



UNIVERSITAT DE
BARCELONA

CRAI

Centre de Recursos per a
l'Aprenentatge i la Investigació

Science of Synthesis

Science of Synthesis és un recurs produït per Thieme que recull el text complet de la metodologia sintètica desenvolupada, des de principis del 1800 fins a l'actualitat, en els camps de la Química Orgànica i Organometàlica

Pantalla inicial de cerca

The screenshot shows the Thieme Science of Synthesis search interface. At the top, there is a navigation bar with 'Home', 'Query', 'Results', 'Full Text', and 'Explore Contents'. A 'MySOS' login link is visible in the top right. Below the navigation bar, there is a 'FUNCTIONS' sidebar with options like 'Use ChemDraw', 'Upload Molfile...', and 'Reset Query'. The main area features a search input field labeled 'Enter your Query' and a 'Full Text' dropdown. Below the search field is a 'Drawing' editor with a toolbar containing various chemical drawing tools. A yellow sticky note is pinned to the left side of the interface, containing the text: 'For optimal results please keep structure and reaction searches simple and use filter options on the Results Tab.' Callouts point to various features: 'Accés com a usuari registrat' points to the MySOS link; 'Cerca al text complet' points to the search input field; 'Informació sobre la cerca avançada' points to an information icon; and 'Editor d'estructures. No necessita Java' points to the drawing editor. At the bottom, there are 'Clear Drawing' and 'Submit' buttons.

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents

MySOS

FUNCTIONS

- Use ChemDraw
- Upload Molfile...
- Reset Query

Enter your Query

Full Text

Drawing

Clear Drawing Submit

For optimal results please keep structure and reaction searches simple and use filter options on the Results Tab.

Accés com a usuari registrat

Cerca al text complet

Informació sobre la cerca avançada

Editor d'estructures. No necessita Java

Return to Top

Accés com a usuari registrat (MySOS)

The screenshot displays the Thieme Science of Synthesis MySOS interface. The top navigation bar includes 'Home', 'Query', 'Results', 'Full Text', and 'Explore Contents', along with a 'MySOS' link. A 'Log on' section contains fields for 'Username' and 'Password', and a 'Log on' button. A 'FUNCTIONS' menu lists options like 'Log on', 'Create account', and 'Forgot password'. A second screenshot shows the 'Enter your Query' section with a 'Full Text' input field, a 'Drawing' toolbar, and a 'Submit' button. A yellow sticky note provides search tips: 'For optimal results please keep structure and reaction searches simple and use filter options on the Results Tab.' Callout boxes explain the registration and login process.

Per accedir com a usuari registrat (MySOS)

Si volem accedir a MySOS, primer hem de crear-nos un compte personal

Ens identifiquem a MySOS

L'accés a MySOS ens permet gravar cerques i executar-les posteriorment

For optimal results please keep structure and reaction searches simple and use filter options on the Results Tab.

Tipus de cerques



- Text complet
- Avançada
- Estructural:
 - Substàncies
 - Reaccions
- Combinada: text complet i estructura

Cerca de text

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents

FUNCTIONS

- Use-ChemDraw
- Upload Molecule...
- Reset Query

Enter your Query

Full Text

ferrocene

ferrocene
ferrocenebisphosphine
ferroceneboronic
ferrocenecarbaldehyde
ferrocenecarbaldehydes
Ferrocenecarbonyl
ferrocenecarboxamide
ferrocenecarboxylate
ferrocenecarboxylic
ferrocenediyl
ferrocenes
Ferrocenes
ferrocenestellurolate
ferrocenethiolate

Drawing Submit

For optimal results please keep structure and reaction searches simple and use filter options on the Results Tab.

Al posar el terme de cerca, s'obre el diccionari i ens dona diferents variacions possibles del terme.

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents MySOS Log out

REFINE

RETRIEVE:

- Title (25)
- Full Text (465)

SORT LIST:

- By relevance
- By publication date

FUNCTIONS

- Upload Molecule
- Save Molecule
- Log Out
- Search Molecules
- Download Hits
- Reset

Results (Articles found containing your search term, structure or reaction)

Page: 1

21 Three Carbon-Heteroatom Bonds: Amides and Derivatives; Peptides; Lactams #1 of 467

Mahajan, Y. R.; Weinreb, S. M., *Science of Synthesis*, (2005) 21, 1.
...acids, chiral nucleophiles such as cinchona alkaloids (e.g., quinine), or chiral ferrocene
...2+2] Cycloaddition of an Imine with a Ketene in the Presence of a Chiral Ferrocene Derivative
> Show Full Text > Show TOC

1 Compounds with Transition Metal-Carbon n-Bonds and Compounds of Groups 10 - 8 (Ni, Pd, Pt, Co, Rh, Ir, Fe, Ru, Os) #2 of 467

Lautens, M., *Science of Synthesis*, (2001) 1, 1.
Reactions of Ferrocene Complexes
Many of the ferrocene complexes described in this section are useful in the synthesis of ligands for catalytic reactions...
> Show Full Text > Show TOC

Organometallic Complexes of Iron #3 of 467

1.7 Product Class 7: Organometallic Complexes of Iron
Stephenson, G. R., *Science of Synthesis Knowledge Updates*, (2014) 1, 1.
...chemistry is more closely related to the organic chemistry of the ligands. Ferrocene affords an architecture in which substituents on the two coplanar cyclopentadienyl ligands are...
> Show Full Text > Show TOC

Organometallic Complexes of the Actinides #4 of 467

2.13 Product Class 13: Organometallic Complexes of the Actinides
Batrice, R. J.; Karmel, I.-S.; Eisen, M. S., *Science of Synthesis Knowledge Updates*, (2012) 4, 99.
...the discovery of the first organometallic complexes, often erroneously assumed to be the preparation of ferrocene,
> Show Full Text > Show TOC

Organometallic Complexes of Titanium #5 of 467

Resultats de la cerca: Es pot accedir al text complet i a la taula de continguts.

La cerca es fa al títol i també, al text complet.

Cerca avançada

- Operadors booleans (S'han de posar en majúscules):
 - AND: cerca diferents termes alhora al mateix document.
 - OR: cerca els termes al mateix document. No cal que hi siguin tots.
 - NEAR: els termes de cerca han d'estar a prop entre ells dins del document.
- Truncament (*): Es pot posar tan al final com a principi del terme *XXX*, XXX*, *XXX
- "XXX XX": es busca el terme o frase exacta de dins de les cometes.
- Cerca de metadades. S'han d'utilitzar els següents prefixos davant del terme de cerca:
 - **Section, volume o page:** número de secció, volum o pàgina dins del SOS.
 - **author:** autors que han contribuït al SOS.
 - **year:** any de publicació del volum del SOS.
 - **title:** títol de la secció.
 - **ref-author:** autor de les referències citades.
 - **ref-year:** any de publicació de les referències citades.
 - **journal:** títol de la revista de les referències citades.
 - **cas-rn:** número de registre del CAS.
 - **doi:** Digital Object Identifier (DOI).
 - **namereaction:** nom de la reacció.

Cerca avançada

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents

FUNCTIONS

- Use-ChemDraw
- Upload Molfie...
- Reset Query

Enter your Query

Full Text

organocatal* AND year:2010

Drawing

Termes de cerca amb truncament, operador booleà i prefix

Resultats amb el text complet corresponent

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents

REFINE

SORT HITLIST:

- By relevance
- By publication date

Update

FUNCTIONS

- Select all hits
- Deselect all hits
- Reset all hits

Results (Articles found containing your search term, structure or reaction)

Page: 1 of 10

- Alkenes
47.1.3.1.2.4 Method 4: Reactions Using Chiral **Organocatalysts**
Fringuelli, F.; Piematti, D.; Pizzo, F.; Vaccaro, L., *Science of Synthesis*, (2010) 47, 679.
Method 4: Reactions Using Chiral **Organocatalysts**
In addition to organometallic asymmetric catalysts, asymmetrically induced **organocatalytic** reactions have attracted intense interest.
Show Full Text Show TOC
- 41 Nitro, Nitroso, Azo, Azoxy, and Diazonium Compounds; Azides, Triazenes, and Tetrazenes
Banert, K., *Science of Synthesis*, (2010) 41, 1.
is conducted in the presence of an enantiopure **organocatalyst**, the product
Show Full Text Show TOC
- Alkenes
47.1.3.1.3.1.3 Variation 3: With **Organocatalysts**
Fringuelli, F.; Piematti, D.; Pizzo, F.; Vaccaro, L., *Science of Synthesis*, (2010) 47, 700.
Variation 3: With **Organocatalysts**
Certain **organocatalysts** can be used to increase the reactivity and selectivity of enantioselective cycloadditions. Most of these promoters are aza-**organocatalysts**.
Show Full Text Show TOC
- Nitroalkanes
47.1.3.1.2.4 Method 4: Reactions Using Chiral **Organocatalysts**
DOI: 10.1055/66-36-047-00352
Fringuelli, F.; Piematti, D.; Pizzo, F.; Vaccaro, L., *Science of Synthesis*, (2010) 47, 679.
In addition to organometallic asymmetric catalysts, asymmetrically induced **organocatalytic** reactions have attracted intense interest.^{[1]-[10]} The advantages of an **organocatalyst** over a metal promoted process are (i) no metals contaminate the reaction products, (ii) the catalysts are simple and stable molecules that can be easily modified, (iii) an aprotic atmosphere, inert solvents, and even aqueous media can be used, and (iv) the catalyst is easily immobilized on a solid support. The most generally employed strategy to perform an organo-catalyzed Diels-Alder cycloaddition is to generate an active minimum ion from an α -sulfonamide substituted aldehyde and its enone (the **organocatalyst**) that lowers the LUMO of the diophile (analogous to the effect caused by a Lewis acid catalyst), making the cycloaddition reaction go faster.^[11] Final hydrolysis of the intermediate adduct releases the product and regenerates the amine. The efficiency of the process depends upon the rate of the minimum ion generation.^[12] Among the proposed chiral **organocatalysts**, the (R)-binaphthyl-based diamine **20b** exhibits unprecedentedly high enantioselectivity (81–95%) in the asymmetric Diels-Alder reaction of an α,β -unsaturated aldehyde with cyclohexadiene in dichloromethane or (D)-fluoromethylbenzene as the solvent (Scheme 1.14).^[13] Analogous eno selectivity is observed when performing the same type of cycloaddition with a cyclic hydroxide in a compact camphor-derived framework combined with trifluoromethanesulfonic acid and working in aqueous medium.^[14] The pyridone derivative **20c**, combined with trifluoroacetic acid, is an effective catalyst in the enantioselective synthesis of cyclohexenone-benzaldehyde (Scheme 1.14).^[15]

Scheme 1.14 Synthesis of Cyclohexenone by Diels-Alder Reactions Promoted by Chiral **Organocatalysts**^{[14]-[15]}

Cerca avançada

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents

FUNCTIONS

- Use ChemDraw
- Upload Mofile...
- Reset Query

Enter your Query

Full Text

"Wittig chemistry"

Drawing

Es cercarà exactament el terme o frase que es troba entre cometes

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents

REFINE

RETRIEVE

- Full Text (6)
- Reaction (2)

SORT BY:

- By relevance
- By publication date

FUNCTIONS

- Select all hits
- Deselect all hits
- Reset all hits

Results (Articles found containing your search term, structure or reaction)

2.6.1 Product Subclass 1: Metal-Carbene Complexes

Schrock-type carbene complexes, those of group 6 metals present marked nucleophilic reactivity undergo Wittig chemistry with α

46.1.1.1 Method 1: Synthesis from Phosphorus Ylides and Enones or Enals

1.7.8.17.2.14 Method 14: Applications in Oligomers and Polymers

With simple achiral cocenes, Wittig chemistry builds up 1-(chloromethyl)-3,5-bis(

20.8.4.1.2

ation 3: Acylation by Carboxylic Acids

Wittig chem

15.

with Formation of the 1-2 and 3-4 Bonds

pend on aza-Wittig chemistry for the 1

Resultats de cerca

2 F.L. Fieser: η^5 -Carben-Komplexe über Heterofunktion am C-Atom

III) über Heterofunktion am Carben-C-Atom

1. ein Metall-Komplex mit Carben, Diäthenyl-Verbindungen bzw. Alkyl- η^5 -Cyclopentadienyl-Liganden

Die Herstellung von Carben-Komplexen gelingt gelegentlich durch Übertragung des Carben-Liganden aus einem anderen η^5 -Komplex, z. B.:

$$K^+M^+CO_3^{2-} + Ph_2C=CH-C_5H_4M^+ \xrightarrow{O_2, \text{BF}_3 \cdot OEt_2} K^+M^+CO_3^{2-} + Ph_2C=C_5H_4M^+$$

$M = Cr, Mo$

η^5 -Cyclopentadienyl-Liganden: η^5 -Cp, η^5 -Cp*

Die Herstellung von Carben-Komplexen gelingt gelegentlich durch Übertragung des Carben-Liganden aus einem anderen η^5 -Komplex, z. B.:

Die Komplexe Typen werden nach Zahl der gebundenen C-Atome geordnet. Weiterhin unterscheiden man zwei Gruppen der Liganden:

- Die, die über eine große Zahl von C-Atomen gebunden werden (η^5 , η^6 und η^7 -Liganden, die als solche eine Kohlenwasserstoff-Struktur besitzen)
- Die, die über eine geringe Zahl von C-Atomen gebunden werden, aber η^5 , η^6 und η^7 -Liganden, die in einem Metall-Atom (z.B. η^5 -Cp) gebunden sind

Beide Gruppen sind die Herstellungsmethoden oft sehr ähnlich. Alkine können entweder über zwei oder über vier π -Elektronen gebunden werden und in letzterem Falle werden sie an ein Metall-Atom (z.B. η^5 -Cp) als η^5 -Ligand gebunden. Zur Benennung nach dem „System“ ist nur die Zahl der Metall-C-Kontakte wichtig ohne Rücksicht auf die Bindungszahl.

a) η^5 -Komplexe

η^5 -Carben-Komplexe

Alle Komplexe, die formal mit einer M-C-Doppelbindung beschrieben werden können, werden als Carben-Komplexe bezeichnet. Mit wenigen Ausnahmen besitzen die beschriebenen Carben-Komplexe elektronenreiche Substituenten, so daß die M-C-Bindung nur teilweise Doppelbindungscharakter anzeigt.

2.6.1 Product Subclass 1: Metal-Carbene Complexes

DOI: 10.1055/sos-SD-002-00315

Polk, R.; Smith, K. M., Science of Synthesis, (2003) 2, 283.

While group 6 complexes containing carbonyl ligands (Fischer-type) are most common for chromium, those without carbonyl ligands (Schrock-type, also called alkylidene complexes) are more typical of molybdenum and tungsten. Although a few chromium examples are known,^[1] our attention will be almost completely devoted to molybdenum and tungsten systems. These complexes are generally found in high oxidation states (2-6) and supported by electronegative, σ -donor ligands (alkoxy, amido, imido). These ligands have the possibility of stabilizing low-coordination environments by σ -donation in excess of the valence requirement (e.g., σ -2x Mo=O or W=O or imido derivatives), resulting in tetrahedral species. Often, however, these complexes allow expansion of the coordination sphere by formation of dimers (e.g., halide bridged) or by addition of two-electron donor with formation of five-coordinate and occasionally six-coordinate species, the formation of which is more likely for tungsten than for molybdenum and when the metal bears electron-withdrawing ligands.^[2]

Group 6 metal-carbene complexes are most stable when devoid of β -hydrogen atoms on the carbene ligand, the latter leading to decomposition by 1,2-H migration and formation of alkene derivatives.^[3] The carbene ligand usually bears hydrogen or alkyl substituents, and is normally considered as a nucleophilic $(-CR^2R^3)^-$ ligand for the purpose of formal oxidation state assignment. Like all other Schrock-type carbene complexes, those of group 6 metals present marked nucleophilic reactivity and undergo Wittig chemistry with α -molecules, the thermodynamics favoring the Mo=C and Re=C combination when X is harder than Y.^[4] This reaction, however, does not represent particular advantages over classical Wittig reagents for organic synthesis, a major use being the metal removal at the end of organic transformations carried out on carbene complexes (e.g., alkene metathesis, see Section 2.6.1.5).

References

[1] Harding, M. M.; Mokide, G.; Mackay, J. P.; Probst, J.; Lucas, S. W., *Inorg. Chem.*, (1998) 37, 2432.

[2] Suppan, K. D.; Watanabe, K. E., *J. Am. Chem. Soc.*, (1996) 118, 10311.

[3] Freudenberger, J. M.; Schrock, R. R., *Organometallics*, (1995) 4, 1037.

[4] Schrock, R. R.; Hurdock, J. S.; Bazzan, S. C.; Robbins, J.; O'Hare, M.; O'Regan, M., *J. Am. Chem. Soc.*, (1990) 112, 3075.

Related Information

1. Houben-Weyl, (1965) E 10-1, 2.

Houben-Weyl escanejat

Text complet. Conté cites del Houben-Weyl i dona accés al corresponent document escanejat.

Cerca de substàncies per estructura

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents | Log out

FUNCTIONS

- Use ChemDraw
- Upload Molfile...
- Save Query...
- Load Query...
- Reset Query

Enter your Query

Full Text

Drawing

C N O S F

Clc1ncnc1

Clear Drawing Submit

Es poden incorporar arxius amb extensió .mol

For optimal results please keep structure and reaction searches simple and use filter options on the Results Tab.

L'editor permet dibuixar l'estructura de cerca. No cal tenir Java instal·lat.

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents | MySOS | Log out

REFINE

FILTER BY:

- Reaction Reactant (131)
- Reaction Product (109)
- Molecule (2)
- Reaction Catalyst (2)
- Reaction Reagent (1)

FILTER BY MATCH TYPE:

- Substructure Match (149)

SORT HITLISTS:

- By relevance
- By publication date

Update

FUNCTIONS

- Update hitlist
- Save hitlist
- Load hitlist
- Select all hits
- Deselect all hits
- Reset all hits

Results (Articles found containing your search term, structure or reaction)

Page: 1 of 10

- Pyrimidines #1 of 149
16.12.4.1.4.2.1 Formation of Stannylpyrimidines
von Angerer, S., Science of Synthesis Knowledge Updates, (2011) 1, 356.
Show Reaction Show Full Text Show TOC Show Single Step Reactions
- Aryllicon Cross-Coupling Reactions #2 of 149
1.2.1.3.6.2.2 Brønsted Base Activation
Denmark, S.; Chang, W.-T. T., Science of Synthesis: Cross Coupling and Heck-Type Reactions, (2012) 1, 419.
Show Reaction Show Full Text Show TOC Show Single Step Reactions
- Organotin Cross-Coupling Reactions #3 of 149
1.3.1.2.3.3 Coupling Using a (β-Oxoiminato)(phosphine)palladium Complex
Pitaval, A.; Echevarren, A. M., Science of Synthesis: Cross Coupling and Heck-Type Reactions, (2012) 1, 542.
Show Reaction Show Full Text Show TOC Show Single Step Reactions
- Pyrimidines #4 of 149
16.12.4.1.4.3.3 Palladium-Catalyzed Cross Coupling with Organostannanes (Stille Reaction)
von Angerer, S., Science of Synthesis Knowledge Updates, (2011) 1, 371.
Show Reaction Show Full Text Show TOC Show Single Step Reactions
- Purines #5 of 149
16.17.3.4.1.2.1 Variation 1: Chlorination with Phosphoryl Chloride
Seel, F.; Ramzeva, N.; Rosemeyer, H., Science of Synthesis, (2004) 16, 1042.
Show Reaction Show Full Text Show TOC Show Single Step Reactions
- Purines #6 of 149
16.17.3.2.1 Method 1: Dehalogenation
Science of Synthesis, (2004) 16, 1000.
Show Reaction Show Full Text Show TOC Show Single Step Reactions

Els resultats inclouen substàncies i reaccions que contenen l'estructura que ens interessa. Es poden refinar.

Es poden gravar llistes de resultats i recuperar-les més tard

Cerca de reaccions

Per cercar reaccions cal dibuixar l'estructura de qualsevol component de la reacció. No és necessari dibuixar la reacció completa

FUNCTIONS

- Use ChemDraw
- > Upload Molfile...
- > Save Query...
- > Load Query...
- > Reset Query

Enter your Query

Full Text

Drawing

Clear Drawing Submit

REFINE

FILTER BY:

- Reaction (11)

FILTER BY MATCH TYPE:

- RX-UNKNOWN Hits (9)

SORT HITLIST:

- By relevance
- By publication date

Update

FUNCTIONS

- > Update hitlist
- > Save hitlist
- > Load hitlist
- > Select all hits
- > Deselect all hits
- > Reset all hits

Results (Articles found containing your search term, structure or reaction)

Page: 1 of 10

- Enolates
32.5.2.2.6 Method 6: Protonation and Deuteration of Enolates
Trauner, D., *Science of Synthesis*, (2008) 32, 573.
Show Reaction Show Full Text Show TOC Show Single Step Reactions
- Aryl Ketones with the Carbonyl in a Ring
26.8.3.1.9.3 Variation 3: By [4+2] Aromatic Ring Formation
Campagne, J. M.; Six, Y., *Science of Synthesis*, (2005) 26, 1031.
Show Reaction Show Full Text Show TOC Show Single Step Reactions
- Seven-Membered and Larger-Ring Cyclic Ketones
26.12.1.3.5 Variation 5: Electrocyclic Ring Expansions
Scott, P. J. H., *Science of Synthesis Knowledge Updates*, (2013) 4, 290.
Show Reaction Show Full Text Show TOC Show Single Step Reactions
- Palladium-Alkene Complexes
1.2.4.7.2 Oxy-Cope Rearrangement
Takacs, J. M.; Vayalakkada, S., *Science of Synthesis*, (2001) 1, 371.
Show Reaction Show Full Text Show TOC Show Single Step Reactions

Reaction

R1C(OH)C(R2)C(R3)C(R4)C=C $\xrightarrow[\text{THF, 25 } ^\circ\text{C}]{\text{PdCl}_2(\text{NCPH})_2 (0.1 \text{ equiv})}$ R1C(OH)C(R2)C(R3)C(R4)C=C \rightarrow R1C(OH)C(R2)C(R3)C(R4)C=O

For optimal results please keep structure and reaction searches simple and use filter options on the Results Tab.

Es poden indicar els àtoms on té lloc la reacció.

A la pantalla de resultats és possible visualitzar directament la reacció

Cerca combinada

Diferents opcions per refinar els resultats

Als resultats apareix el terme cercat i l'estructura

Thieme Science of Synthesis

Home Query Results Full Text Explore Contents MySOS

FUNCTIONS

- Use-ChemDraw
- Upload Molfile...
- Reset Query

Enter your Query

Full Text

epoxidation

Drawing

Clear Drawing Submit

Return to Top

For optimal results please keep structure and reaction searches simple and use filter options on the Results Tab.

És possible fer una cerca de text i estructura a la vegada.

Text complet

Science of Synthesis

Home Query Results Full Text Explore

REFINE

FILTER BY:

- Reaction Reactant (20)
- Reaction Product (1)

FILTER BY MATCH TYPE:

- Exact Match (15)
- Substructure Match (2)

RETRIEVE:

- Title (8)
- Full Text (17)
- Nomenclature (5)

SORT HITLIST:

- By relevance
- By publication date

Update

FUNCTIONS

- Select all hits
- Deselect all hits
- Reset all hits

Results (Articles found containing your query in title or reaction)

Page: 1 of 10

37 Ethers

Forstner, C. J.; Science of Synthesis, (2008) 37, 1.

synthesis by carbonyl **epoxidation**), and methods for epoxide preparation are organized into four categories: alkene **epoxidation** mediated by metals (Section), alkene **epoxidation**

Show Reaction Show Full Text Show TOC Show Single Step Reactions

Reaction Reactant

0.7 mol% NaOCl, PhCl >98%

indinavir

Synthesis from Alkenes by Metal-Mediated Oxidation #2 of 17

NAVIGATION #13 of 17

Science of Synthesis

Well-known procedures for the synthesis of epoxides include the Harwood-mediated Sharpless reaction for chiral alkenes (Scheme 2),^[1]

Scheme 2 Sharpless Asymmetric **epoxidation** [14]

Another widely used procedure is the manganese-mediated Jacobsen **epoxidation**, as exemplified in the synthesis of a precursor to the HIV protease inhibitor indinavir (Scheme 3).^[14]

Scheme 3 Jacobsen Asymmetric **epoxidation** [14]

Visualització dels resultats

The screenshot shows the 'Science of Synthesis' search results page. The top navigation bar includes 'Home', 'Query', 'Results', 'Full Text', and 'Explore Contents'. The 'Results' section displays a list of search results with checkboxes, titles, and brief descriptions. A 'REFINE' sidebar on the left allows filtering by 'Title (25)' and 'Full Text (465)'. A 'FUNCTIONS' sidebar on the right includes 'Collapse Tree'. A 'Text complet' callout points to the word 'ferrocene' in the search results. A 'Taula de continguts' callout points to the 'Explore Contents' sidebar on the right, which lists various chemical classes and sub-classes.

A la cerca de text podem refinar els resultats. El nostre terme de cerca pot trobar-se al títol o al text complet

Taula de continguts

Text complet

Visualització dels resultats

Reset all hits

SHOW REACTION SHOW FULL TEXT SHOW TOC SHOW SINGLE STEP REACTIONS #4 of 9

Palladium-Alkene Complexes

1.2.4.7.2 Oxy-Cope Rearrangement
Takacs, J. M.; Vayalakkada, S., *Science of Synthesis*, (2001) 1, 371.

Show Reaction Show Full Text Show TOC Show Single Step Reactions

Reaction

Des dels resultats de la cerca de reaccions s'accedeix al text complet

Query | Results | Text | Explore

0 Hits

NAVIGATION

Previous / Next

1.2.4.7.2 Oxy-Cope Rearrangement

DOI: 10.1055/sos-SD-001-00238

Takacs, J. M.; Vayalakkada, S., *Science of Synthesis*, (2001) 1, 371.

The oxy-Cope rearrangement is a synthetically useful variant on the Cope rearrangement. While the full experimental details are not reported, it was found that in certain cases the palladium(II)-catalyzed rearrangement of **245** is quite facile (Scheme 71).^[246] For example, **245** (R¹ = R² = Me; R³ = R⁴ = H) undergoes palladium-catalyzed rearrangement to unsaturated ketone **247** under mild conditions ([PdCl₂(NCPh)₂ (0.1 equiv), THF, 25°C, 3 h) and in quantitative yield. The reaction presumably proceeds via a palladacyclohexyl cation (as illustrated in Scheme 67) to afford an intermediate enol **246**, which tautomerizes to the observed ketone. Bis(benzonitrile)dichloropalladium is a superior catalyst to other common palladium(II) complexes, e.g. [PdCl₂(cod)], [PdCl₂(PPh₃)₂], or Pd(OAc)₂. The reaction proceeds with good control over the geometry of the newly formed double bond (the observed E/Z is greater than 9:1) and can be used to construct macrocyclic rings [R¹, R² = (CH₂)₄ or (CH₂)₁₀]. One rather unusual limitation on the reaction is that in substrate **245** the substituents R¹ and R³ must be alkyl, neither can be hydrogen. The reasons for this requirement are not clear.

Scheme 71 Palladium(II)-Oxy-Cope Rearrangements^[246]

Text complet

Explore Contents

- Science of Synthesis
 - Organometallics
 - Ni, Pd, Pt, Co, Rh, Ir, Fe, Ru, and Os Compounds (Groups 10-8) (Vol. 1)
 - Organometallic Complexes of Nickel
 - Organometallic Complexes of Palladium
 - Palladium-Diene Complexes
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 - Allylic Ester Rearrangement

S'arriba a la taula de continguts (TOC), tant des de la pantalla de resultats com des del text complet

R ¹	R ²	R ³	R ⁴	Time (h)	Ratio (E/Z)	Yield (%) of 247	Ref
Me	H	Me	H	3		100	[246]
Me	CH ₂ CH=CMe ₂	Me	H	3	100	76	[246]
(CH ₂) ₄		Me	H	24	9	55	[246]
(CH ₂) ₁₀		Me	H	6	100	65	[246]

* The reaction failed for R¹ = R² = Me; R³ = H; R⁴ = Me or H and R¹ = R² = R⁴ = H; R³ = Me.

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Compendium with Four
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Heteroatom Bonds
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21 Three Carbon—Heteroatom Bonds: Amides and Derivatives; Peptides; Lactams

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This volume covers the synthesis of compounds containing an amide moiety, including peptides and lactams. These compounds have been divided into groups depending on the type of amide and the nature of the substituents around the amide functionality. These groups are shown in Table 1, together with the sections in which they appear.

Table 1 Classes of the Amide-Bond-Containing Compounds Covered in Volume 21

Product Class	Structural Formula(s)	Section
simple amides	$R^1C(O)NH_2$, $R^1C(O)NHR^2$, $R^1C(O)NR^2R^3$	21.1
triacylamines and diacylamines	$R^1C(O)NC(O)R^2C(X)R^3$, $R^1C(O)NR^2C(O)R^3$	21.2
<i>N</i> -[α -(heteroatom)alkyl]-substituted alkanamides	$R^1C(O)NR^2CX_2R^3$, $R^1C(O)NR^2CXR^3R^4$	21.3
<i>N</i> -aryalkanamides, ynamides, enamides, dienamides, and allenamides	$R^1C(O)NR^2Ar^1$, $R^1C(O)NR^2C=CR^3$, $R^1C(O)NR^2CR^2=CR^4R^5$	21.4
α -heteroatom-substituted alkanamides	$R^1C(X)C(O)NR^2R^3$, $R^1CX_2C(O)NR^2R^3$, $R^1CHXC(O)NR^2R^3$	21.5
alk-2-ynamides, arenecarboxamides, and alk-2-enamides	$R^1C\equiv CC(O)NR^2R^3$, $Ar^1C(O)NR^1R^2$, $R^1R^2C=CR^3C(O)NR^4R^5$	21.6
β -heteroatom-substituted alkanamides	$R^1C(X)CH_2C(O)NR^2R^3$, $R^2CX_2CH_2C(O)NR^2R^3$, $R^2CH(X)CH_2C(O)NR^2R^3$	21.7
α -lactams		21.8

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