

Derwent Journal of Synthetic Methods

MDL's electronic, structure-searchable version of the Derwent Journal of Synthetic Methods combines up-to-date chemical reaction information from worldwide journal and patent sources with the power and convenience of MDL's reaction retrieval systems.

The top screenshot shows the MDL Database Browser search interface. It features a search bar, a field index on the left, and a search results area displaying a chemical reaction structure. The search type is set to 'Reaction Substructure'.

The bottom screenshot shows the search results page for a specific reaction. It displays the chemical structure of the reaction and a table of reaction details.

Product no.	% Yield	Grade	%CS	%ds	%de	%ee	Reactant no.	Reactant Grade
1	92							

Step no.	Catalysts and Solvents	Catalyst ID	Solvent ID
1	Non-Binchinger (Amberlyst A 20 tetracarboxylic dihydrogenate) THF	5211	1011

Reaction Details: R2340001004 Reaction Variation 1 of 14

External Registry No.: 19937573Y

Publ: A

Step: 1 Step

Conditions: Reference

Reference: Bolchini, G. P., Cainelli, G., Umari-Bonchi, A., J Organomet Chem 1993, 243 (2), 155.

This query seeks reactions that selectively reduce chloro-substituted nitrobenzene derivatives to the corresponding anilines. The query retrieves a synthetic procedure carried out under mild conditions using inexpensive starting material.

Your resource for new synthetic methods

MDL's electronic version of the *Derwent Journal of Synthetic Methods* provides a selection of current chemical reaction literature from more than 150 journal and patent sources worldwide.

Updated once a year with approximately 3,000 new reactions, it contains detailed information about:

- New synthetic procedures
- High-yield functional group transformations
- Improvements to existing synthetic methods
- Representative example reactions from the most significant new patents



WWW.MDL.COM



Powering
the Process
of Invention™

MDL®

MDL Information Systems, Inc.

14600 Catalina Street
San Leandro, CA 94577
TEL: (510) 895-1313
FAX: (510) 483-4738

About MDL

Over 1,000 life science companies supercharge their discovery engines with MDL software solutions to generate fresh ideas and make breakthrough discoveries. By synchronizing and streamlining the sharing and management of vital information and knowledge, we enable scientists to work more efficiently and invent drugs faster. This saves time, money, and lives. In support of our customers and the momentous challenges they face, everything we do must be reliable, resourceful, innovative, and insightful.

The screenshot displays the MDL Database Browser interface in Microsoft Internet Explorer. The main window shows a table with columns for Step no., Catalysts and Solvents, Catalyst ID, and Solvent ID. Below this, there are sections for Detailed Data, Conditions, and References. A table titled 'Reaction Variation 4 of 14' shows product and reactant information. Another table below shows catalyst and solvent details for a specific step.

Step no.	Catalysts and Solvents	Catalyst ID	Solvent ID
1	(M)2NH ₂ O ₂ CH ₂ (1.6%) Rf(CO)18 420 (1.44 Parts) 2-Ethoxyethanol (3 Part)	513 9822	4130 1228

Product no.	% Yield	Grade	tics	tds	tdc	hse	Reactant no.	Reactant Grade
1	99.7							

Step no.	Catalysts and Solvents	Catalyst ID	Solvent ID
1	Et ₃ N (Small amount, on silica, 1 part) n-Bu ₄ N ⁺ (Small amount, 2 parts) Hexane	858 7802	5427

The database is organized to easily examine the various reagents used to produce the same reaction. There are 14 methods to carry out the synthetic procedure shown here. Note the extremely high yield conditions (99.7%) reported in the European Patent source (Reaction Variation 4).

Coverage beyond THEILHEIMER

The *Derwent Journal of Synthetic Methods* extends the coverage of MDL's THEILHEIMER database. THEILHEIMER abstracts reactions from the literature published from 1946 to 1980. The *Derwent Journal of Synthetic Methods* begins where THEILHEIMER ends, covering the literature from 1980 to the present, using the same selection criteria. In addition, the *Derwent Journal of Synthetic Methods* includes worldwide patent literature information selected by the leader in patent coverage—Derwent Information.

Benefits at a glance

The *Derwent Journal of Synthetic Methods* is an indispensable tool for the synthetic chemist because it provides:

- An extension to the THEILHEIMER database to include current literature
- Useful synthetic methods from recent worldwide chemical literature
- Reaction abstracts from patents filed by the world's leading chemical and pharmaceutical companies
- Reaction cross-references to the *Synthetic Methods of Organic Chemistry*

For more information about the *Derwent Journal of Synthetic Methods*, please contact an MDL sales representative or visit www.MDL.com.

MDL Information Systems, Inc.
an Elsevier company

MDL is a registered trademark in the United States, and DiscoveryGate and "Powering the Process of Invention" are trademarks or service marks of MDL Information Systems, Inc. Other names used herein may be the trademarks or registered trademarks of their respective holders, in the United States and other countries.

© Copyright 2003 MDL Information Systems, Inc.
All rights reserved.
DJSM/01-03/5k