

# Searching CrossFire Gmelin

A Supplement to  
***Searching CrossFire Databases-***  
***based on CrossFire Beilstein*** Training Guide

Chapter 1  
Introduction

Training Guide



CrossFire<sup>®</sup> Commander  
Version 7.1



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Training Guide

## Chapter 1 Introduction

### CrossFire<sup>®</sup> Commander Version 7.1

### Training Guide

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## Searching CrossFire Gmelin

### ***Key points***

- Welcome to the *Searching CrossFire Gmelin* module.
- In this module, you will use the CrossFire Commander 7.1 to search the Gmelin database.
- The focus of this course is to present only information that is unique to the Gmelin Database.
- General information about how to use the CrossFire Commander can be found in the manual “Searching CrossFire Databases- based on CrossFire Beilstein”.

### ***Notes***

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## Module objectives

- ❑ Review the definition of a Gmelin compound
- ❑ Review Sources & Time Coverage of Gmelin
- ❑ Use your knowledge of searching with the XFire Commander 7.1 to retrieve information from Gmelin
- ❑ Retrieve lists of Gmelin compounds based on
  - ❑ structural criteria incorporating query features
  - ❑ characterization criteria
  - ❑ physical and chemical property values

### ***Key points***

- In this module, you will learn the qualifications used to define a compound as a Gmelin compound.
- You will learn how to apply the features learned on XFire Commander 7.1 to the Gmelin database, with specific examples.
- You will view how to find desired information resulting from structural criteria, various characterization criteria, and physical or chemical property values.

### ***Notes***

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## What is a Gmelin compound?

### Compounds included in Gmelin:

- All compounds without carbon
- Elemental carbon
- Alloys and multi-component systems with carbon components, carbides, and carbideoxides, carbonic acids and the thio- and seleno-analogues, as well as small molecules like CO, CS, CO<sub>2</sub>, CS<sub>2</sub>, or phosgene.
- Substances, which contain carbon, containing at least one “Gmelin element”

### *Key points*

- The Gmelin database contains structures, synthesis, and property data for compounds that meet the criteria shown.
- The Gmelin database covers all compounds without carbon.
- The compounds in Gmelin are available with their structures. However, only molecular structures are indexed. Compounds such as alloys, glasses, and ceramic materials have no structures in the database.

### *Notes*

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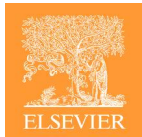
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## Elements included in Gmelin

	Ia	IIa	IIIb	IVb	Vb	VIb	VIIb	VIIIb	Ib	IIb	IIIa	IVa	Va	VIa	VIIa	VIIIa		
1	H															He		
2	Li	Be										B	C	N	O	F	Ne	
3	Na	Mg										Al	Si	P	S	Cl	Ar	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra																
Lan			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
Act			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

Elements, in combination with carbon, included in Gmelin are shaded in the periodic table.

### Key points

- The elements, in combination with carbon, included in the Gmelin database are shaded in the periodic table.

### Notes

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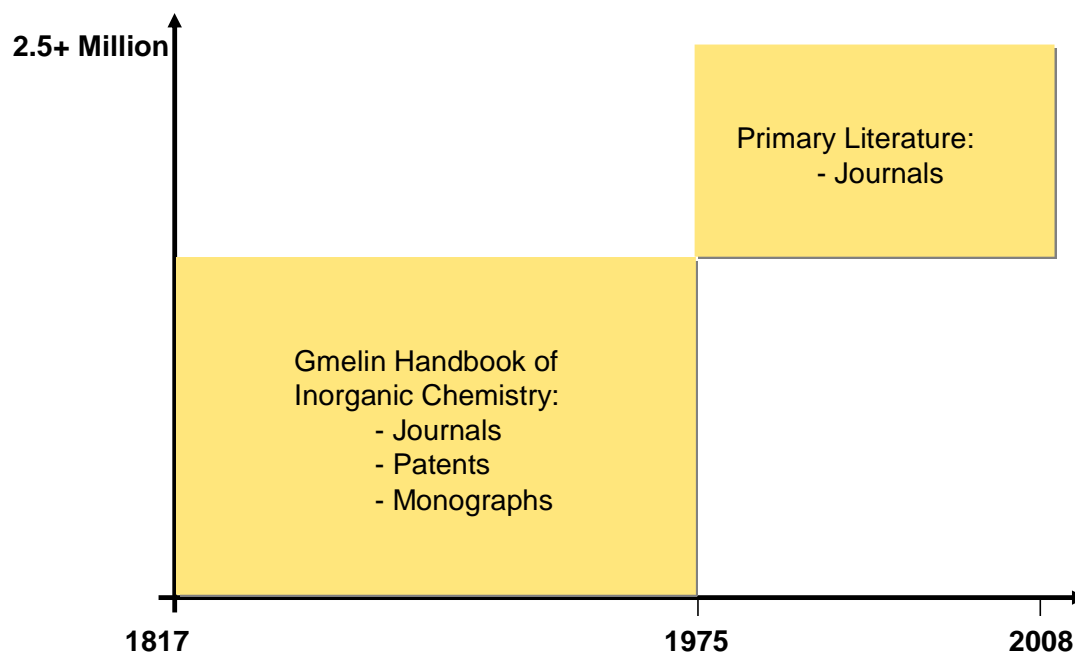
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## Sources



### Key points

- Data is excerpted from the following sources to include in the Gmelin database.
- From 1817 until 1975, data was taken from the Gmelin Handbook of Inorganic Chemistry (journals, patents, and monographs) and included values for all physical properties.
- From 1975 until present, data is taken from the primary literature (journals).

### Notes

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## Time coverage

- ❑ Time coverage from 1772 to present
- ❑ Gmelin Handbook of Inorganic Chemistry from its beginning in 1817 up to 1975
- ❑ Primary literature from 1975 onwards, currently about 62 journals

### *Key points*

- This slide shows a summary of the time frames for the excerption of data.
- The list of the journals considered in the Gmelin database is available at <http://info.crossfiregmelin.com/GMJournals.pdf>

### *Notes*

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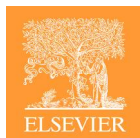
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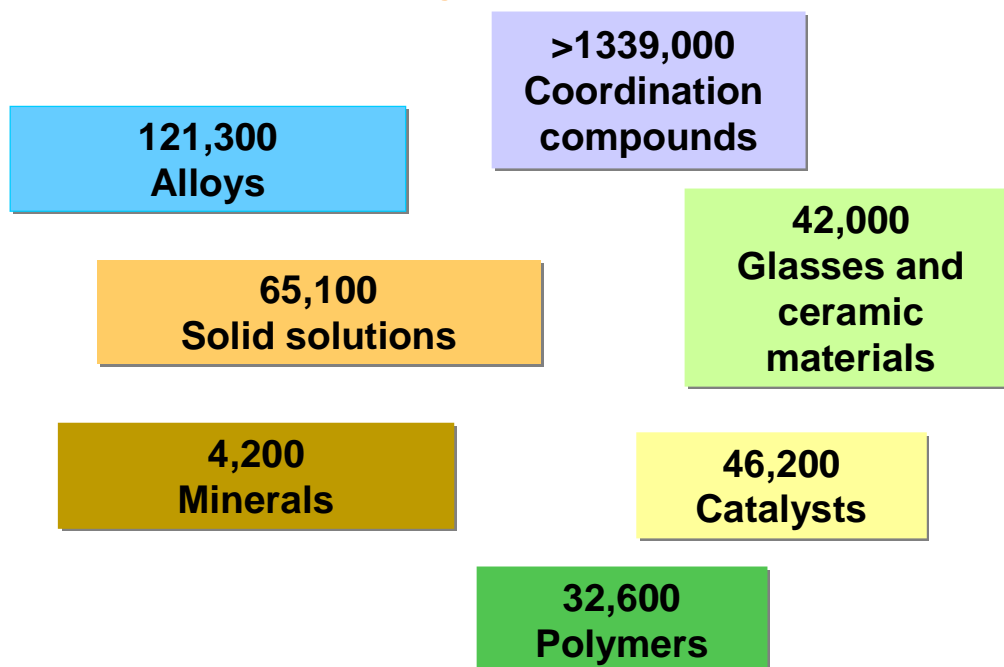
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## Compound types



### *Key points*

- This slide displays the types and frequency of the compounds found in this database.
- There are greater than 1339,000 coordination compounds, and approximately 121,300 alloys, 65,100 solid solutions, 42,000 glass and ceramic materials, 46,200 catalysts, 32,600 polymers, and 4,200 minerals (GM0704).
- The residual compounds are other inorganic compounds, such as an element (chemical), small molecules (like water), inorganic salts, solid-state compounds, and organic reactants.

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