Searching Inorganic Substances in SciFinder®
Agenda

• Today’s presenter
• CAS databases
• Explore Substances options
• When and how to use names, molecular formulas, or structures
• Demonstration
• Summary
• Training and learning resources
Today’s presenter

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Associate Librarian
University at Buffalo (State University of New York)
Substance content in SciFinder

- CAS REGISTRY℠ - the most authoritative collection of disclosed substance information
- World standard CAS Registry Number®

As of August 2011
Information from a substance answer

Substance Identifier "stannous fluoride" > substances (1)

1 Substance 0 Selected

Select All Deselect All | Sort by: CAS Registry Number

CAS Registry Number: 7783-47-3

View Substance Detail
Explore by Structure
Synthesize this...
Get Reactions where Substance is a
Get Commercial Sources
Get Regulatory Information
Get References
Export as Image
Export as molfile
Send to SciPlanner
Substance roles and properties

CAS Registry Number: 7783-47-3

SnF2

Tin fluoride (SnF2); Difluorostannylene; Fluoristan; Gel-Tin; Stannous fluoride; Stannous fluoride (SnF2); Stop; Tin bifluoride; Tin difluoride; Tin(II) fluoride

Deleted CAS Registry Numbers: 12324-56-0; 12324-60-6

~1,772 References


<table>
<thead>
<tr>
<th>CAS Role</th>
<th>Patents</th>
<th>Nonpatents</th>
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<tbody>
<tr>
<td>Analytical Study</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Biological Study</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Formation, Nonpreparative</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Miscellaneous</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Occurrence</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Preparation</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Process</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Properties</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Prophetic in Patents</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Reactant or Reagent</td>
<td>✓</td>
<td></td>
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<tr>
<td>Uses</td>
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</table>

Experimental Properties: Biological Density Electrical

<table>
<thead>
<tr>
<th>Biological Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Median Lethal Dose (LD50)</td>
<td>188.2 mg/kg</td>
</tr>
<tr>
<td>Median Lethal Dose (LD50)</td>
<td>128.4 mg/kg</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Density Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>4.57 g/cm³</td>
</tr>
<tr>
<td>Density</td>
<td>4.57 g/cm³</td>
</tr>
<tr>
<td>Density</td>
<td>4.57 g/cm³</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Electrical Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electric Conductance and Electric Resistance</td>
<td>See full text</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Spectra Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluorine-19 NMR Spectrum</td>
<td>See spectrum</td>
</tr>
</tbody>
</table>
Explore Substances options

- Chemical Structure
- Markush
- Molecular Formula
- Substance Identifier

Characteristic(s)
- Single component
- Commercially available
- Included in reference(s)

Class(es)
- Alloys
- Coordination compounds
- Incompletely defined
- Mixtures
- Polymers
- Organics, and others not listed

Studies
- Analytical
- Biological
- Preparation
- Reactant or reagent
Substance Identifier

- **Searches**
  - CAS Registry Number® (CAS RN) - assigned to every unique compound
  - Formal chemical names (CAS Index Names)
  - Synonyms, including trade names and code designations
Search by Substance Identifier if you have a…

- CAS RN from another source (e.g., article, MSDS, [www.commonchemistry.org](http://www.commonchemistry.org))

- Simple chemical/trade name for a…
  - Base element (Germanium)
  - Elemental particle (Top quark)
  - Specific mineral (Rutile)
  - Specific alloy (AISI H11; Hastelloy® C-276)
  - Specific salt or other common inorganic substance
Cautions when searching chemical names

• Retrieval generally requires an exact match
• No variants are retrieved, e.g., ionic species, isotopes, mineral forms, or hydrates
• The more complex the name, the more likely an exact match will fail, although SciFinder will attempt to find answers

Options: Molecular formula (MF) or structure searching often required to retrieve important variants.
Basic molecular formula conventions

• Recommend input of elements in Hill system order

• Used for
  – Most simple ionic salts, oxides, sulfides, and hydroxides (e.g., CsHO, BrNa)
  – Some simple minerals (e.g., FeS [troilite])
  – Homogeneous metal clusters (e.g., Au55)
Multicomponent substances

• Periods [.] separate components

• Formally known as ‘dot disconnect formulas’

• Most common convention for inorganics (e.g., H₂O₄S.2Na)

• Ratios often shown in separate composition table
Multicomponent substances: Salts/hydrates

1. Substance Detail
7757-82-6
(Component: 7664-93-9)

H₂O₄S₂·2Na
Sulfuric acid sodium salt (1:2)

1. Substance Detail
10102-17-7
(Component: 13686-28-7)

H₂O₃S₂·5H₂O·2Na
Thiosulfuric acid (H₂S₂O₃), sodium salt, hydrate (1:2:5)
## Multicomponent substances: Alloys

<table>
<thead>
<tr>
<th>Component</th>
<th>Component Percent</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni</td>
<td>78</td>
</tr>
<tr>
<td>Fe</td>
<td>21</td>
</tr>
<tr>
<td>Mn</td>
<td>0.3</td>
</tr>
</tbody>
</table>

**Fe . Mn . Ni**

Nickel alloy, base, Ni, Fe, Mn (Permalloy 78)

<table>
<thead>
<tr>
<th>Component</th>
<th>Component Percent</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>64</td>
</tr>
<tr>
<td>Ni</td>
<td>36</td>
</tr>
<tr>
<td>Mn</td>
<td>0.3</td>
</tr>
</tbody>
</table>

**Fe . Mn . Ni**

Iron alloy, base, Fe 64, Ni 36, Mn 0.3
Multicomponent substances: Tabular inorganics

• Tabular Inorganic Substances (TIS) definition
  • Structure is unknown, or
  • Does not exist as a discrete molecule, or
  • Has a 3D lattice structure, or
  • Has a nonstoichiometric fraction composition or range of compositions

• TIS include complex carbonates, phosphates, and oxides
Tabular inorganics examples

1. **Substance Detail 860021-07-4**

<table>
<thead>
<tr>
<th>Component</th>
<th>Component Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>2</td>
</tr>
<tr>
<td>O4P</td>
<td>1.5</td>
</tr>
<tr>
<td>V</td>
<td>1</td>
</tr>
<tr>
<td>Ag</td>
<td>3.5</td>
</tr>
</tbody>
</table>

**Ag . O4 P . O . V**

Silver vanadium oxide phosphate (Ag3.5VO2(PO4)1.5)

2. **Substance Detail 208391-95-1**

<table>
<thead>
<tr>
<th>Component</th>
<th>Component Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>2</td>
</tr>
<tr>
<td>O4P</td>
<td>1</td>
</tr>
<tr>
<td>V</td>
<td>1</td>
</tr>
<tr>
<td>Ag</td>
<td>2</td>
</tr>
</tbody>
</table>

**Ag . O4 P . O . V**

Silver vanadium oxide phosphate (Ag2VO2(PO4))
Alternate molecular formulas

- Multicomponent substances with specific ratios assigned a second molecular formula
  - Simple molecular formula with the component ratios and no dots which is searchable using molecular formula query screen

- Example: Molybdenum Silver Oxide (Ag₂Mo₂O₇) assigned two molecular formulas
  - Ag.Mo.O (standard dot disconnect)
  - Ag₂Mo₂O₇ (alternate MF)
Search by molecular formula for...

• **All forms of an element (isotopes, ions, etc.)**
  – Can refine results to only isotope-containing

• **All forms of a mineral**
  – O2Ti retrieves Brookite, Rutile, and Anatase
  – Al.HO.O5.Si2 or Al2H4O9Si2 retrieves Kaolinite
Molecular formula searching for metals

• Alloys with a fixed number of elements
  – ‘Al.Cu.Fe.Mg.Mn.Si’ retrieves every alloy with exactly those elements

• Cermets (alloys with non-metallic elements)
  – ‘CW.Co’ retrieves all cobalt tungsten carbides (any ratio)

• Intermetallics
  – Cu3Sn (alternate molecular formula) retrieves the copper-tin intermetallic with that specific ratio
Molecular formula searching is good for...

- Elements and minerals (Br, Ca.H2O4S.2H2O)
- Simple ionic salts, oxides, hydroxides, and sulfides (MgO, FeH2O2)
- Oxygen-containing acid based salts (H3O4P.3Na)
- Specific hydrates (Cu.H2O4S.5H2O)
- Alloys and related compounds (Fe.Ni.Mn)
- Tabular Inorganic Substances (TIS)
Searching coordination compounds

1. Draw structure and select search type
Searching coordination compounds

2. Check “Show Precision Analysis” and “Coordination Compounds”
Searching coordination compounds

3. Select “Conventional Substructure [or Exact]” on Precision Candidates screen.
Sample substructure search results
Structure searches are also useful for…

- All hydrates of a given salt (Demo)
- Specific ions (e.g., Ge$^{4+}$)
  - Draw atom and assign proper charge
- Alloys and TIS where additional elements may be present
  - Draw in each element/species as a separate fragment
  - Run exact structure search checking “Show Precision Analysis” and “Organics and others not listed” boxes
  - `Choose “Conventional Exact” option in the Precision Candidate window"
Demonstration

Use of Silver Vanadium phosphate oxides in battery applications.

Structure search for copper sulfate hydrates
Review of key tips and techniques

- Search CAS RN or simple name, if available
- Keep in mind molecular formula conventions (especially dot disconnects for inorganics)
- Prefer structure searching if name or molecular formula are long and complex
- Test query/known compound similar to the substance of interest to verify how it is represented by CAS
- Precision Analysis is an important tool
## Advantages of substance searching in SciFinder

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Comprehensive</strong></td>
<td>Database of more than 62 million organic and inorganic substances</td>
</tr>
<tr>
<td><strong>Current</strong></td>
<td>Updated daily</td>
</tr>
<tr>
<td><strong>Flexible</strong></td>
<td>Multiple search options (chemical name, CAS RN, molecular formula, structure)</td>
</tr>
<tr>
<td><strong>Integrated</strong></td>
<td>Obtain additional information for retrieved substances (e.g., reactions, commercial suppliers, references, patents, and properties)</td>
</tr>
</tbody>
</table>
Training and learning resources

• Product help messages
• Open Practice Sessions, Virtual Classes
• Interactive training tutorials and e-seminars on CAS Learning Solutions
  learningsolutions.cas.org
Browsing for SciFinder training materials

Welcome to CAS Learning Solutions! We invite you to explore our full range of instructor-led and self-directed training.

Here is what you can do from this page:

- **Calendar** - View upcoming instructor-led events and register for them.
- **Search Training** - Find instructor-led and self-directed training by keyword.
- **My Selections** - Keep track of your favorite resources and activities.
- **Browse for Training** - Find instructor-led and self-directed training by topic.
- **My Upcoming Sessions** - See calendar events for which you have registered.

### Browse for Training

- All SciFinder Topics
- Overview and New Features
- Reference Searching
- **Substance Searching**
- Reaction Searching
- Patent Searching
- SciFinder 2007 Client Version
### Substance searching tutorials

<table>
<thead>
<tr>
<th>Code</th>
<th>Title</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>231.100</td>
<td>Substance Searching Chemical Abstracts Service</td>
<td>This collection contains SciFinder learning resources that explain the various search techniques and analysis tools that you can use to find substances of interest. Request this collection to add it...</td>
</tr>
<tr>
<td>231.110</td>
<td>Introduction to Substance Searching CAS</td>
<td>(15-minute interactive tutorial) This module presents an overview of how to: Search by substance identifier. Use a retrieved substance as the basis for a new search. Search for similar structures, exact structures, and substructures. View substance details. Analyze and refine the answer set by structure characteristics, substance role, elements, and atom attachments.</td>
</tr>
<tr>
<td>231.410</td>
<td>SciFinder Fundamentals Part 2: Basic Substance Search and Analysis Techniques</td>
<td>(45-minute recorded e-Seminar from September 2010) Build your knowledge of basic search and analysis techniques that will get the results you need to support your research. This seminar covers: CAS Registry content. Overview of the Explore Substances functions. Definitions of Substance Identifier, Molecular Formula, Exact Structure, Substructure, Similarity, and Markush searches. Tools for analyzing and refining your answer set. Tips and techniques for drawing stru...</td>
</tr>
<tr>
<td>233.110</td>
<td>Search by Exact Structure Chemical Abstracts Service</td>
<td>(5-minute interactive tutorial) Learn how to retrieve substances that match the structure query. You will be shown how to: Draw a chemical structure. Retrieve substances that match the structure query. Limit the search to substances that have specific characteristics. Refine the substance answer set.</td>
</tr>
<tr>
<td>233.115</td>
<td>Search by Substructure Chemical Abstracts Service</td>
<td>(0-minute interactive tutorial) Learn how to search for substances that contain a substructure of interest. You can limit the types of substitution allowed on the substructure by applying special query features. You will be shown how to: Conduct a substructure search. Evaluate the answers retrieved, and then refine the answer set by modifying the chemical structure. Block substitution on the structure query. Use structure variables. Refine the answer set by using u...</td>
</tr>
</tbody>
</table>
Questions?