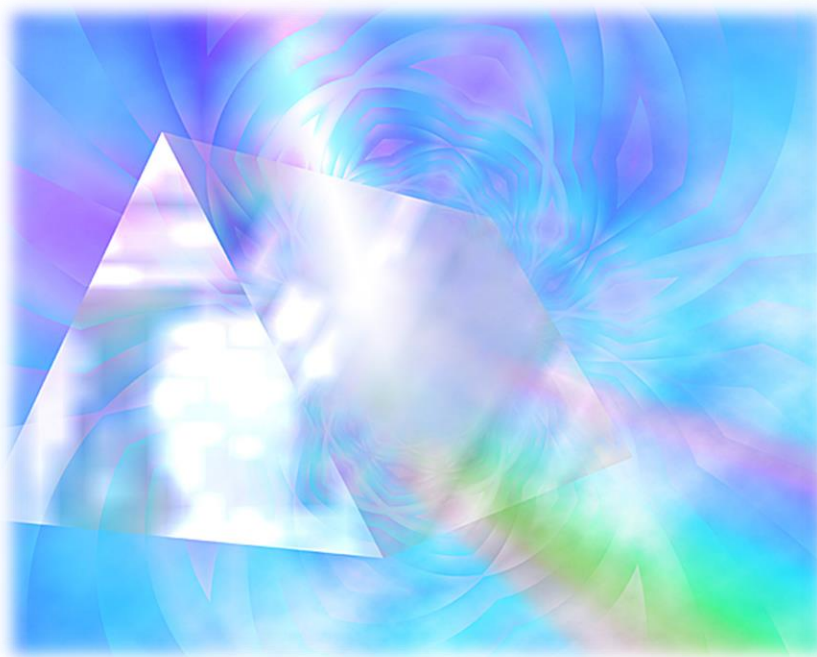


無機結晶構造データベース(ICSD) のご紹介

まずは検索画面から。



■検索初期画面（ベーシックサーチ画面：よく使われる検索項目を1ページにまとめた画面）

ICSD

Welcome to ICSD Web. IP authenticated

FIZ Karlsruhe | Contact
Close session

Login

LoginId:

Password:

Login Personalized

Lost password? Personalize account

Content Selection

☒ Experim. inorganic structures

☐ Experim. metal-organic str.

☐ Theoretical structures

Basic Search & Retrieve

Bibliography

Authors Year of Publication

Title of Journal

Title of Article

Chemistry

Composition Periodic Table

Number of Elements

Cell

Cell Parameters

Cell Volume Tolerance +/- %

Symmetry

Space Group Symbol Space Group Number

Crystal System Centering

Exp. Info. & Ref. Data

New Data Only ☐

PDF Number Temperature K

ICSD Collection Code Pressure MPa

Count Basic Search

Search Action

Run Query Clear Query

Search Summary

Basic Search: -

Query History

Number of queries: 0

Clear Query History

Structure Type

Experimental Information

DB Info

Query Management

Manage Queries

List Combined Queries

Create Combined Query

ICSD links

ICSD News

実験値(無機化合物or金属有機化合物)か計算値かの選択が可能。初期設定では, 無機化合物の実験によって求められた構造のみを検索。

周期表から元素を選択して検索可能。

ICDDのPDF番号から検索可能。

Search Chemistry Visual Search mode

↓	↓												↓					
→	H												He					
→	Li	Be										B	C	N	O	F	Ne	
→	Na	Mg	↓	↓	↓	↓	↓	↓	↓	↓	↓	Al	Si	P	S	Cl	Ar	
→	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
→	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
→	Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
→	Fr	Ra		Rf	Db													

→	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
→	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

→ Metals → Transition Metals → Non-Metals

Click on element or select period and/or group.

☐ Restrict total number of elements to selected number of elements

OK Cancel

■ 詳細検索画面例(アドバンスドサーチ画面)

格子定数からの検索画面

Cell Search

Cell Length a Cell Angle α

Cell Length b Cell Angle β

Cell Length c Cell Angle γ

Cell Volume Units of Length

Calc. Density g/cm³

Global Tolerance +/- %

Reduce Cell Parameters ☐ Search Cell Data

Centering

化合物情報からの検索画面

Chemistry Search

Composition Number of Elements

Structural Formula Formula Weight

Chemical Name

ANX Formula AB Formula

Mineral Name

Mineral Name IMA

Mineral Group

Mineral Series

Structure typeでの検索画面

Structure Type Search

Pre Defined Structure Types

Structure Type e.g. "Mg2SiO4" or "Olivine" or "Mg2GeS4" or "Si(2)"

Structure Type	Alias	Prot.	Mem.	Sys.	Sp. Gr.	Wyc.
((C2)2O2Dy12)18	421641	2	HE	P6/M	I11 K	
((C2H5)4N)4(SCN)8Pu	238915	4	TE	I4/MMM	n4 m3	
((C3H7)4N)2Mn(H2O)4ReOS8(CN)6	91172	2	TE	I4/M	i5 h4 e	
((C4H9)2NH2)26Cd12In48S97	281499	3	CU	I-43D	e12 d	
((CH3)2H2N)6(SO4)2Co2(C2O4)3	162958	2	CU	P4132	e7 d c	
((CH3)2NH2)2CoCl4	110562	6	MO	P121/N1	e23	
((CH3)2NH2)2In2Sb2S7	185457	4	MO	C12/C1	f14 e	
((CH3)2NH2)2MnBr4	240877	7	MO	14	e11	
((CH3)2NH2)2MnBr4	240877	7	MO	P121/N1	e23	
((CH3)2NH2)2TiCl6	281532	5	OR	PNNM	h g4 a	
((CH3)2NH2)2TiCl6	281532	5	OR	PNNM	h3 g6	
((CH3)2NH2)3Mo12SiO4OHO35	240978	2	TG	R-3MH	i6 h14	
((CH3)2NH2)3Sb2Cl9	172431	2	MO	P1C1	a38	
((CH3)2NH2)4(BiCl6)Cl	53593	7	OR	P21212	c9 b a	
((CH3)2NH2)4(NdCl6)Cl	155692	5	OR	P22121	c21 b	

(1 of 820)

There are 12296 lines with predefined Structure Type definitions for " ". Double-click on an entry in the table above to transfer this type to the search field 'Structure Type'.

結晶学データ、
化合物情報、
構造タイプ、
測定情報、
書誌情報
などからの
詳細な検索
が可能。

■ 検索の掛け合わせ画面

ICSD

Welcome to ICSD Web. IP authenticated

FIZ Karlsruhe | Contact
Close session

Login

LoginId:

Password:

Login Personalized

Lost password? Personalize account

Content Selection

☒ Experm. inorganic structures
☐ Experm. metal-organic str.
☐ Theoretical structures

Navigation

Basic search & retrieve

Advanced search & retrieve

Bibliography

Cell

Chemistry

Symmetry

Crystal Chemistry

Structure Type

Experimental Information

DB Info

Query Management

Manage Queries

List Combined Queries

Create Combined Query

Basic Search & Retrieve

Bibliography

Authors

Title of Journal

Title of Article

Chemistry

Composition Na Cl Periodic Table

Cell

Cell Parameters

Cell Volume

Symmetry

Space Group Symbol Space Group Number

Crystal System Centering

Exp. Info. & Ref. Data

New Data Only

PDF Number Temperature

ICSD Collection Code Pressure

Search Action

Run Query Clear Query

Query History

Number of queries: 5

Clear Query History

2019-08-14T04:30	903
2019-08-14T04:30	2166
2019-08-14T04:29	6
2019-08-14T04:29	1955
2019-08-14T04:29	225

「Manage Queries」で検索名やコメントの編集が可能。
「Create Combined Query」で複数の検索の掛け合わせが可能。

Create Combined Query

Name:

Comment:

Available Queries:

	Query Name	Date	Query Type	# of hits	Saved
☐	2019-08-14T04:30	2019-08-14T04:30	Basic	903	
☐	2019-08-14T04:30	2019-08-14T04:30	Basic	2166	
☐	2019-08-14T04:29	2019-08-14T04:29	Basic	6	
☐	2019-08-14T04:29	2019-08-14T04:29	Basic	1955	
☐	2019-08-14T04:29	2019-08-14T04:29	Basic	225	

Must have (AND):
☐ ☐ No records found.

Must have at least one of (OR):
☐ ☐ No records found.

Must not have (NOT):
☐ ☐ No records found.

検索履歴が30件まで自動で保存。

検索掛け合わせ画面。AND/OR/NOT検索が可能。

次に検索結果画面を紹介します。



■レコード画面例1

ICSD Welcome to ICSD Web. IP authenticated

Entry 329 of 4373

Collection Code 62388

Back to Query Back to List

CCDC Export Cif Print Feedback to Editor

Summary

Struct. formula	Ca Mo6 S8	Structure type	Mo6PbS8
Cell parameter	6.5146(5) 6.5146(5) 6.5146(5) 89.63(1) 89.63(1) 89.63(1)	Space group	R -3 R (148)
Cell volume	276.46 [Å ³]	Z	1
Temperature	room temperature	Pressure	atmospheric
Data quality	High quality	R-value	0.032
Author	Kubel, F.; Yvon, K.;	Title	Matrix Effect in Chevrel Phases Containing Divalent Metal Cations. The Structure of Rhombohedral CaMo6S8
Reference	Journal of Solid State Chemistry (1988) 73, p. 188-191	Fulltext	Get full text by DOI Search full text by Google Scholar
See also	CCDC structures depot OQMD - Open Quantum Materials Database Materials Project property set 1/1		

Details

Visualization

Expand all Collapse all

CIF形式での出力やプリンターでの印刷

レコードの
サマリー

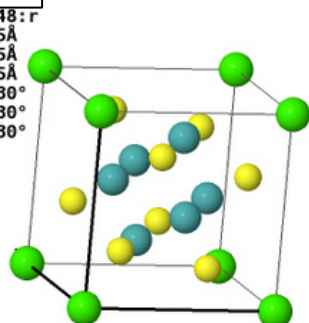
←関連外部サイトへのリンク

↓ここからレコードの詳細。
次ページにも続く。

粉末X線回折パターン
の計算表示

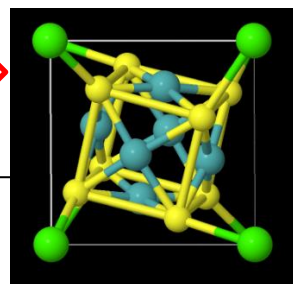
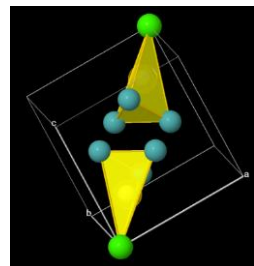
3次元構造の表示

148 #148: r
a=6.515Å
b=6.515Å
c=6.515Å
α=89.630°
β=89.630°
γ=89.630°

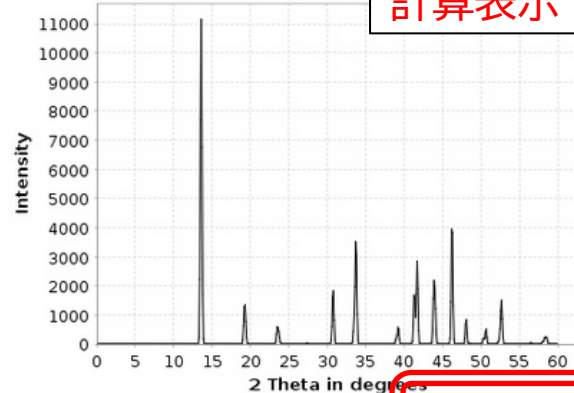


Interactive Visualization

原子間距離・角度の表示、
配位状況の表示等が可能。

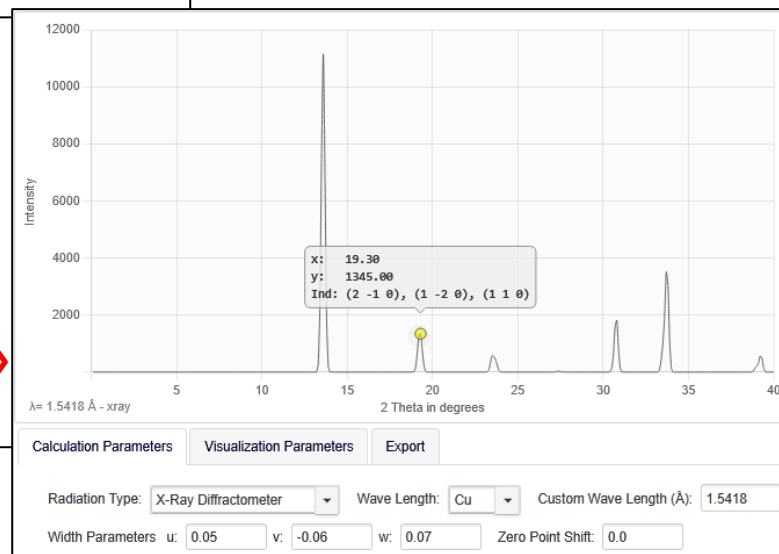


Powder Pattern



Interactive Visualization

線源の選択や任意の波長の設定、
中性子回折パターンの表示、横軸
の表示範囲の変更などが可能。



λ= 1.5418 Å - xray

Calculation Parameters Visualization Parameters Export

Radiation Type: X-Ray Diffractometer Wave Length: Cu Custom Wave Length (Å): 1.5418

Width Parameters u: 0.05 v: -0.06 w: 0.07 Zero Point Shift: 0.0

■レコード画面例2

Chemistry

Sum. formula

Ca₁ Mo₆ S₈

Struct. formula

Ca Mo₆ S₈

Molecular weight

872.2320 [u]

Z

1

ANX formula

AB6X8

AB formula

AB6C8

Chemical name

Calcium hexamolybdenum octasulfide

Published Crystal Structure Data

Cell parameter

6.5146(5) 6.5146(5) 6.5146(5) 89.63(1) 89.63(1) 89.63(1)

Space group

R-3 R (148)

Cell volume

276.46 Å³

Z

1

Crystal system

trigonal

Crystal class

-3

Laue class

-3

Structure type

Mo₆PbS₈

Pearson symbol

hR15

Wyckoff sequence

f2 c a

Axis ratios

a/b

1.0000

b/c

1.0000

c/a

1.0000

Calc. density

5.24 [g/cm³]

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	TF
Ca	1	+2.00	1 a	0	0	0	1	
Mo	1	+2.33	6 f	0.22568(7)	0.41774(7)	0.55977(7)	1	
S	1	-2.00	6 f	0.3783(2)	0.1269(2)	0.7445(2)	1	
S	2	-2.00	2 c	0.2391(2)	0.2391(2)	0.2391(2)	1	

EL	Lbl	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Mo	1	0.0050(2)	0.0045(2)	0.0051(2)	0.0000(1)	-0.0003(1)	-0.0004(1)
S	1	0.0089(5)	0.0054(5)	0.0083(5)	-0.0013(4)	0.0007(4)	0.0009(4)

Standardized Crystal Structure Data

Cell parameter

9.1832 9.1832 11.3563 90.000 90.000 120.000

Space group

R-3 H (148)

Cell volume

829.38 Å³

Z

1

Crystal system

trigonal

Crystal class

-3

Laue class

-3

Structure type

Mo₆PbS₈

Pearson symbol

hR15

Wyckoff sequence

f2 c a

Axis ratios

a/b

1.0000

b/c

0.8086

c/a

1.2366

Transformation info

cell volume changed: R-3R(z=1) -> R-3H(z=3) REMARK Transformed from rhombohedral cell.-> R-3 TRANS a-b,b-c,a+b+c y,x,-z

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	TF
Ca	1	+2.00	3 a	0.0000	0.0000	0.0000	1.000000	
Mo	1	+2.33	18 f	0.1587	0.1754	0.4011	1.000000	
S	1	-2.00	18 f	0.0437	0.3387	0.0832	1.000000	
S	2	-2.00	6 c	0.0000	0.0000	0.2391	1.000000	

EL	Lbl	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Mo	1	0.005000	0.004500	0.005100	0.000000	-0.000300	-0.000400
S	1	0.008900	0.005400	0.008300	-0.001300	0.000700	0.000900

化合物情報、
分子式タイプ、
鉱物名など

文献中に記
載されている
格子定数、空
間群、原子座
標などの結
晶学データ

スタンダード
なセッティン
グに変換した
場合の格子定
数、空間群、
原子座標など
の結晶学デー
タ

■レコード画面例3

▼ Distances and Angles

Select pairs of elements Select from atom position

Atom A

☒ Ca
☒ Mo
☒ S

☒ (un)select all

Atom B

☒ Ca
☒ Mo
☒ S

☒ (un)select all

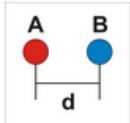
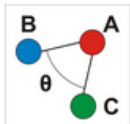
Atom C

☐ Ca
☐ Mo
☐ S

☒ (un)select all

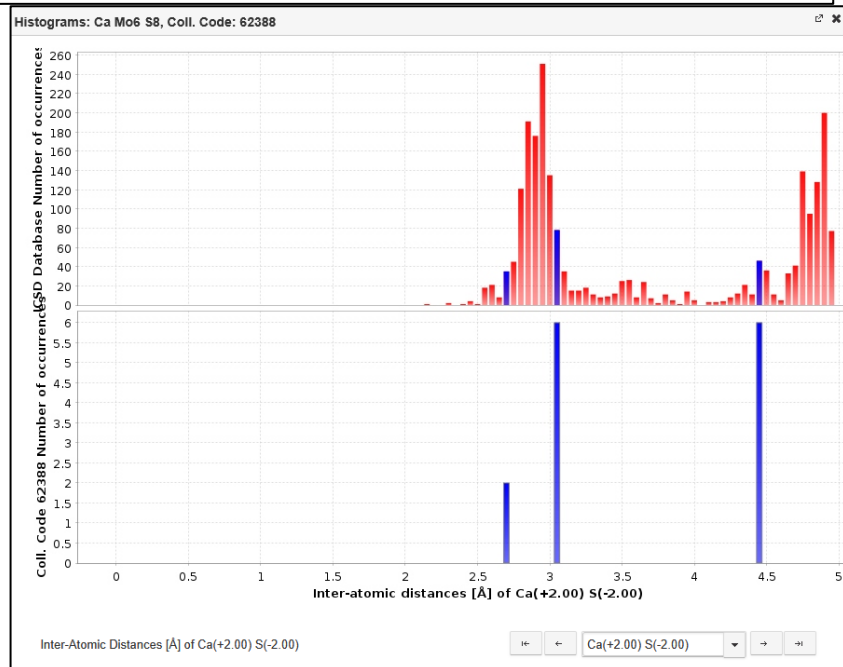
Histograms

Calculate

特定の原子間距離の分布のプロットが可能。
(例: $\text{Ca}^{2+} - \text{S}^{2-}$ 間の距離)

原子間距離・角度の計算が可能。



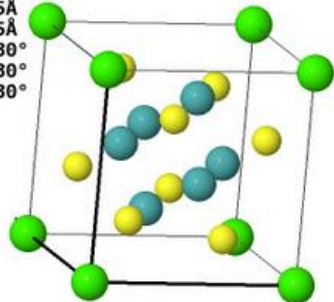
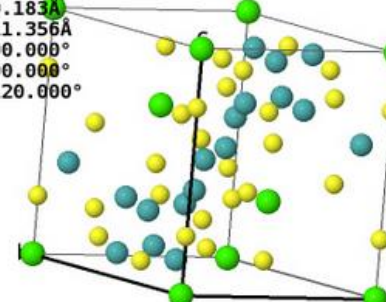
Distances Angles

download

Atom A			Atom B			Symmetry	Distance [Å]
Lbl	Ox	Wyck	Lbl	Ox	Wyck		
Ca1	+2.00	1a	S2	-2.00	2c	x,y,z 555	2.715
			S2	-2.00	2c	-z,-x,-y 444	2.715
Mo1	+2.33	6f	Mo1	+2.33	6f	z,x,y 555	2.667
			Mo1	+2.33	6f	y,z,x 555	2.667
			Mo1	+2.33	6f	-z,-x,-y 555	2.724
			Mo1	+2.33	6f	-y,-z,-x 555	2.724
Mo1	+2.33	6f	S1	-2.00	6f	x,y,z 555	2.447
			S1	-2.00	6f	-z,-x,-y 555	2.452
			S1	-2.00	6f	y,z,x 555	2.511
			S1	-2.00	6f	-y,-z,-x 455	2.563
Mo1	+2.33	6f	S2	-2.00	2c	x,y,z 555	2.399

■レコード画面例4

書誌情報: DOI、Google Scholarのリンクあり。一部はabstractも収録。

▼ Bibliography	
Author	Kubel, F.; Yvon, K.;
Reference	Journal of Solid State Chemistry (1988) 73, p. 188-191
Get full text	by Google Scholar
▼ Experimental information	
Temperature	room temperature
Radiation type	X-Ray
R-value	0.032
PDF calc.	01-085-1269
Remarks	Temperature factors available
▼ Additional information	
Comments	Hexagonal setting: 9.183, 11.35
Warnings	At least one temperature factor missing in the paper.
Materials Project	Entry at Materials Explorer (1/1)
OQMD	Entry in the Open Quantum Materials Database (OQMD)
▼ Compare Published and Standardized Structure	
Published Crystal Structure	Standardized Crystal Structure
148 #148: r a=6.515Å b=6.515Å c=6.515Å α=89.630° β=89.630° γ=89.630° 	148 #148: a, b, c a=9.183Å b=9.183Å c=11.356Å α=90.000° β=90.000° γ=120.000° 

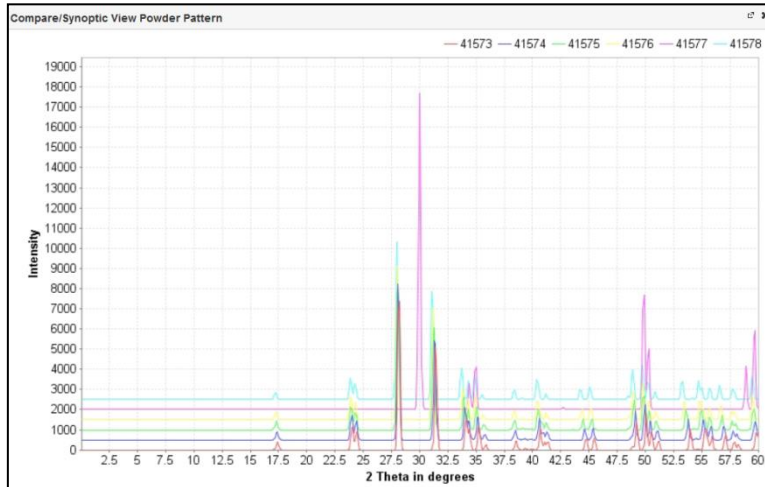
測定情報

Additional Information

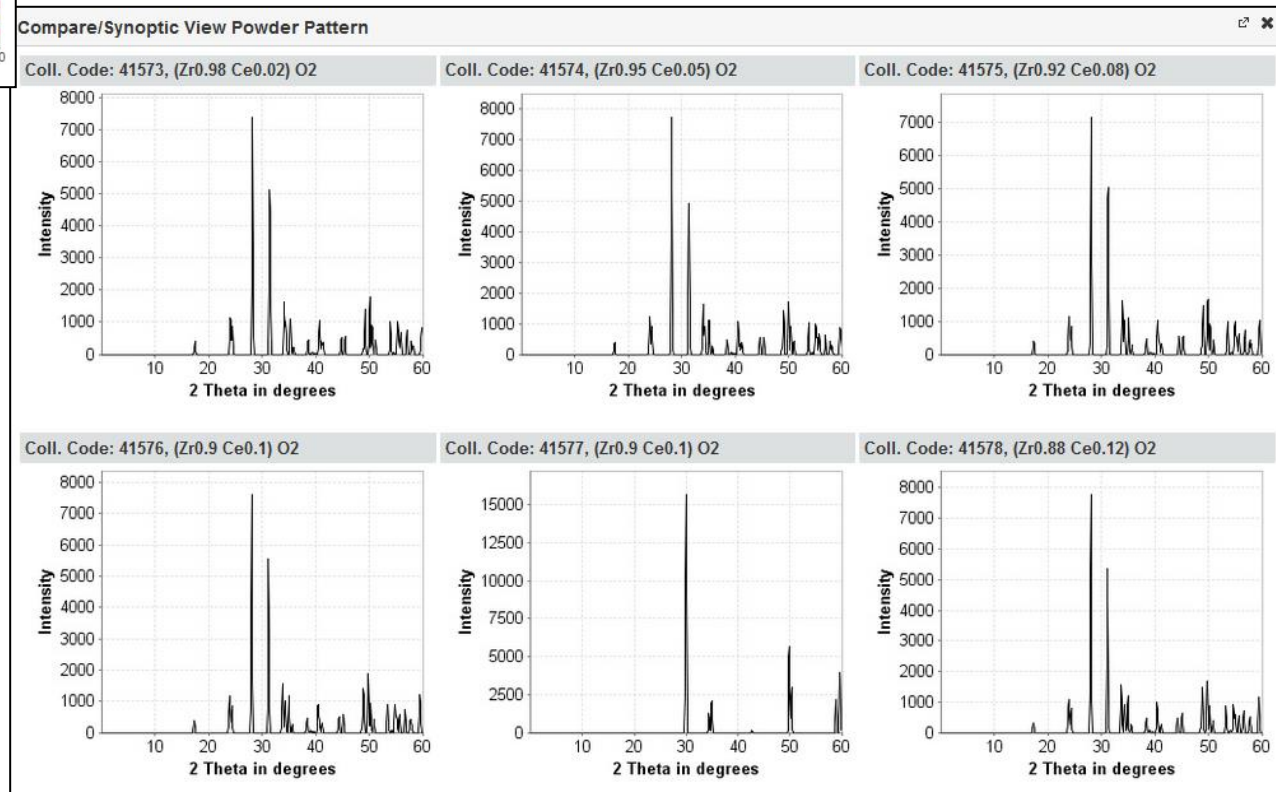
文献中に記載されている構造とスタンダードセッティングに変換した構造の比較。

★文献から結晶学データを収録するだけでなく、製作元の専門スタッフが、Additional informationのComment/Warning欄に、データの矛盾点や不足情報、コメントなどの価値ある付加情報を記載。

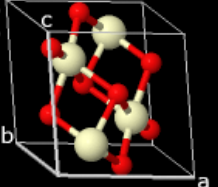
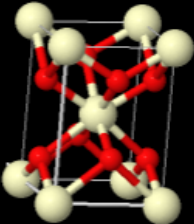
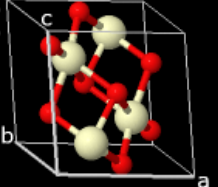
■その他の機能1



複数のレコードの粉末パターン
重ね合わせ表示や比較も可能。



■その他の機能2

Coll. Code: 41573, (Zr _{0.98} Ce _{0.02}) O ₂	Coll. Code: 41574, (Zr _{0.95} Ce _{0.05}) O ₂	Coll. Code: 41575, (Zr _{0.92} Ce _{0.08}) O ₂
HM: P 1 21/c 1 #14 a=5.158Å b=5.213Å c=5.325Å α=90.000° β=99.183° γ=90.000°  ICSD	HM: P 1 21/c 1 #14 a=5.171Å b=5.221Å c=5.339Å α=90.000° β=99.116° γ=90.000°  ICSD	HM: P 1 21/c 1 #14 a=5.185Å b=5.228Å c=5.354Å α=90.000° β=99.051° γ=90.000°  ICSD
Coll. Code: 41576, (Zr _{0.9} Ce _{0.1}) O ₂	Coll. Code: 41577, (Zr _{0.9} Ce _{0.1}) O ₂	Coll. Code: 41578, (Zr _{0.88} Ce _{0.12}) O ₂
HM: P 1 21/c 1 #14 a=5.196Å b=5.229Å c=5.367Å α=90.000° β=99.004° γ=90.000°  ICSD	HM: P 42/n m c S #137 a=3.630Å b=3.630Å c=5.213Å α=90.000° β=90.000° γ=90.000°  ICSD	HM: P 1 21/c 1 #14 a=5.207Å b=5.225Å c=5.382Å α=90.000° β=98.924° γ=90.000°  ICSD

複数のレコードの
構造比較も可能。

■ ICSDの機能や表示についてご質問や、オンラインでのご説明のご要望などがございましたら、
化学情報協会 科学データ情報室 < crystal@jaici.or.jp >までお問い合わせください。

以上