

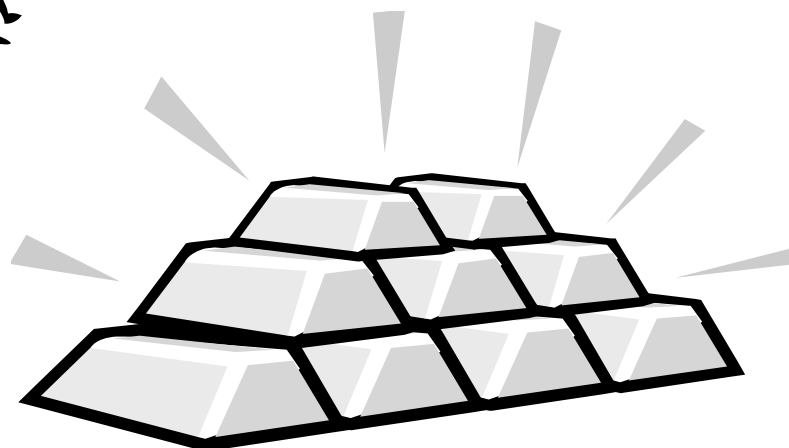
 SciFinder®
インターネットセミナー

無機化合物の検索

JAICI
化学情報協会

1

SciFinder で無機化合物
は検索できるの？



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本日の流れ

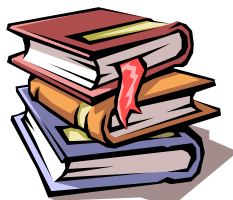
- 1 物質の収録について
- 2 お勧めの検索方法
- 3 ヒットした回答件数が多い場合の対処法

本日の流れ

- 1 物質の収録について
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物質の収録について

文献
(論文や特許)



CASのアナリスト



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人手で文献より物質を収録！

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物質の収録について

収録件数	約 1 億 4 千万件
収録物質	有機化合物, 高分子, たんぱく質, 核酸, 無機化合物 , 素粒子など

金属, 合金, 配位化合物(金属錯体),
鉱物, セラミックス, など

無機化合物が

約400万件も収録！

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無機化合物の分類

	区別する観点
無機化合物	構成元素・組成比
合金(例外1)	構成元素・重量%
鉱物(例外2)	組成式・結晶構造
配位化合物(例外3)	分子式・分子構造

通常は、**構成元素・組成比**により区別

無機化合物の例

<input type="checkbox"/> 13. Substance Detail 145114-32-5 ~64 	<input type="checkbox"/> 14. Substance Detail 107875-70-7 ~54 												
<table border="1"><thead><tr><th>Component</th><th>Component Ratio</th></tr></thead><tbody><tr><td>O</td><td>1.6</td></tr><tr><td>Si</td><td>1</td></tr></tbody></table>	Component	Component Ratio	O	1.6	Si	1	<table border="1"><thead><tr><th>Component</th><th>Component Ratio</th></tr></thead><tbody><tr><td>O</td><td>1.2</td></tr><tr><td>Si</td><td>1</td></tr></tbody></table>	Component	Component Ratio	O	1.2	Si	1
Component	Component Ratio												
O	1.6												
Si	1												
Component	Component Ratio												
O	1.2												
Si	1												
O . Si Silicon oxide (SiO _{1.6})	O . Si Silicon oxide (SiO _{1.2})												

構成元素・組成比で区別

例外1. 合金の例

7. Substance Detail
12700-79-7

~166

Component	Component Percent
Fe	100
Mn	0.2
Si	0.2

Fe . Mn . Si
Steel, Fe 100,Mn 0.2,Si 0.2

Experimental Properties

8. Substance Detail
71849-08-6

~155

Component	Component Percent
Fe	96
Si	3.4
Mn	0.1

Fe . Mn . Si
Iron alloy, base, Fe 96,Si 3.4,Mn 0.1

重量%で区別

例外2. 鉱物の例

2. Substance Detail
1317-80-2

~12936

$O = Ti = O$

O₂ Ti
Rutile (TiO₂)

Experimental Properties

3. Substance Detail
1317-70-0

~9086

$O = Ti = O$

O₂ Ti
Anatase (TiO₂)

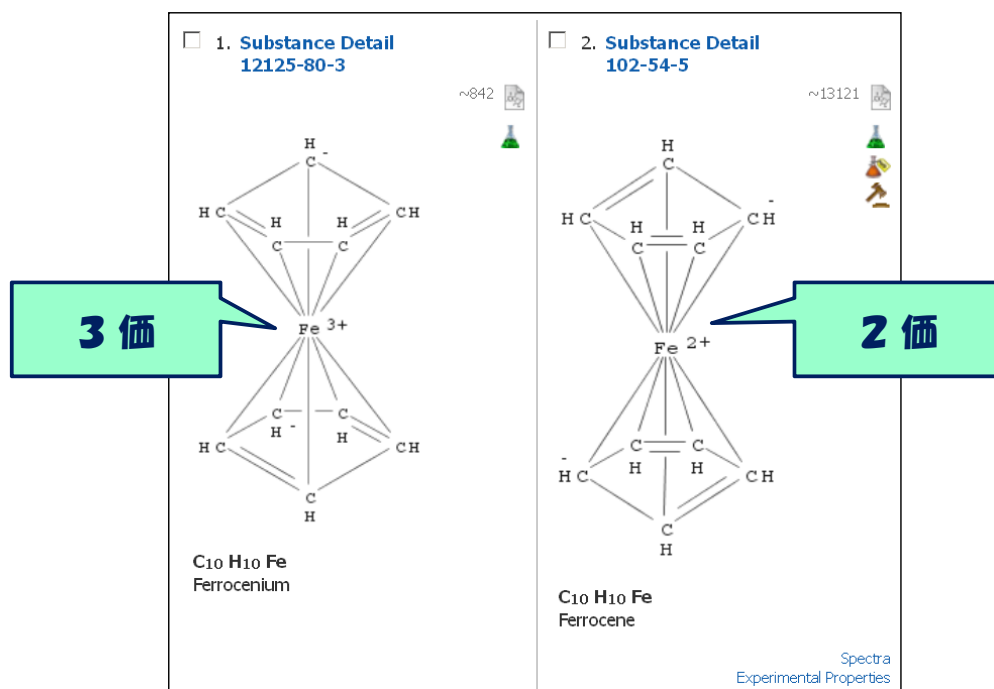
Experimental Properties

ルチル型

アナターゼ型

結晶構造で区別

例外3. 配位化合物の例

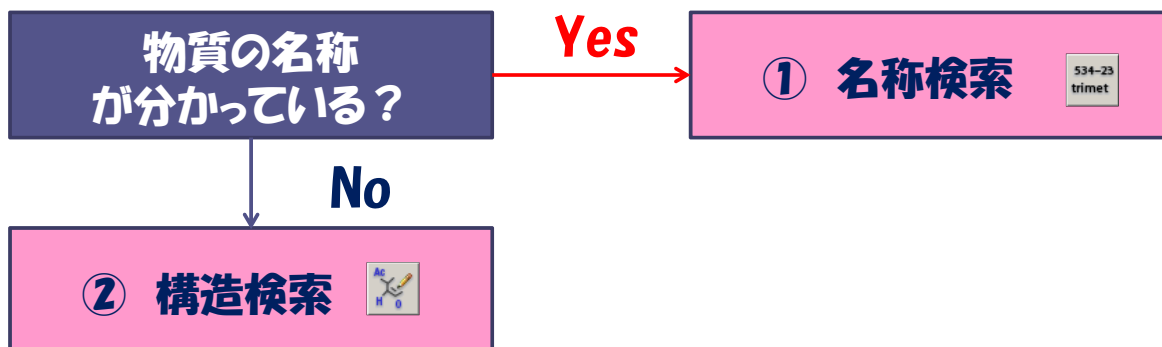


構造式が少しでも異なれば区別

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お勧めの検索方法



① 名称検索

The screenshot shows the SciPlanner search interface. On the left is a sidebar with categories: REFERENCES, SUBSTANCES, and REACTIONS. Under SUBSTANCES, "Substance Identifier" is highlighted with a red box. The main area is titled "SUBSTANCES: SUBSTANCE IDENTIFIER" and contains a search input field with the text "barium titanate", "lithium aluminum hydride", and "quartz". Below the input field are examples and a "Search" button. A yellow speech bubble with the text "名前からヒット" (Hit from name) points to the search results. The results are displayed in three columns:

- 1. Substance Detail 16853-85-3 (Component: 19469-81-9) showing the chemical structure of lithium aluminum hydride (Li^+ and AlH_4^-).
- 2. Substance Detail 14808-60-7 showing the chemical structure of quartz (SiO_2).
- 3. Substance Detail 12047-27-7 showing the chemical formula BaO_3Ti and the name Barium titanium oxide (BaTiO_3).

② 構造検索

他のもっとも

Component	Component Percent
Fe	98 - 99
Mn	0.60 - 0.90
C	0.43 - 0.50
Si	0 - 0.35
S	0 - 0.050
P	0 - 0.040

Component	Component Percent
Fe	99
Mn	0.4 - 0.6
Si	0.1 - 0.3
C	0.1 - 0.2
S	0 - 0.1

C . Fe . Mn . S . Si
Steel, (Q235)

15

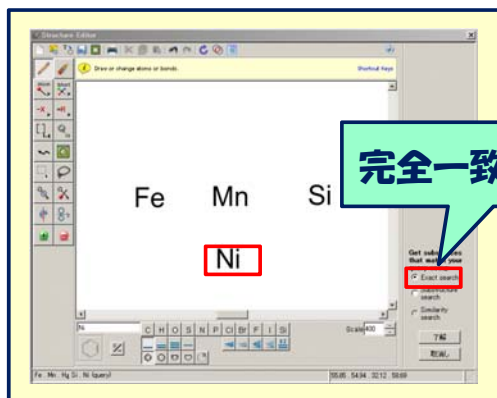
本日の流れ

1 物質の収録について

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① 構成元素の追加



Analyze **Refine** Sort by: CAS Registry Number ↓

0 of 341389 Substances Selected

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Chemical Structure:

Fe Mn Si

Click image to change structure or view detail
Search type: **Exact Structure**

1. **Substance Detail**
1444102-92-4 ~1

Component	Component Percent
Fe	37 - 88
Cr	7 - 17
Ni	4 - 14
V	1 - 5
Co	0 - 5
Cu	0 - 5
Ti	0 - 5
W	0 - 5

ニッケルも含む

10. **Substance Detail**
75711-25-0 ~25

Component	Component Percent
Fe	52 - 63
Cr	27 - 31
Ni	3 - 5
Si	2.8 - 4.2
Mn	1.5 - 4
C	2.5 - 3.3

C . Cr . Fe . Mn . Ni . Si
Iron alloy, base, Fe 52-63,Cr 27-31, Ni 3-5,Si 2.8-4.2,Mn 1.5-4,C 2.5-3.3 (PG-S-1)

② 構成元素による限定

Analyze **Refine**

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Chemical Structure:

Fe Mn Si
Ni

Click image to change structure or view detail
Search type: **Exact Structure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component**
- Are in specific substance classes
- Are in specific types of studies

Refine

チェック

記載した構成元素のみ

1. **Substance Detail**
37188-31-1 ~34

Component	Component Percent
Fe	60
Mn	40
Si	0.3
Ni	0.2

Fe . Mn . Ni . Si
Iron alloy, base, Fe,Mn,Ni,Si (G 40)

③ 物質の分類による限定

Analyze Refine

Refine by:

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Chemical Structure:

Fe Mn Si
Ni

Click image to change structure or view detail
Search type: **Exact Structure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
 - Alloys
 - Coordination compounds
 - Incompletely defined
 - Mixtures
 - Polymers
 - Organics, and others not listed
- Are in specific types of studies

Refine

- Alloys (合金)
- Coordination (配位化合物) compounds
- Incompletely defined
- Mixtures
- Polymers
- Organics, and others not listed
- Are in specific types of studies


「合金」や「配位化合物」など物質の分類で限定!

1. Substance Detail 8049-19-2

Component	Component Percent
Fe	75 - 82
P	18 - 25

Fe . P
Iron alloy, base, Fe,P (Ferrophosphorus)

2. Substance Detail 132-16-1



C₃₂H₁₆FeN₄
Iron, [29H,31H-phthalocyaninato(2-)-κ^N₃,κ^N₄]-, (SP4-1)-

Spectra Experimental Properties

④ 物質の文献数によるソート

文献数でソート

Sort by: Number of References

Answers per Page [50] View: [] [] []

0 of 1243 Substances Selected Page: 1 of 25

1. Substance Detail 37188-31-1

~34

Component	Component Percent
Fe	60
Mn	40
Si	0.3
Ni	0.2

Fe . Mn . Ni . Si
Iron alloy, base, Fe,Mn,Ni,Si (G 40)

2. Substance Detail 113746-00-2

~31

Component	Component Percent
Fe	64
Ni	36
Mn	0.3
Si	0.1

Fe . Mn . Ni . Si
Iron alloy, base, Fe 64,Ni 36,Mn 0.3,Si 0.1 (9CI)

3. Substance Detail 105421-68-9

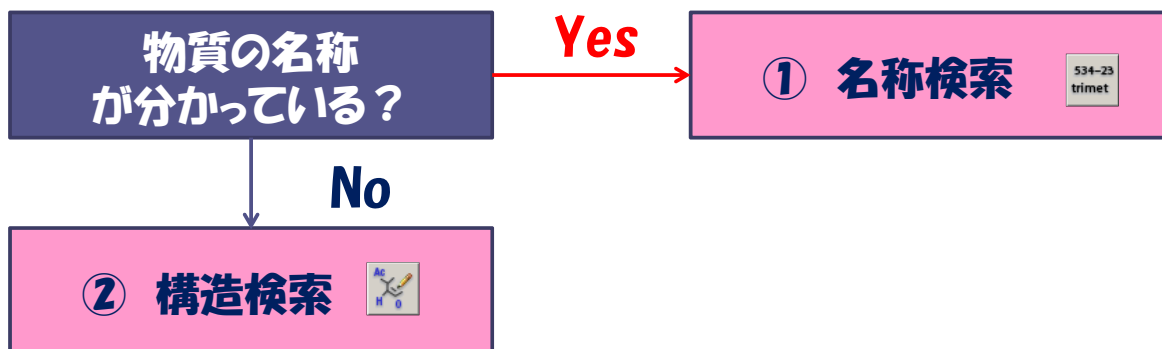
~20

Component	Component Percent
Fe	63
Ni	36
Mn	0.4
Si	0.2

Fe . Mn . Ni . Si
Iron alloy, base, Fe 63,Ni 36,Mn 0.4,Si 0.2

まとめ

無機化合物の検索方法について 紹介しました。



補足1：物性値の確認

☐ 1. Substance Detail
12047-27-7

~32073

Substance
Image
Cannot Be
Displayed
12047-27-7

Ba O₃ Ti
Barium titanium oxide (BaTiO₃)

Spectra
Experimental Properties

物性値！

CAS Registry Number: 12047-27-7

Ba O₃ Ti
Barium titanium oxide (BaTiO₃)

Substance Image Cannot Be Displayed 12047-27-7

Alternate CAS Registry Numbers: 12542-89-6
Deleted CAS Registry Numbers: 7707-45-3, 12556-53-0, 52869-64-0, 70599-62-7, 160462-52-2, 203796-96-7, 208713-64-8, 225239-81-6, 229640-62-4, 237795-05-4, 358369-13-8, 412932-53-7, 554462-75-4, 683228-79-7, 895905-07-0, 892125-11-0, 928048-64-0, 942045-70-7, 1028693-40-4, 1059109-97-2, 1080453-86-6, 1183962-04-0, 121557-74-1, 122599-65-3, 1260244-95-6, 126929-25-1, 1297529-82-8, 1313220-99-3, 132524-06-7, 133071-50-3, 1337864-79-5, 1345468-64-5, 135332-98-5, 1354327-81-3, 1363176-84-4, 137020-17-7

Experimental Properties: Acoustic Chemical Density Electrical Electronic Flow and Diffusion Interface Magnetic Mechanical Nuclear Optical and Scattering Spectra Structure-related Thermal

Spectra Properties	Value	Condition	Note
Electron Spectrum	See full text	1 of 4	(3)CAS
ESR Spectrum	See full text	1 of 15	(3)CAS
IR Absorption Spectrum	See spectrum		(4)BIORAD
IR Absorption Spectrum	See spectrum		(4)BIORAD
IR Absorption Spectrum	See spectrum		(4)JAST
IR Absorption Spectrum	See full text	1 of 52	(4)CAS
IR Emission/Luminescence Spectrum	See full text	1 of 3	(4)CAS
IR Reflectance Spectrum	See full text	1 of 5	(4)CAS
IR Spectrum	See full text	1 of 12	(4)CAS
Metal NMR Spectrum	See full text	1 of 4	(5)CAS
Microwave Spectrum	See full text	1 of 2	(5)CAS
NMR Spectrum	See full text		(5)CAS
Photoelectron Spectrum	See full text	1 of 18	(6)CAS
Raman Spectrum	See full text	1 of 91	(6)CAS
UV and Visible Absorption Spectrum	See full text	1 of 17	(7)CAS
Emission/Luminescence Spectrum	See full text	1 of 30	(6)CAS
UV and Visible Reflectance Spectrum	See full text	1 of 6	(8)CAS
UV and Visible Spectrum	See full text	1 of 10	(8)CAS
X-Ray Absorption Spectrum	See full text	1 of 7	(8)CAS
X-Ray Emission/Luminescence Spectrum	See full text	1 of 4	(8)CAS
X-Ray Reflectance Spectrum	See full text		(8)CAS
X-Ray Spectrum	See full text	1 of 5	(8)CAS
Structure-related Properties	Value	Condition	Note
Crystal Lattice Parameters	See full text	1 of 112	(5)CAS
Crystal Structure	See full text	1 of 40	(6)CAS
Neutron Diffraction Pattern	See full text	1 of 3	(5)CAS
Particle Size	See full text	1 of 254	(5)CAS
Pore Size	See full text	1 of 9	(6)CAS
Porosity	See full text	1 of 9	(6)CAS
Specific Surface Area	See full text	1 of 48	(7)CAS
X-Ray Diffraction Pattern	See full text	1 of 507	(5)CAS

補足2：文献検索オプション

Get References ⓘ

Limit results to:

<input type="checkbox"/> Adverse Effect, including toxicity	<input type="checkbox"/> Prophetics in Patents
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Preparation
<input type="checkbox"/> Biological Study	<input type="checkbox"/> Process
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

For each sequence, retrieve:

Additional related references, e.g., activity studies, disease studies.

物性

用途

Get Cancel