereochemistry for the double bond between the rings was identical in both drawings. We all did.

Under that assumption, these two molecules are indeed not the same. However, if the E/Z stereochemistry is actually not the same for that double bond, ... well, you get the point. Perhaps this was not the best of examples, as it is quite conventional to use 2D coordinates to determine E/Z stereochemistry... we even have a special drawing style to indicate the E/Z stereochemistry is *unknown*. Then again, how often does the organic chemist really use that.

A more convincing example was also drawn in the pub, and I should have given that one. Peter [posted those later](#). These involve a [spiro compounds](#). Here too, I assumed that the stereochemistry around the spiro carbon was identical. My bad. There was one person in the pub who spotted the problem: David Jessop.

Underlying issue, of course, is those stupid 2D drawings. Jmol has been around for more than 10 years now (and non-free tools too), and we still use 2D drawings... why, oh why? 3D coordinates and explicit hydrogens, that is what our molecular data should be represented with. Henry does this right, over and over again, in his brilliant [blog](#). Well, most of the time anyway. Look for the 'Click for 3D' statements behind the figures, and just give it a try, e.g. in [this post on I\(CN\)7](#).

BTW, a clear example of [McPrinciple #2](#).