

Science of Synthesis

Your expert guide to
making molecules



We transform synthesis!



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Your expert guide to making

Science of Synthesis at a glance

The largest collection of evaluated organic synthetic methods available worldwide:

- Access to more than 20,000 reliable synthetic methods
- Evaluated by world-renowned experts
- Author-written reviews of organic transformations
- Easy to navigate by product class or reaction type

Chemistry in context

Each review typically includes:

- Introduction and background
- Discussion of the methods
- Synthetic schemes
- Scope and limitations
- Preparative details
- All relevant references (linked outbound)

Why is SoS unique?

SoS gives you all the important information you need, fast and in one place!

Science of Synthesis provides critical reviews on synthetic methodology in organic and organometallic chemistry. It is organized systematically and logically based on the product, specifically the main functional group being made.

Its insightful, didactic reviews include knowledge that you can't find anywhere else.

SoS at your institution

A license to SoS helps support excellence in:

- Cost efficiency: Potential savings on document delivery; archive options; manageable training effort due to intuitive interface
- Teaching: Using SoS as a teaching tool helps your institution create highly skilled chemists
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- Service: Providing users with online access to SoS helps clear the shelves and frees up library space

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6.1.4.2 Fragmentation of Quaternary Center Alcohols with Halogen Trapping

DOI: 10.1055/sos-SD-229-00118

Thullen, S. M.; Ashley, M. A.; Rovis, T., *Science of Synthesis: Photocatalysis in Organic Synthesis*, (2019)

This strategy can also be employed in the presence of other radical trapping reagents, such as halogen reagents, to generate the corresponding alkyl halides 15 after β -scission and subsequent trapping with an electrophilic halide reagent (Scheme 4).^[14] Fluorination, chlorination, and bromination have all been demonstrated to proceed in good to excellent yields.

Scheme 4 Alcohol Fragmentation and Ketone Formation with Distal Halogenation^[14]

14

X	Halide Source (Equiv)	Catalyst (mol%)	Collidine (Equiv)	Solvent	Time (h)	Yield (%)
F	Selectfluor (4)	2	1	d_2 -MeCN/ D_2O (1:1)	3	52
Cl	CCl_2 (20)	5	3	$PhCF_3$	18	98
Br	$CBrCl_3$ (3)	3	3	CH_2Cl_2	24	95

5-Fluoro-1-(4-methoxyphenyl)pentan-1-one (15, X = F); Typical Procedure

A screw-cap culture tube (16 × 125 mm) fitted with a PTFE/silicone septum (methoxyphenyl)cyclopentan-1-ol (14; 96 mg, 0.5 mmol), redistilled collidine [Ir(dFCF₃ppy)₂(5,5'-dCF₃bpy)]PF₆ (11 mg, 0.01 mmol, 2 mol%), and Se then evacuated and backfilled with N₂ (3 ×). Degassed d_2 -MeCN (5 mL) an suspension. The mixture was sparged with N₂ for 20 min. The mixture was inside a beaker, and stirred at rt with a fan to cool the reaction setup. After washed with H₂O, extracted with EtOAc, and then purified by column chromatography (52%).

References

[14] Yajla, H. G.; Wang, H.; Tarantino, K. T.; Orbe, H. S.; Knowles, R. R.

Science of Synthesis is the largest resource for evaluated reviews of synthetic methods and features a clear and consistent presentation and discussion of the reactions, as well as the direct inclusion of experimental procedures.

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Who are the experts?

The Science of Synthesis editorial board, led by Professor Alois Fürstner, comprises world-renowned organic chemists from both academia and industry. Together with some 2,500 volume editors and authors, they continuously add to, develop, and improve Science of Synthesis.

The screenshot displays the 'Science of Synthesis' website interface. At the top, there are navigation tabs for 'Full Text', 'Explore Contents', and 'Training & Support'. Below this is a large tree view titled 'Explore Contents' under the heading 'Science of Synthesis'. The tree is organized into several main categories:

- Organometallics
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 - Proton-Coupled Electron Transfer for Ketyl Radical Generation
 - Intramolecular Ketyl-Alkene Cyclizations
 - Intramolecular Asymmetric Aza-Pinscol Reaction
 - Homodimerization of Ketyl Radical Derivatives
 - Fragmentation of Quaternary Center Alkoxy Groups for Ketone Formation
 - Fragmentation of Quaternary Center Alcohols with Hydrogen-Atom Trapping
 - Fragmentation of Quaternary Center Alcohols with Halogen Trapping
 - Proton-Coupled Electron Transfer for Amidyl Radical Formation
 - Organocatalysis with Amines in Photocatalysis
 - Copper-Based Photocatalysts for Visible-Light-Mediated Organic Transformations
 - Gold in Photocatalysis
 - Palladium in Photocatalysis
 - Nickel in Photocatalysis
 - Acridinium Dyes and Quinones in Photocatalysis

All methods are clearly organized in a logical structure based on the functional group to be synthesized and can be explored in the context of other methods.

What can I get from SoS?

Science of Synthesis answers questions such as:

- What is the best method to use? Are there alternatives?
- What is the background to the field of research I am interested in?
- What is the context of a transformation in relation to other methods?*
- Which experimental procedures should I use?
- Am I going to need specialist equipment?
- What should I avoid based on the experience of experts working in the field?

What can I use SoS for?

SoS helps if you are:

- Starting out in a new area of chemistry
- Writing a paper
- Preparing for a talk
- Writing a thesis
- Looking for a new way of teaching advanced synthesis

Why choose Science of Synthesis?

Save time and resources by finding the most important information fast!

A community of experts provides reliable knowledge that is readily applicable in the lab:

- Unique insights to help you choose the best approach
- Tips and tricks to solve your synthetic problems
- All necessary information in one place
- Inclusion of procedures for immediate consideration

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"Science of Synthesis is an indispensable tome of chemical information organized in an intuitive and logical way. It contains information on nearly every aspect of chemical reactivity and, for me, is the "go-to" resource for rapidly learning about a new area. I use it regularly in preparation for classes and for consulting visits – it simply gives me the information I need far more easily than any search

engine is capable of – and very often contains references and insight that cannot be found anywhere else."

Phil Baran

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"Science of Synthesis has done a nice job of establishing a useful resource for synthetic chemists including some important contributions from my industry colleagues. It's important to remember that industry has considerable expertise here, and this provides a powerful forum for scientific exchange."

Rebecca Ruck

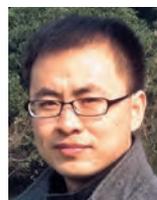
Merck Sharp & Dohme Corp., NJ, USA



"To me, the true value of Science of Synthesis is its systematic approach to reprocess the state-of-the-art for any functional group. When I quickly need a competent overview of the chemistry of this or that class of compounds, Science of Synthesis is my immediate choice. Conventional review articles do usually not provide this information."

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