



Finding Chemical Safety Information

(Post-Workshop Version, revised 2023-07-21)

Also see: <https://guides.library.stanford.edu/lab-safety>

GRACE BAYSINGER, CHEM & CHEM ENG LIBRARIAN EMERITA, STANFORD UNIVERSITY (GRACEB@STANFORD.EDU)

MEGHAN LAFFERTY, CHEMISTRY, CHEMICAL ENGINEERING, & MATERIALS SCIENCE LIBRARIAN, UNIVERSITY OF MINNESOTA (MLAFFERT@UMN.EDU)

RALPH STUART, ENVIRONMENTAL SAFETY MANAGER, KEENE STATE COLLEGE, RALPH.STUART@KEENE.EDU

UMN RAMP REFRESHER AND CSL BUILDING WORKSHOP, JUNE 27-28, 2023

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Introduction

FINDING CHEMICAL
SAFETY INFORMATION

Safety Statement *Science of Synthesis*

Warning! Read carefully the following: Although this reference work has been written by experts, the user must be advised that the handling of chemicals, microorganisms, and chemical apparatus carries potentially life-threatening risks. For example, serious dangers could occur through quantities being incorrectly given. The authors took the utmost care that the quantities and experimental details described herein reflected the current state of the art of science when the work was published. However, the authors, editors, and publishers take no responsibility as to the correctness of the content. Further, scientific knowledge is constantly changing. As new information becomes available, the user must consult it. Although the authors, publishers, and editors took great care in publishing this work, it is possible that typographical errors exist, including errors in the formulas given herein. Therefore, **it is imperative that and the responsibility of every user to carefully check whether quantities, experimental details, or other information given herein are correct based on the user's own understanding as a scientist.** Scale-up of experimental procedures published in **Science of Synthesis** carries additional risks. In cases of doubt, the user is strongly advised to seek the opinion of an expert in the field, the publishers, the editors, or the authors. When using the information described herein, the user is ultimately responsible for his or her own actions, as well as the actions of subordinates and assistants, and the consequences arising therefrom.

Safety Statement in *Science of Synthesis*

Although authors, editors, publishers, take great care in publishing a work, incorrect quantities or typographical errors may occur.

Scientific knowledge is constantly changing. As new information becomes available, a user must consult it.

Scale-up of experimental procedures carries additional risks.

Warning statements based on a prescribed list of reagents used in a reaction are embedded in the full text of *SoS*.



- Chemical Substances
 - Name
 - CAS Registry Number
 - Structure
 - Class of substance
- Physical Properties
 - Experimental
 - Predicted
- Reactions
 - Experimental
 - Predicted
- Comments & Caveats:
 - Properties vary by physical state (liquid, solid, gas) and by concentration levels
 - Experimental methods are usually the most detailed in journal articles
 - Confirm information by using > 1 source
 - Unknowns: it is possible to search for unknowns using physical appearance (e.g., color), properties, and keywords.

Common Ways to Search for Chemical Safety Information

Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
CAS Common Chemistry	Includes basic data on ~500,000 commonly used and regulated substances.	Find substance identifiers & basic compound properties.	Annually	Open access /API	CAS
PubChem	A “21 st century handbook” w/ data from over 925 data sources covering more than 115 million chemicals.	Laboratory Chemical Safety Summary Datasheets and reactivity information from government hazmat sources.	Daily	Open access / API	NLM/NIH
CAMEO Chemicals	Covers 9,000 hazardous chemicals. Identifies reactions and precautions for pairs of chemicals at commercial scale.	Reactivity alerts, hazmat profile plus emergency response guidance.	Annually	Open access	NOAA/EPA
Pistoia Alliance Chemical Safety Library	Catalogs hazardous reactions to alert scientists to potentially dangerous experiments.	Laboratory scale reaction incidents reported by users or from the literature.	Crowd-sourced	Open access	CAS/Pistoia Alliance
Knovel	Has ~12,000 sci-tech handbooks plus interactive & visualization tools.	Full-text and tables to chemical safety handbooks.	1-3 Months	Subscription	Elsevier
Organic Syntheses	Provides detailed, reliable, and carefully checked procedures for the synthesis of organic compounds. Reproducibility is checked Editorial Board members.	Beginning August 2017, the first Note in every article is devoted to addressing safety aspects of the procedures described in the article.	1 Volume/Year. Includes Pre-Pub articles	Open Access	Organic Syntheses, Inc.
Science of Synthesis	Expert reviews of best synthetic methods for organic & organometallic compounds.	Safety warnings are highlighted the full text description of a method.	3-4 Times/Year plus Pre-Pub articles	Subscription / API	Thieme
SciFinder-n	Comprehensive database in chemistry and chemical engineering. Reactions for organic & organometallic compounds.	References, substances, and reactions. Includes properties, safety notes & methods for reactions.	Daily	Subscription	CAS
Reaxys	Core database (includes Beilstein, Gmelin, Chem Patents) w/ content going back to 1771. Reactions for organic, organometallic, and inorganic compounds.	Identification, reactions, and properties data plus “Laboratory Use and Handling” in “Other Data.”	Weekly	Subscription	Elsevier
Dimensions	Multidisciplinary database for articles, preprints, conference proceedings, & books.	Ability to do a full-text search for finding safety info such as methods.	Daily	Open access (Publications)	Digital Science

Summary of Sources Covered in UMN Workshop

“Foundational” - Chemical Safety Information Databases

Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
CAS Common Chemistry	Includes basic data on ~500,000 commonly used and regulated substances.	Find substance identifiers & basic compound properties	Annually	Open access /API	CAS
PubChem	A “21 st century handbook” w/ data from over 925 data sources covering more than 115 million chemicals.	Laboratory Chemical Safety Summary Datasheets and reactivity information from government hazmat sources	Daily	Open access / API	NLM/NIH
CAMEO Chemicals	Covers 9,000 hazardous chemicals. Identifies reactions and precautions for pairs of chemicals at commercial scale.	Reactivity alerts, hazmat profile plus emergency response guidance	Annually	Open access	NOAA/EPA
Pistoia Alliance Chemical Safety Library (CSL)	Catalogs hazardous reactions to alert scientists to potentially dangerous experiments.	Laboratory scale reaction incidents reported by users or from the literature	Crowd-sourced	Open access	CAS/Pistoia Alliance

a relatively new and developing foundational resource

Advanced Undergraduate - Chemical Safety Information Databases

CAS Common Chemistry, PubChem, & CAMEO Chemicals plus

Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
Knovel	Has ~12,000 sci-tech handbooks plus interactive & visualization tools.	Full-text and tables to chemical safety handbooks.	1-3 Months	Subscription	Elsevier
Organic Syntheses	Provides detailed, reliable, and carefully checked procedures for the synthesis of organic compounds. Reproducibility is checked by an Editorial Board member.	Beginning August 2017, the first Note in every article is devoted to addressing the safety aspects of the procedures described in the article.	1 Volume/Year. Includes Pre-Pub articles	Open Access	Organic Syntheses, Inc.
E-EROS (Encyclopedia of Reagents for Organic Synthesis)	Gives detailed information on more than 5,250 reagents and catalysts	Handling, Storage, and Precautions: (storage lifetime under certain conditions, dry box, etc.; incompatibilities with solvents and other reagents; emphasizes personal safety) [in Abstract]	Up to 200 new or updated articles added annually	Subscription, Open access to abstracts	Wiley
SciFinder-n	Comprehensive database in chemistry and chemical engineering. Reactions for organic & organometallic compounds.	References, substances, and reactions. Includes properties, safety notes & methods for reactions.	Daily	Subscription	CAS
Not Voodoo X	Collect of Lessons Learned and lab mishaps with a "vote up" mechanism to indicate similar experiences	Data related to undergraduate organic chemistry research	As needed	Publicly available	Univ of Rochester

Research & Specialty Labs - Chemical Safety Information Databases

Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
Knovel	Has ~12,000 sci-tech handbooks plus interactive & visualization tools.	Full-text and tables to chemical safety handbooks.	1-3 Months	Subscription	Elsevier
E-EROS (Encyclopedia of Reagents for Organic Synthesis)	Gives detailed information on more than 5,250 reagents and catalysts	Handling, Storage, and Precautions: (storage lifetime under certain conditions, dry box, etc.; incompatibilities with solvents and other reagents; emphasizes personal safety) [in Abstract]	Up to 200 new or updated articles added annually	Subscription, Open access to abstracts	Wiley
Science of Synthesis	Expert reviews of best synthetic methods for organic & organometallic compounds.	Safety warnings are highlighted the full text description of a method.	3-4 Times/Year plus Pre-Pub articles	Subscription / API	Thieme
SciFinder-n	Comprehensive database in chemistry and chemical engineering. Reactions for organic & organometallic compounds.	References, substances, and reactions. Includes properties, safety notes & methods for reactions.	Daily	Subscription	CAS
Reaxys	Core database (includes Beilstein, Gmelin, Chem Patents) w/ content going back to 1771. Reactions for organic, organometallic, and inorganic compounds.	Identification, reactions, and properties data plus "Laboratory Use and Handling" in "Other Data."	Weekly	Subscription	Elsevier
Dimensions	Multidisciplinary database for articles, preprints, conference proceedings, & books.	Ability to do a full-text search for finding safety info such as methods.	Daily	Open access (Publications)	Digital Science

EH&S Professionals – Chemical Safety Information Databases

Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
Knovel	Has ~12,000 sci-tech handbooks plus interactive & visualization tools.	Full-text and tables to chemical safety handbooks.	1-3 Months	Subscription	Elsevier
CCOHS – Academic Support Program	Collection of environmental and occupational health and safety databases, selected and priced specifically for the academic community.	Includes access to SDS, CHEMINFO, RTECS, OSH References, Toxicology, plus more. CHEMpendium, a supplemental product, offers cross-database search capabilities.	Monthly	Subscription	Canadian Centre for Occupational Health and Safety
E-EROS (Encyclopedia of Reagents for Organic Synthesis)	Gives detailed information on more than 5,250 reagents and catalysts	Handling, Storage, and Precautions: (storage lifetime under certain conditions, dry box, etc.; incompatibilities with solvents and other reagents; emphasizes personal safety) [in Abstract]	Up to 200 new or updated articles added annually	Subscription, Open access to abstracts	Wiley
SciFinder-n	Comprehensive database in chemistry and chemical engineering. Reactions for organic & organometallic compounds.	References, substances, and reactions. Includes properties, safety notes & methods for reactions.	Daily	Subscription	CAS
Dimensions	Multidisciplinary database for articles, preprints, conference proceedings, & books.	Ability to do a full-text search for finding safety info such as methods.	Daily	Open access (Publications)	Digital Science