



Science of Synthesis

Thieme

- Thieme promove os mais recentes avanços na prática clínica e é conhecida pela alta qualidade didática de seus livros, revistas e produtos eletrônicos.
- Além de publicar 70 novos títulos de livros a cada ano, a Thieme publica mais de 140 revistas médicas e científicas tanto em formato impresso tradicional quanto em formato eletrônico
- Possui uma longa história na área da saúde, atuando há mais de 125 anos.



Science of Synthesis

- É o único recurso que fornece revisão crítica de texto completo, bem como da metodologia sintética atual nos campos da química orgânica e organometálica.
- Escrito por químicos para químicos, a SOS fornece recomendações de especialistas de mais de 1.750 colaboradores, bem como informações únicas sobre o escopo e as limitações dos métodos sintéticos.

The screenshot shows the homepage of the Thieme Science of Synthesis database. It features a navigation bar at the top with links for 'Query', 'Results', 'Full Text', 'Explore Contents', and 'Training & Support'. A search bar is prominently displayed in the center, allowing users to search by word, author name, or DOI. Below the search bar, there are several categorized sections for exploring the science of synthesis, including Trends & Innovation, Functional Groups, Heteroarenes, Organometallics, and Hydrocarbons.

A página inicial é dividida em quatro partes:

1. Barra de navegação superior
2. Área de login pessoal

3. Caixa de pesquisa por texto e citação, além de busca por estrutura e/ou reação
4. Área de destaque

A página do conteúdo é dividida em três partes:

1. Ferramentas de refinamento lateral
2. Ferramentas de visualização de resultados
3. Resultados de busca

The screenshot shows the Thieme Science of Synthesis interface. At the top, there are navigation links for Help, Safety Statement, About Science of Synthesis, and About Thieme Chemistry. Below this is the Thieme logo and the title 'Science of Synthesis'. A menu bar contains 'Query', 'Results', 'Full Text', 'Explore Contents', and 'Training & Support'. A 'MySOS' button is located on the right.

Annotation 1: A red box highlights the 'REFINE' sidebar on the left. It includes sections for 'FILTER BY:' (with checkboxes for 'No role assigned (272)', 'Reaction catalyst (1673)', 'Reaction product (2796)', 'Reaction reactant (2230)', 'Reaction reagent (113)', and 'Reaction solvent (3)'); 'FILTER BY MATCH TYPE:' (with checkboxes for 'Exact (92)', 'Similar (166)', and 'Substructure (4529)'); and 'SORT HITLIST:' (with radio buttons for 'By relevance' and 'By publication date', and an 'Update' button).

Annotation 2: A red box highlights the 'Results' header area. It shows 'Results (Articles found containing your search term, structure or reaction)', a 'Hide All Reactions' button, and pagination controls (Page: 1, # 10). Below this are buttons for 'Select Page', 'Update Hit List', 'Delete Hits After This Page', and 'Reset Hit List'.

Annotation 3: A large red box highlights the main results area. It shows a section for 'Lead Compounds' (#1 of 4655) with the title '5.3 Product Class 3: Lead Compounds' and a citation: 'Moloney, M. G., *Science of Synthesis*, (2003) 5, 619.' It includes navigation links for 'Hide Reaction', 'Show Full Text', 'Show TOC', and 'Show Single Step Reactions'. Three chemical reactions are displayed:

- $R^1Pb(OAc)_3 \xrightarrow[53-81\%]{5 \text{ mol\% } Pd_2(dba)_3 \cdot CHCl_3, CHCl_3, \text{rt, 10 min}} R^1-R^1$
 $R^1 = Ph, Ar^1, 2\text{-thienyl}, C \equiv CR^2$
- $Ar^1Pb(OAc)_3 + R^1B(OH)_2 \xrightarrow[71-80\%]{5 \text{ mol\% } Pd_2(dba)_3 \cdot CHCl_3, 10 \text{ mol\% } CuI, NaOMe (6 \text{ equiv}), DME/MeCN (1:1)} Ar^1-R^1$
 $Ar^1 = Ph, 4\text{-MeOC}_6\text{H}_4, 2\text{-furyl}, 3\text{-furyl}, 2\text{-thienyl}; R^1 = Ph, Ar^2, (E)\text{-CH=CHPh}$
- $Ar^1Pb(OAc)_3 + Ar^2I(Ph^+ BF_4^-) \xrightarrow[62-75\%]{5 \text{ mol\% } Pd_2(dba)_3 \cdot CHCl_3, NaOMe (4 \text{ equiv}), MeOH/MeCN (1:1), \text{rt, 3 h}} Ar^1-Ar^2$
 $Ar^1 = Ph, 4\text{-MeOC}_6\text{H}_4, 2\text{-thienyl}; Ar^2 = Ph, 4\text{-MeOC}_6\text{H}_4, 2\text{-thienyl}, (E)\text{-CH=CHPh}$

Below this is a section for 'Monoarylcopper(I) Compounds' (#2 of 4655) with the title '3.4.1.3.4 Method 4: Biaryl Syntheses from Aryl Halides and Copper(I) Salts' and a citation: 'Heaney, H.; Christie, S., *Science of Synthesis*, (2004) 3, 361.' It includes navigation links for 'Hide Reaction', 'Show Full Text', 'Show TOC', and 'Show Single Step Reactions'. A chemical reaction is shown:

$$\text{C}_6\text{H}_4(\text{CO}_2\text{Me})\text{I} \xrightarrow[97\%]{\text{copper thiophene-2-carboxylate, NMP}} \text{C}_6\text{H}_3(\text{CO}_2\text{Me})_2$$

A página do conteúdo é dividida em três partes:

1. Navegação entre lista de resultados.
2. Ferramentas diversas: Download PDF; imprimir; citação; informações.
3. Navegação entre conteúdos.

1 NAVIGATION
Hit 1 of 491
Previous / Next

2

3

35.3.1.1.6.3 Azide-Induced Oxidative Iodination with Hydrogen Peroxide and Acetic Anhydride

DOI: 10.1055/sos-SD-135-00098

Iskra, J., *Science of Synthesis Knowledge Updates*, (2015) 2, 388.

The environmentally friendly oxidant hydrogen peroxide, acetic anhydride, and sodium azide are used for the **oxidative** iodination of various alkanes and cycloalkanes in an aqueous/organic biphasic mixture (**Scheme 3**).^[4] Acetic anhydride and sodium azide have to be used in excess to improve the efficiency with respect to iodine incorporation using the organic hypervalent iodine precursor. The yields for this reaction are given as the ratio between mmol of isolated iodinated compound per mmol of added molecular iodine. For example, iodocyclopentane (**5**) is obtained in a yield of 1.33 mmol per mmol of molecular iodine.

Scheme 3 Azide-Promoted Iodination in the Presence of Hydrogen Peroxide and Acetic Anhydride^[4]

Iodocyclopentane (5); Typical Procedure:^[4]

CAUTION: Hydrogen peroxide having concentrations of 50% or more is very hazardous and can explode violently, particularly in the presence of certain inorganic salts and easily oxidizable organic material.

CAUTION: Sodium azide can explode on heating and is highly toxic. Contact of metal azides with acids liberates the highly toxic and explosive hydrazoic acid.

Ac₂O (1.2 mL), H₂O (0.5 mL), and NaN₃ (0.20 g, 3 mmol) were sequentially added to a cooled soln (water/ice bath) of I₂ (0.25 g, 1 mmol) in cyclopentane (5 mL). 30% aq H₂O₂ (0.3 mL) was added and the mixture was vigorously stirred at 40 °C for 6 h. The mixture was poured into sat. aq NaHCO₃ (20 mL) this mixture was washed with 5% aq Na₂S₂O₃ (15 mL). The organic layer was dried (Na₂SO₄) and the excess pentane was recovered by distillation. The yellowish residue was purified by column chromatography (hexanes); yield: 0.26 g (1.33 mmol).

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