

Hydrodealkenylative C(Sp³)–C(Sp²) Bond Scission

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SUMMARY

UCLA researchers in the Department of Chemistry and Biochemistry have developed a new chemical reaction that combines ozone, an iron salt, and a hydrogen atom donor to enable hydrodealkenylative cleavage of C(sp³)–C(sp²) bonds in a widely applicable manner.

BACKGROUND

The commercial accessibility of complex molecules very often relies on starting material cost. There is a limit to the natural products, drugs and agrochemicals available for research and commercialization due to the complexity and cost of synthesizing chiral molecules. Traditionally, the assembly of complex molecules from simple precursors, is accompanied, more often than not, by the need to install carbon centers with precisely defined stereochemical arrangements. Despite the bevy of methods available to accomplish such goals, sometimes it can be more efficient and cost-effective to reorganize starting materials already containing the required complexity and/or stereochemistry into the desired molecular structures. Such, deconstructive strategies can provide access to challenging, or otherwise inaccessible, molecular structures. While there are some examples of C(sp²)–C(sp²) bond scissions and C(sp³)–C(sp³) bond fragmentations, general methods for the functionalization of C(sp³)–C(sp²) bonds remain elusive. Given the profuse number of organic molecules containing these linkages, activation of such bonds in a controllable manner would be extremely useful.

INNOVATION

UCLA researchers targeted the less common deconstructive strategy toward complexity—particularly one involving C–C bond scission. The hydrodealkenylative cleavage of C(sp³)–C(sp²) bonds, performed using oxygen, an iron salt, and a hydrogen atom donor. These reactions are simple to operate and reach completion within 30 minutes, delivering their products in high yields—even on decagram scales.

Researchers have used this transformation to produce desirable synthetic intermediates and applied it in the total syntheses of complex molecules. With broad substrate scope and high functional group compatibility, this methodological advance lays new paths for the syntheses of organic molecules with utility in chemistry, biology, and medicine.

APPLICATIONS

- Cost-effective synthesis of chiral building blocks
- Medicinal chemistry methodology

ADVANTAGES

- Mild conditions
- High yielding
- Scalable method
- Broad substrate scope
- High functional group compatibility

STATE OF DEVELOPMENT

The developed methodology has been applied in the synthesis of desirable synthetic intermediates in high yields and up to decagram scale. Expensive chiral building blocks have been prepared from up to 10⁴-fold cheaper starting materials.

PATENT STATUS

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INVENTORS

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OTHER INFORMATION

KEYWORDS

bond fragmentation, C(sp³)–C(sp²)
 bonds, C-C bond scission, organic synthesis, agrochemicals, drugs, hydrodealkenylation

CATEGORIZED AS

- **Materials & Chemicals**
 - Agricultural
 - Biological
 - Chemicals
- **Medical**
 - Research Tools
- **Research Tools**
 - Reagents
- **Agriculture & Animal Science**
 - Chemicals

RELATED CASES

2019-603-0

Country	Type	Number	Dated	Case
United States Of America	Published Application	2022-016958	06/02/2022	2019-603
European Patent Office	Published Application	3944739	02/02/2022	2019-603

RELATED MATERIALS

- ▶ [Smaligo, A. J.; Sriramurthy, V.; Kwon, O. “Carvone-Derived P-Stereogenic Phosphines: Design, Synthesis, and Use in Allene–Imine \[3 + 2\] Annulation” ACS Catal. 2018, 8, 5188–5192.](#)
- ▶ [Smaligo, A. J.; Swain, M.; Quintana, J. C.; Tan, M. F.; Kim, D. A.; Kwon, O. “Hydrodealkenylative C\(sp3\)-C\(sp2\) bond fragmentation” Science, 2019, 364, 681–685.](#)

ADDITIONAL TECHNOLOGIES BY THESE INVENTORS

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