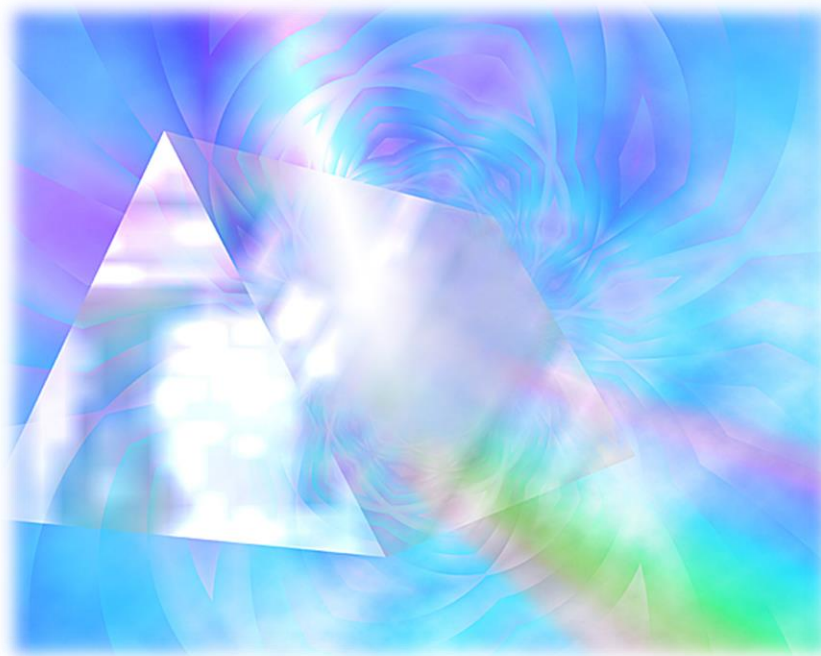


# 無機結晶構造データベース(ICSD) のご紹介

まずは検索画面から.



**JAICI**  
化学情報協会

 **ICSD**  
FIZ Karlsruhe

## ■ 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)

The screenshot displays the ICSD Web interface. On the left, the 'Login' section includes fields for 'LoginId' and 'Password', a 'Login Personalized' button, and links for 'Lost password?' and 'Personalize account'. Below this is the 'Content Selection' section, which is highlighted with a red box. It contains three checkboxes: 'Experim. inorganic structures' (checked), 'Experim. metal-organic str.' (unchecked), and 'Theoretical structures' (unchecked). A red arrow points from the 'Periodic Table' button in the 'Basic Search & Retrieve' section to the 'Search Chemistry Visual Search mode' section. This section features a periodic table with elements highlighted in blue, indicating they are selected for search. Below the periodic table, there are buttons for 'Metals', 'Transition Metals', and 'Non-Metals'. The 'ICSD Collection Code' field is also highlighted with a red box. The 'Search Action' section on the right includes 'Run Query' and 'Clear Query' buttons, a 'Search Summary' section, and a 'Query History' section.

実験値(無機化合物or有機金属化合物)か計算値かの選択が可能.  
初期設定は、無機化合物の実験値のみの検索。

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。

# ■ 詳細検索画面例(アドバンスサーチ画面)

格子定数からの検索画面

ICSD

Welcome to ICSD Web. IP authenticated

Login

LoginId:

Password:

Login Personalized

Lost password? Personalize account

Content Selection

☒ Experim. inorganic structures

☐ Experim. metal-organic str.

☐ Theoretical structures

Navigation

Basic search & retrieve

Advanced search & retrieve

Bibliography

Cell

Chemistry

Symmetry

Crystal Chemistry

Structure Type

Experimental Information

DB Info

Basic Search & Retrieve

Bibliography

Authors

Title of Journal

Title of Article

Chemistry

Composition

Cell

Cell Parameters

Cell Volume

Symmetry

Space Group Symbol

Space Group Number

Crystal System

Centering

Exp. Info. & Ref. Data

New Data Only ☐

Experimental Information Search

Temperature  K

Pressure  MPa

Comments

R-Value

Radiation Type

☐ X-Ray

☐ Electrons

☐ Neutrons

☐ Synchrotron

Sample Type

☐ Powder

☐ Single Crystal

Additional Properties

☐ Twinned Crystal Data

☐ Rietveld Refinement employed

☐ Anharmonic Temperature Factors given

☐ Absolute Configuration determined

☐ Experimental PDF number assigned

☐ Calculated PDF number assigned

☐ NMR Data available

☐ Magnetic Structure available

☐ Correction of earlier work

☐ Temperature Factors available

☐ Cell Constants without s.d.

☐ Only Cell and Structure Type determined

Clear Experimental Info Search

Count Experimental Info Search

Cell Search

Cell Length a

Cell Length b

Cell Length c

Cell Volume

Calc. Density  g/cm<sup>3</sup>

Global Tolerance +/-  %

Reduce Cell Parameters ☐

Centering

Cell Angle  $\alpha$

Cell Angle  $\beta$

Cell Angle  $\gamma$

Units of Length

Search Cell Data

Clear Cell Search

Count Cell Search

Chemistry Search

Composition

Structural Formula

Chemical Name

Mineral Name

Mineral Group

ANX Formula

AB Formula

Formula Weight

Number of Elements

Number of Formula Units

Clear Chemistry Search


Count Chemistry Search

化合物情報からの検索画面

実験情報からの検索画面

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



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  Periodic Table

Cell

Cell Parameters

Cell Volume

Symmetry

Space Group Symbol  Space Group Number

Crystal System

Exp. Info. & Ref. Data

New Data Only ☐

PDF Number

ICSD Collection Code

Clear Basic Search

Search Action

Run Query

Clear Query

検索履歴が30件まで自動で保存.

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

Create Combined Query

Name:

Comment:

Available Queries:

	Query Name	Date	Query Type	# of hits	Saved
<input type="checkbox"/>	2019-08-14T04:30	2019-08-14T04:30	Basic	903	
<input type="checkbox"/>	2019-08-14T04:30	2019-08-14T04:30	Basic	2166	
<input type="checkbox"/>	2019-08-14T04:29	2019-08-14T04:29	Basic	6	
<input type="checkbox"/>	2019-08-14T04:29	2019-08-14T04:29	Basic	1955	
<input type="checkbox"/>	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.

「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.

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



Welcome to ICSD Web. IP authenticated

CIFファイルの出力やプリンターでの印刷

Detailed View

Entry 1 of 1

Back to Query

Back to List

Export Cif

Print

Feedback to Editor

Summary

Collection Code 253901

Struct. formula	Pd Se <sub>2</sub>
Cell parameter	6.7099(13) 4.1542(8) 8.9136(18) 90 92.42(3) 90
Cell volume	248.23 [Å <sup>3</sup> ]
Temperature	293 [K]
Data quality	High quality
Author	Selb, Elisabeth; Tribus, Martina; Heymann, Gunter
Reference	Inorganic Chemistry (2017) 56, (10) p5885-p5891

Space group	I 1 2/a 1 (15)
Z	4
Pressure	atmospheric
R-value	0.0329
Title	Verbeekite, the long-unknown crystal structure of monoclinic PdSe <sub>2</sub>
DOI	10.1021/acs.inorgchem.7b00544

レコードの  
サマリー

Details

Expand all Collapse all

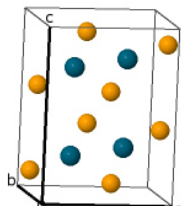
Visualization

↓ここからレコードの詳細。  
次ページにも続く。

Published Crystal Structure

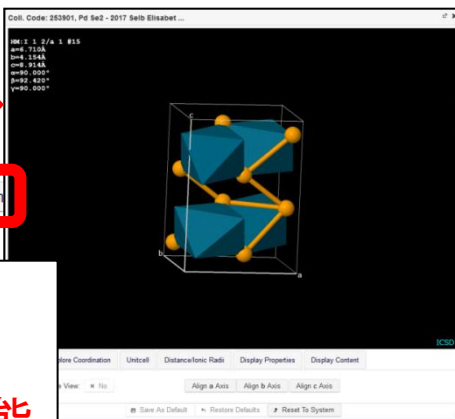
HM:I 1 2/a 1  
a=6.710Å  
b=4.154Å  
c=8.914Å  
α=90.000°  
β=92.420°  
γ=90.000°

3次元構造の表示

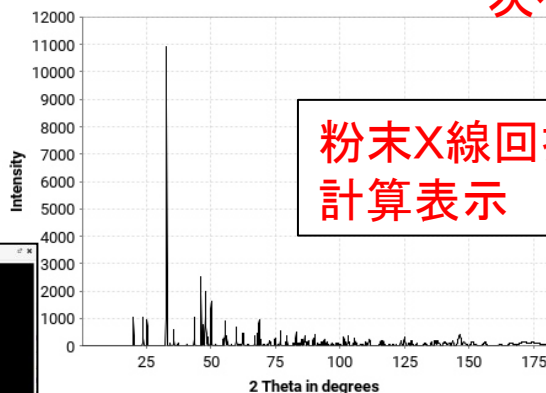


Interactive Visualization

多面体表示や  
原子間距離の表示,  
回転や拡大などが可能



Powder Pattern



粉末X線回折パターンの  
計算表示

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。

## ■レコード画面例2

▼ Chemistry									
Sum. formula	Pd1 Se2			Struct. formula	Pd Se2				
Molecular weight	264.3200 [u]			Z	4				
ANX formula	AX2			AB formula	AB2				
Chemical name	Palladium selenide (1/2)								
Mineral name	Verbeekite								
Mineral origin	synthetic								

▼ Published Crystal Structure Data									
Cell parameter	6.7099(13) 4.1542(8) 8.9136(18) 90 92.42(3) 90			Space group	I 1 2/a 1 (15)				
Cell volume	248.23 Å³			Z	4				
Crystal system	monoclinic			Crystal class	2/m				
Laue class	2/m								
Pearson symbol	mS12								
Wyckoff sequence	f d			Axis ratios	a/b	b/c	c/a		
Calc. density	7.07 [g/cm³]				1.6152	0.4661	1.3284		

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	U
Se	1	-1.00	8 f	0.55509(11)	0.1683(2)	0.10613(9)	1.000000	0.0158(3)
Pd	1	+2.00	4 d	0.2500	0.2500	0.2500	1.000000	0.0148(3)

EL	Lbl	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Se	1	0.0143(4)	0.0184(5)	0.0147(4)	0.0003(3)	0.0013(3)	-0.0009(3)
Pd	1	0.0113(4)	0.0198(5)	0.0134(4)	0.0010(3)	0.0006(3)	-0.0007(3)

▼ Standardized Crystal Structure Data									
Cell parameter	10.9281 4.1542 6.7099 90.000 125.420 90.000			Space group	C 1 2/c 1 (15)				
Cell volume	248.24 Å³			Z	4				
Crystal system	monoclinic			Crystal class	2/m				
Laue class	2/m								
Pearson symbol	mS12								
Wyckoff sequence	f d			Axis ratios	a/b	b/c	c/a		
Transformation info	REMARK Transformed from setting I 1 2/a 1.--> C 2/c TRANS -a-c,b,a				2.6306	0.6191	0.6140		

EL	Lbl	OxState	Wyck Symb	X	Y	Z	SOF	U
Se	1	-1.00	8 f	0.1061	0.1683	0.0510	1	0.0158
Pd	1	+2.00	4 d	0.2500	0.2500	0.5000	1	0.0148

EL	Lbl	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Se	1	0.014300	0.018400	0.014700	0.000300	0.001300	-0.000900
Pd	1	0.011300	0.019800	0.013400	0.001000	0.000600	-0.000700

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

既約格子に変  
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

☐ Pd  
☐ Se

✓ (un)select all

Atom B

☐ Pd  
☐ Se

✓ (un)select all

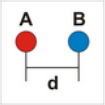

Atom C

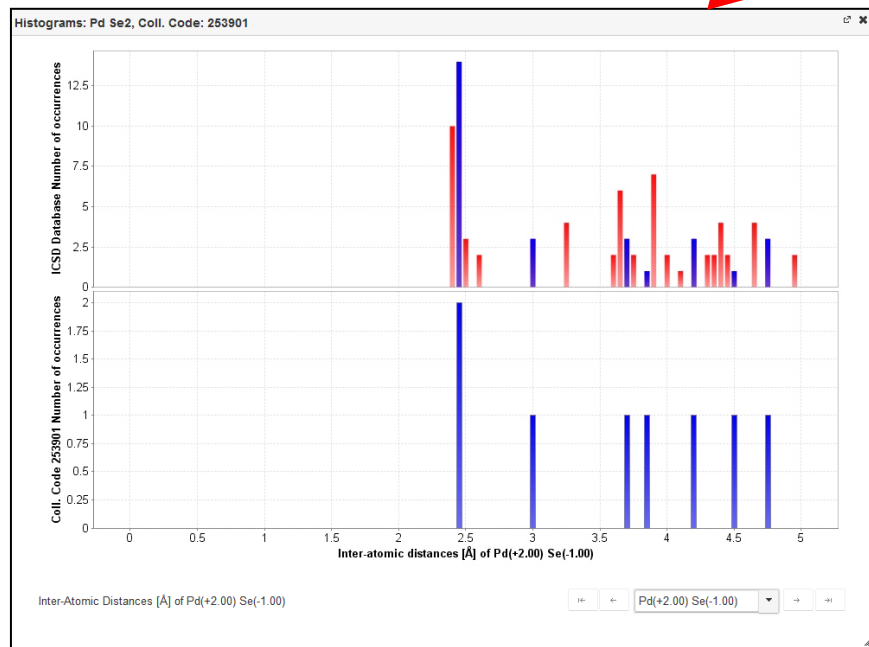
☐ Pd  
☐ Se

✓ (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:  $\text{Pd}^{2+} - \text{Se}^-$  間の距離)

Coll. Code: 253901, Pd Se2 - 2017 Selb Elisabeth ...

Distances    Angles

download

Atom A			Atom B			Symmetry	Distance [Å]
Lbl	Ox	Wyck	Lbl	Ox	Wyck		
Pd1	+2.00	4d	Se1	-1.00	8f	x,y,z 555	2.484
			Se1	-1.00	8f	-x+1/2,-y+1/2,-z+1/2 555	2.484
			Se1	-1.00	8f	-x,y+1/2,-z+1/2 555	2.497
			Se1	-1.00	8f	x+1/2,-y,z 445	2.497
Se1	-1.00	8f	Se1	-1.00	8f	-x,-y,-z 544	2.442

Ionic Radii [%]: ☒ Off    min: 80 max: 120.0

Distance [Å]: ☒ On    min: 0.7 max: 3.0

Save As Default    Restore Defaults    Reset To System

原子間距離・角度の計算が可能。



## ■レコード画面例4

書誌情報: DOI, Google Scholarのリンクあり. Abstractも収録.

▼ Bibliography

書誌情報: DOI, Google Scholarのリンクあり. Abstract

Author	Selb, Elisabeth; Tribus, Martina; Heymann, Gunter	Title	Verbeekite, the long-unknown crystal structure of monoclinic PdSe2
Reference	Inorganic Chemistry (2017) 56, (10) p5885-p5891	DOI	10.1021/acs.inorgchem.7b00544
Abstract	Verbeekite, a monoclinic polymorph of PdSe2, was reported for the first time in 2002 by Roberts et al. The mineral has been discovered in the Musonoi Cu-Co-Mn-U mine, Democratic Republic of Congo, and was named after Dr. Theodore Verbeek, the first geoscientist who studied the palladium mineralization there (1955-1967). Until today, the crystal structure of this very rare mineral has been unknown. By syntheses via multianvil high-pressure/high-temperature methods at 11.5 GPa and 1300 C, synthetic verbeekite could be obtained in a high degree of purity and comparatively good crystal quality, which made it possible to determine the full crystal structure for PdSe2 verbeekite from single-crystal X-ray diffractometer data: I2/a, a = 671.0(2) pm, b = 415.42(8) pm, c = 891.4(2) pm, beta = 92.42(3), V = 248.24(4) AA3, R1 = 0.0368, wR2 = 0.0907 (all data). In contrast to layered PdS2-type PdSe2, verbeekite exhibits a novel crystal structure type of dichalcogenides of the platinum-group metals with (Se2)2- dimer anions connecting the layers. The possibility of different arrangements of the characteristic (Se2)2- dumbbells is the reason for the various polymorphs of the dichalcogenides, with now five known PdSe2 representatives.		
Get full text	by Google Scholar		

▼ Experimental information

Temperature	293 [K]	Pressure	atmospheric
Radiation type	X-Ray	Sample type	Single crystal
R-value	0.0329		
Remarks	Temperature factors available		

実験情報

実験情報

Additional information				
Keywords	Polymorphism	Keywords	Verbeekite type	
Keywords	HT-HP synthesis			
Comments	The deposited CIF at Fiz Karlsruhe (CSD-no. 432630) contains data in space group C2/c and are therefore regarded not to contain a final state		Comments	R = R( <u>refine_ls_R_factor_gt</u> )

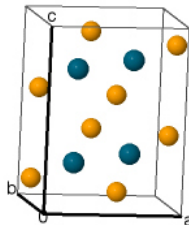
その他の情報: keywords  
ICSD独自のcomments  
warning情報あり

その他の情報: keywordや ICSD独自のcommentや warning情報あり.

▼ Compare Published and Standardized Structure
--

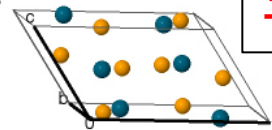
Published Crystal Structure

HM: I 1 2/a 1  
a=6.710Å  
b=4.154Å  
c=8.914Å  
α=90.000°  
β=92.420°  
γ=90.000°



Standardized Crystal Structure

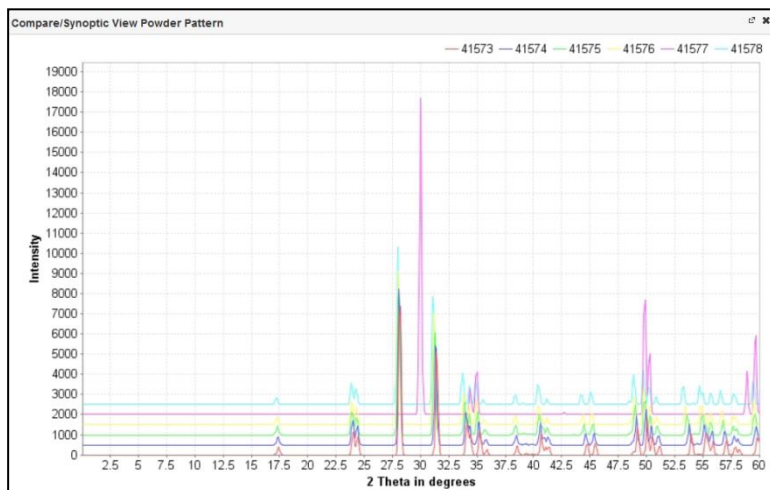
HM: C 1 2/c 1  
a=10.928Å  
b=4.154Å  
c=6.710Å  
α=90.000°  
β=125.420°  
γ=90.000°



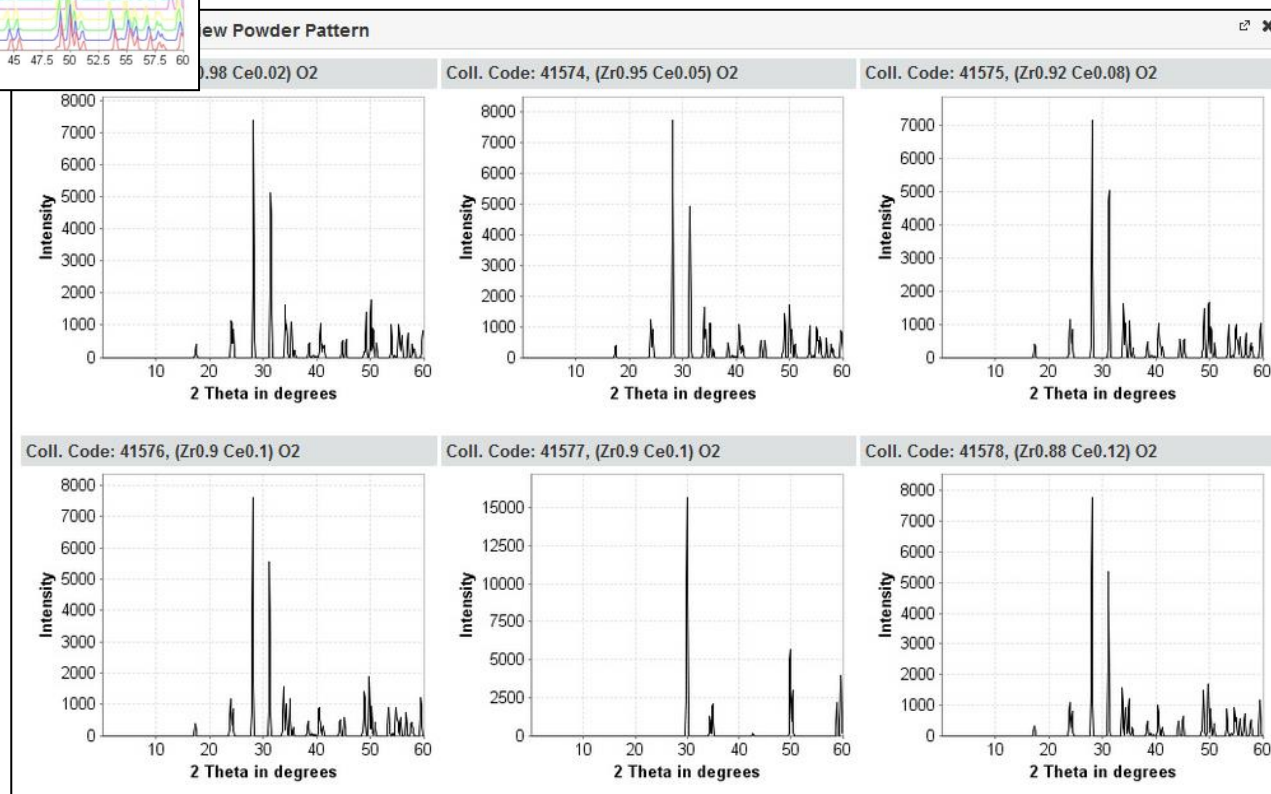
文献中に記載されている格子と既約に変換した格子の比較

★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、データの矛盾点や不足情報、コメントなどの付加情報をcomment/warning欄に記載. 9



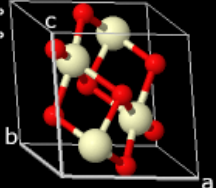

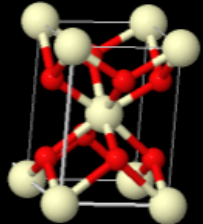
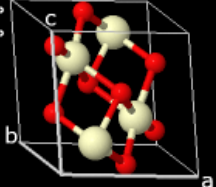
## ■その他の機能1



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

Compare/Synoptic View Structures		
Coll. Code: 41573, (Zr <sub>0.98</sub> Ce <sub>0.02</sub> ) O <sub>2</sub> 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°	Coll. Code: 41574, (Zr <sub>0.95</sub> Ce <sub>0.05</sub> ) O <sub>2</sub> 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°	Coll. Code: 41575, (Zr <sub>0.92</sub> Ce <sub>0.08</sub> ) O <sub>2</sub> 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	ICSD	ICSD
Coll. Code: 41576, (Zr <sub>0.9</sub> Ce <sub>0.1</sub> ) O <sub>2</sub> 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°	Coll. Code: 41577, (Zr <sub>0.9</sub> Ce <sub>0.1</sub> ) O <sub>2</sub> 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°	Coll. Code: 41578, (Zr <sub>0.88</sub> Ce <sub>0.12</sub> ) O <sub>2</sub> 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	ICSD	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](mailto:crystal@jaici.or.jp) >までお問い合わせください.