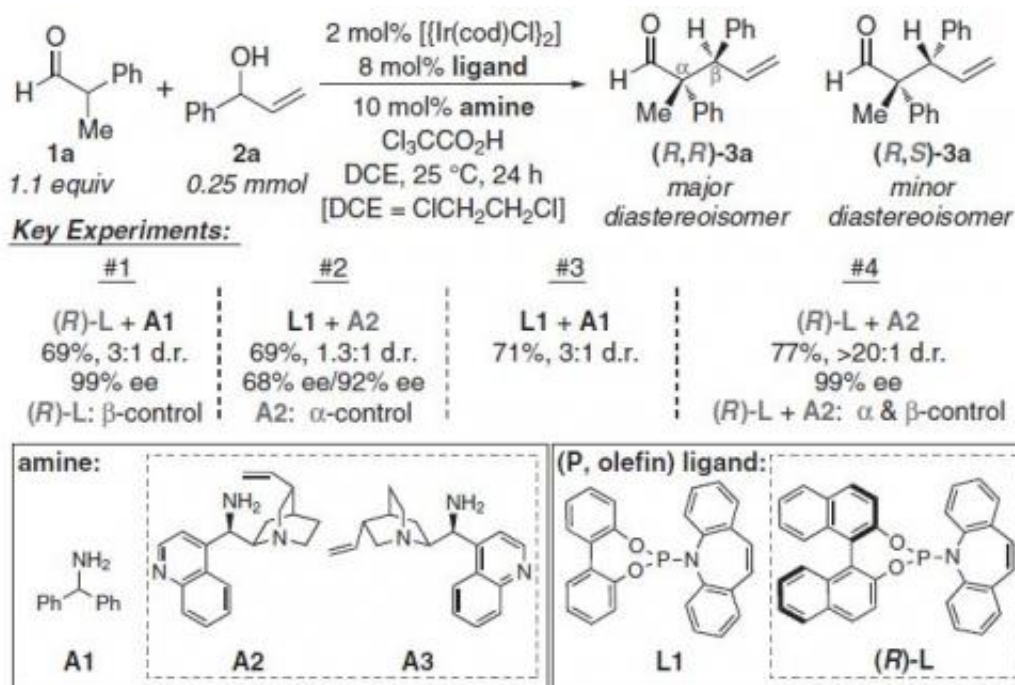


New method of producing stereoisomers developed

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Key experiments in the evaluation of diastereocontrol. Credit: *Science* 31 May 2013; Vol. 340 no. 6136 pp. 1065-1068 DOI: 10.1126/science.1237068

(Phys.org) —A new study by chemists in Switzerland is likely to change the way many stereoisomer molecules are synthesized for industrial, agricultural, or medical uses.

[Chemical reactions](#) often produce molecules called stereoisomers, which have the same molecular formula but a different arrangement of the

atoms within them. If pairs of molecules are mirror images but not superimposable, they are called enantiomers; if they are not [mirror images](#) and also not superimposable they are diastereomers. The different arrangements are around chiral centers (or stereocenters) that in [organic molecules](#) are usually [carbon atoms](#) bonded to four different groups.

The number of stereoisomers of a molecule is dependent on the number of chiral centers (n), and is equal to 2^n , and so if there are two chiral centers there will be four possible stereoisomers. The differences between stereoisomers may appear small, but they can produce large differences in the way the molecules behave. In pharmaceutical molecules, for example, different stereoisomers often have dramatically different effects on the body.

The current practice in controlling which stereoisomer is produced is to use a single catalyst that binds to one of the substrates. To produce another stereoisomer, the substrate, catalyst or reaction conditions usually have to be changed, and it can be difficult or impossible to generate all the stereoisomers required using this technique. This is especially true for large molecules having multiple chiral centers.

In the new study, led by Simon Krautwald of the Eidgenössische Technische Hochschule (ETH) in Zürich, the researchers used two chiral catalysts and showed that they could control the production of all four possible stereoisomers in their chemical reaction involving a molecule with two chiral centers.

In their reaction, the team used one of two [iridium](#) phosphoramidate catalysts to activate a secondary allyl alcohol, which then reacted with an [aldehyde](#) that was in turn activated by one of two amine pseudoenantiomers.

The researchers showed that each catalyst controlled the stereoselectivity of one of the substrates but had no effect on the chiral center derived from the other substrate. They also demonstrated that using the two chiral catalysts together gave them almost perfect control of each chiral center, allowing them to select which of the four stereoisomers would be produced by selecting which combination of catalysts was used.

The results of the study are important in organic chemistry because of the different physical properties and biological effects stereoisomers often have. The new method should allow multiple [stereoisomers](#) to be generated simply by changing the catalysts, rather than changing reagents, catalysts, and/or reaction conditions, which was often required previously.

More information: Enantio- and Diastereodivergent Dual Catalysis: α -Allylation of Branched Aldehydes, *Science* 31 May 2013: Vol. 340 no. 6136 pp. 1065-1068 [DOI: 10.1126/science.1237068](https://doi.org/10.1126/science.1237068)

Abstract

An important challenge in asymmetric synthesis is the development of fully stereodivergent strategies to access the full complement of stereoisomers of products bearing multiple stereocenters. In the ideal case, where four products are possible, applying distinct catalysts to the same set of starting materials under identical conditions would in a single step afford any given stereoisomer. Herein, we describe the realization of this concept in a fully stereodivergent dual-catalytic synthesis of γ,δ -unsaturated aldehydes bearing vicinal quaternary/tertiary stereogenic centers. The reaction is enabled by chiral iridium and amine catalysts, which activate the allylic alcohol and aldehyde substrates, respectively. Each catalyst exerts high local stereocontrol irrespective of the other's inherent preference.

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