

Science of Synthesis

Quick Start Guide

The screenshot displays the Science of Synthesis interface. The main heading is "21.1.7.1.2.1 With O-Acylhydroxylamines". Below this, a reaction scheme shows the conversion of an O-acylhydroxylamine (9) to an amide (11) using potassium acyltrifluoroborate (10) in the presence of t-BuOH/H₂O (1:1) at 0-20 °C. The reaction is labeled as Scheme 3.

Below the reaction scheme is a table summarizing the yields and references for various R¹ and R² groups:

R ¹	R ²	Yield (%)	Ref
Bn	(CH ₂) ₂ Ph	87	[31]
4-TolCH ₂	(CH ₂) ₂ Ph	83	[31]
CHMePh	(CH ₂) ₂ Ph	79	[31]
(CH ₂) ₂ CH=CH ₂	(CH ₂) ₂ Ph	83	[31]
(CH ₂) ₂ Me	(CH ₂) ₂ Ph	84	[31]
(CH ₂) ₂ Ph	(CH ₂) ₂ Ph	90	[31]
Ph	(CH ₂) ₂ Ph	83	[31]
4-Tol	(CH ₂) ₂ Ph	83	[31]
2-Tol	(CH ₂) ₂ Ph	88	[31]
4-ClC ₆ H ₄	(CH ₂) ₂ Ph	70	[31]
1-naphthyl	(CH ₂) ₂ Ph	80 ^a	[31]
(CH ₂) ₂ Ph	(CH ₂) ₂ Ph	82 ^b	[31]

Your expert guide to making molecules



Query

Navigation

Query

Search SOS

Results

Hitlist of search results

Full Text

Descriptions of transformations with experimental procedures

Explore Contents

Overview of all transformations by functional group

Training & Support

Training materials, general information and news

Name to structure tool

Simply type a name, click convert, and the structure appears ready for searching

Upload

Load an existing structure/reaction (e.g. from a ChemDraw file)

Thieme Science of Synthesis

Search Query (keyword, author name, DOI etc.)

Convert Query (keyword, author name, DOI etc.)

Convert (name, trace or systematic name)

Smart Search (default)

Explore Science of Synthesis

Trends & Innovation	Functional Groups	Heterocycles
Advances in Organoborane Chemistry Towards Organic Synthesis	X-CAC, X=C=C, X ₂ C=C, C=C Compounds	Small-Ring Heterocycles, Five-Membered Heterocycles with One Heteroatom
Asymmetric Organocatalysis	Nitriles, Succinimides, and Derivatives	Fused Five-Membered Heterocycles with One Heteroatom
Biosynthesis in Organic Synthesis	Acid Halides, Carboxylic Acids, Esters, Anhydrides, Peroxy Acids	Five-Membered Heterocycles with One Chalcogen and One Additional Heteroatom
C-H Bonding Studies in Organic Synthesis	Amides and Derivatives, Hydrides, Lactams	Six-Membered Heterocycles with One Heteroatom
Catalytic Oxidation in Organic Synthesis	Thio-, Esteryl-, and Tellurocarboxylic Acids, Sulfide Acids, Ortho Acids	Phosphorane Derivatives
Catalytic Reduction in Organic Synthesis		Five-Membered Heterocycles with Three or More Heteroatoms

Text search

Open/close the drawing panel

Information on search options

Citation search

Search for a Science of Synthesis article by bibliographic information, author name, etc.

Structure and reaction search

Search type for structure/reaction searches

Explore SOS by topic

To start a search, please go to

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Ranked search results

After structure or reaction hit is displayed, a scheme showing the hit is displayed. Text searches show text snippets displaying the search term in context.

Navigate within hitlist pages

Show full-text review

Filter results

Sort hitlist

Save/load hitlist

Only available if logged in to MySOS.

Show context of method in breadcrumb navigation

Navigation within hitlist

R ¹	R ²	Yield (%)	Ref.
Ph	(CH ₂) ₂ Ph	87	(1)
4-TolCH ₃	(CH ₂) ₂ Ph	83	(1)
4-ClPh	(CH ₂) ₂ Ph	79	(1)
(CH ₂) ₂ CH=CH ₂	(CH ₂) ₂ Ph	83	(1)
(CH ₂) ₂ Ph	(CH ₂) ₂ Ph	84	(1)
(CH ₂) ₂ Ph	(CH ₂) ₂ Ph	90	(1)
Ph	(CH ₂) ₂ Ph	83	(1)
4-Tol	(CH ₂) ₂ Ph	83	(1)
2-Tol	(CH ₂) ₂ Ph	88	(1)
4-ClC ₆ H ₄	(CH ₂) ₂ Ph	70	(1)
1-naphthyl	(CH ₂) ₂ Ph	80 ^a	(1)
(CH ₂) ₂ CH	(CH ₂) ₂ Ph	80 ^a	(1)

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Navigation within the article or volume

Discussion of method, including reaction scheme and scope

***N*-(2-Phenylethyl)-4-phenylbutanamide [11, R¹ = (CH₂)₃Ph; R² = (CH₂)₂Ph]; Typical Procedure: [3]**

O-Benzoyl-*N*-(2-phenylethyl)hydroxylamine [10, R² = (CH₂)₂Ph; 26.1 mg, 0.11 mmol, 1.1 equiv] was dissolved in H₂O/*t*-BuOH (1:1; 1 mL) in a glass vial at rt. Potassium (4-phenylbutanoyl)trifluoroborate [9, R¹ = (CH₂)₃Ph; 25.4 mg, 0.10 mmol, 1.0 equiv] was added and the mixture was shaken until the starting materials had dissolved. After standing for 30 min, the mixture was diluted with EtOAc (20 mL), washed with sat. aq NaHCO₃/H₂O (1:1; 2 × 5 mL) and brine (5 mL), and then dried (Na₂SO₄), filtered, and concentrated. The crude material was triturated with hexanes (2 mL), the hexanes were decanted, and the residue was dried to give the amide product as a white solid; yield: 24 mg (90%).

References

[3] Dumas, A. M.; Molander, G. A.; Bode, J. W., *Angew. Chem. Int. Ed.*, (2012) **51**, 5683.

Selected experimental procedures

Links to primary literature

Special topics

- Free Radicals: Fundamentals and Applications
- Dual Catalysis
- Advances in Organoboron Chemistry
- Photocatalysis
- and further topics

Logical organization of content

Compound class introduction

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Houben-Weyl methods



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Find out how to use SOS effectively for research or teaching.

Video Tutorials

The screenshot shows the Science of Synthesis website interface. At the top, there is a navigation bar with the Thieme logo and the text "Science of Synthesis". Below this, there are tabs for "Query", "Results", "Full Text", "Explore Contents", and "Training & Support". A "Log out" link is visible in the top right corner. The main content area features the slogan "Best methods. Best results." and four primary navigation icons: "People" (represented by a group of people), "User Guides & Documentation" (represented by a book), "Release & Technical Product Information" (represented by gears), and "Contact" (represented by a speech bubble). Each icon has a corresponding list of links below it. The "People" section includes links for Editorial Board, Volume Editors, Author Map, Editorial Office, and Chemists on SOS. The "User Guides & Documentation" section includes Teaching Resources, Quick Start Guide, Video Tutorials, Ranking of Results, Case Studies, Series Preface, and Editorial Guidelines. The "Release & Technical Product Information" section includes What's New and System Requirements. The "Contact" section includes Ask a Scientist and General Help. At the bottom of the page, there is a "Tutorial Videos" section with a video player showing a cartoon illustration of people interacting with the website.

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Within Science of Synthesis you can register for a MySOS personal account. This allows you to login to SOS from outside your institution as well as save and load queries and hitlists.

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- **What is the best synthetic strategy to use?**
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- **What should I avoid based on the experience of other chemists working in the field?**

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