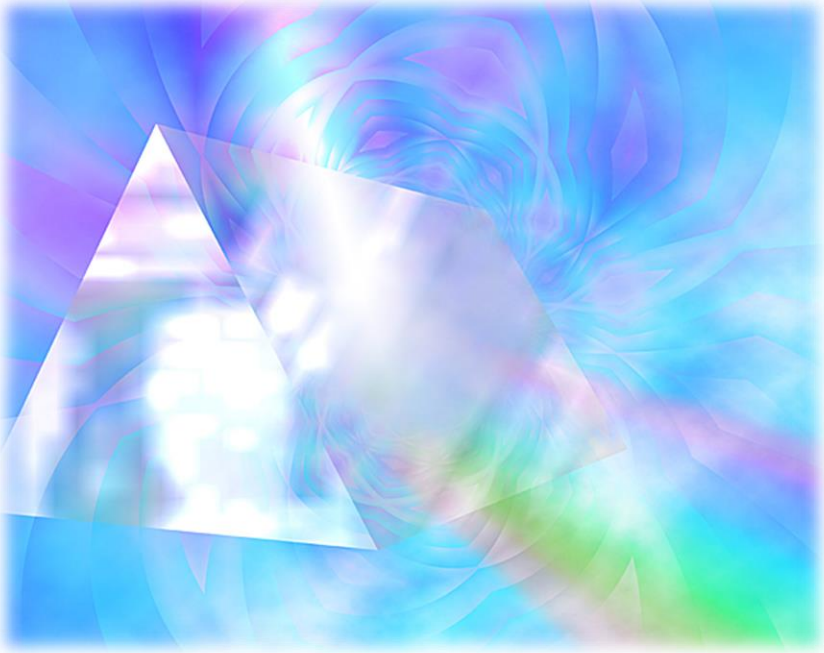
無機結晶構造データベース(ICSD)のご紹介

まずは検索画面から.



JAICI
化学情報協会

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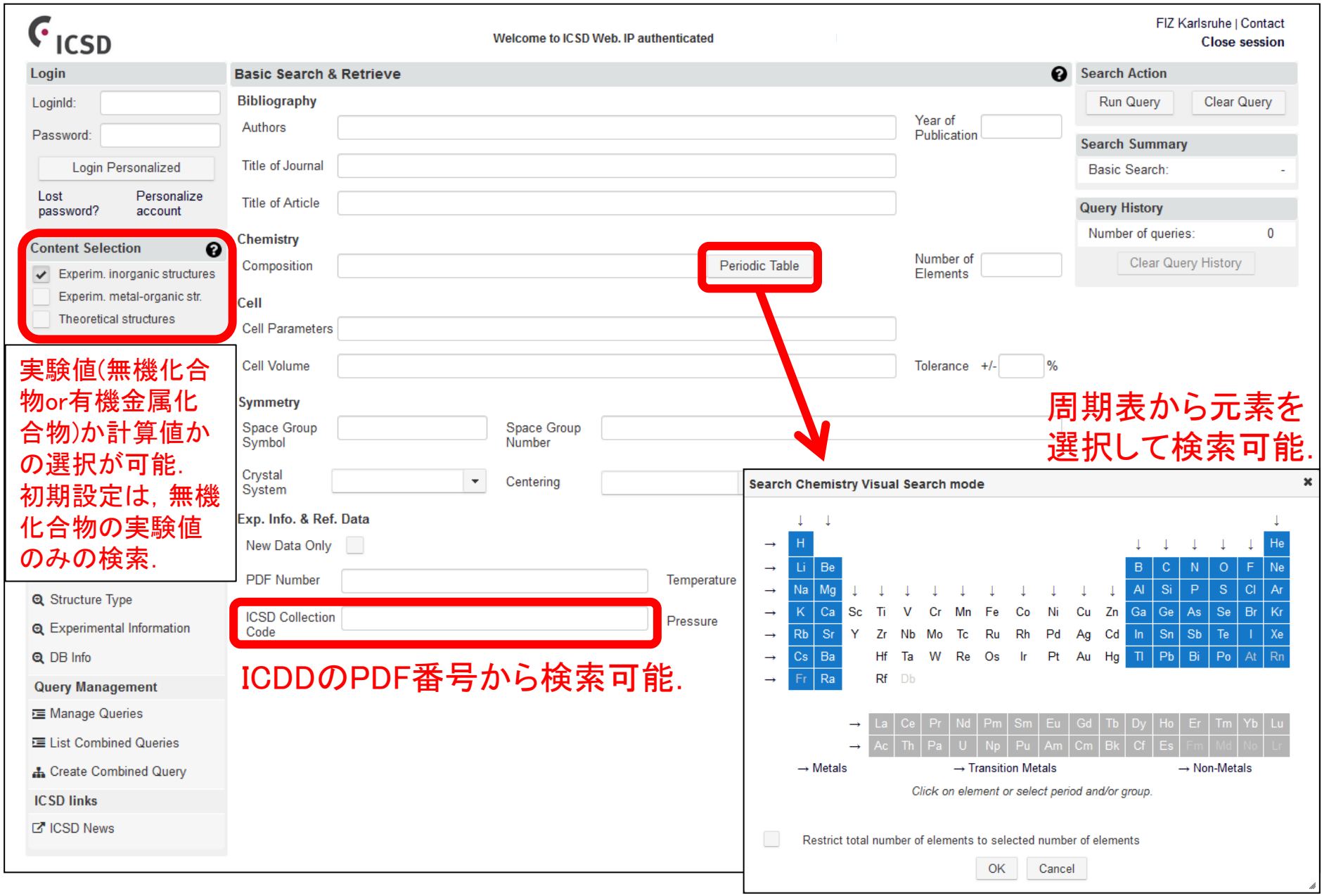
2019年8月作成

■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)



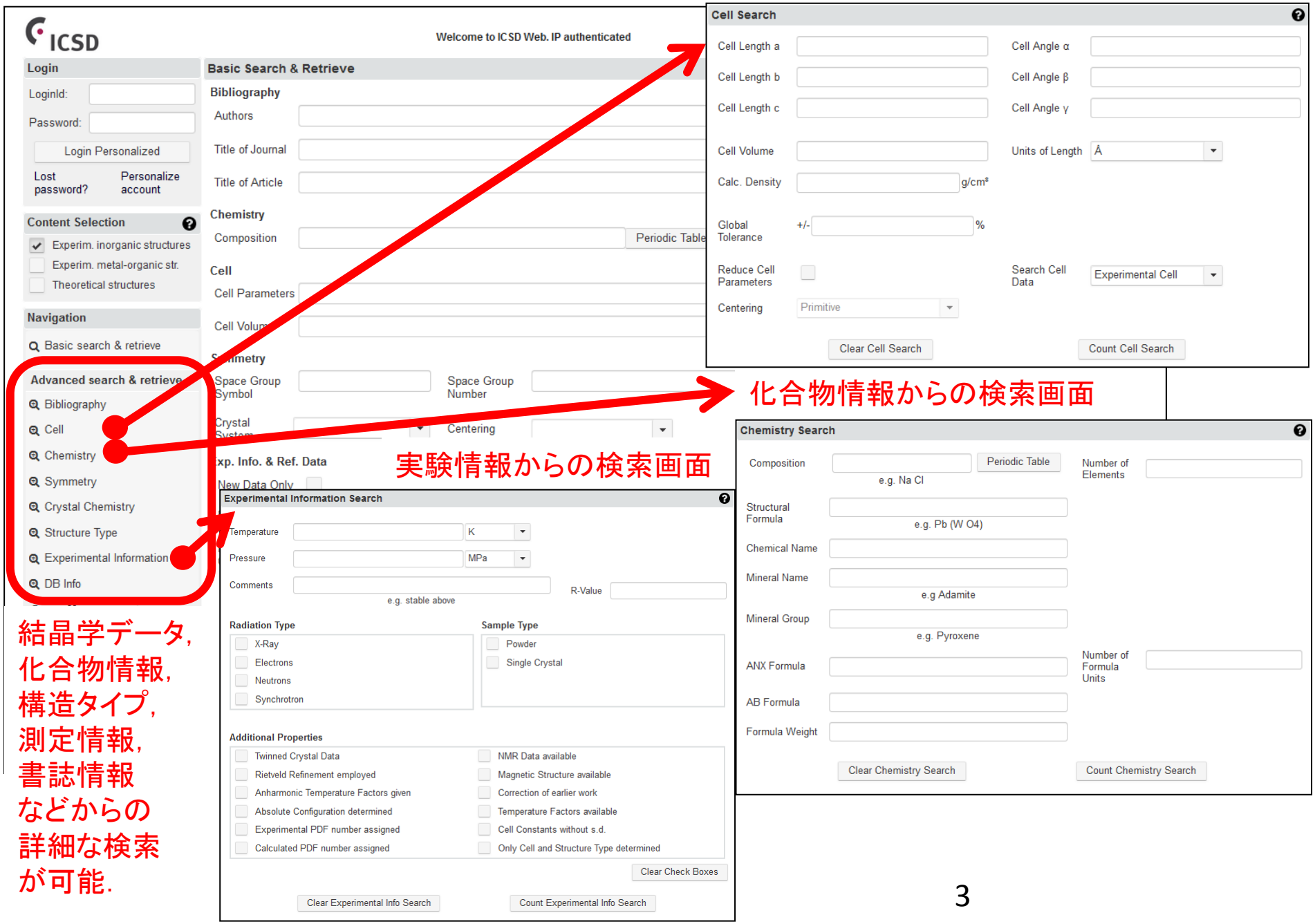
実験値(無機化合物or有機金属化合物)か計算値かの選択が可能.
初期設定は，無機化合物の実験値のみの検索.

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.

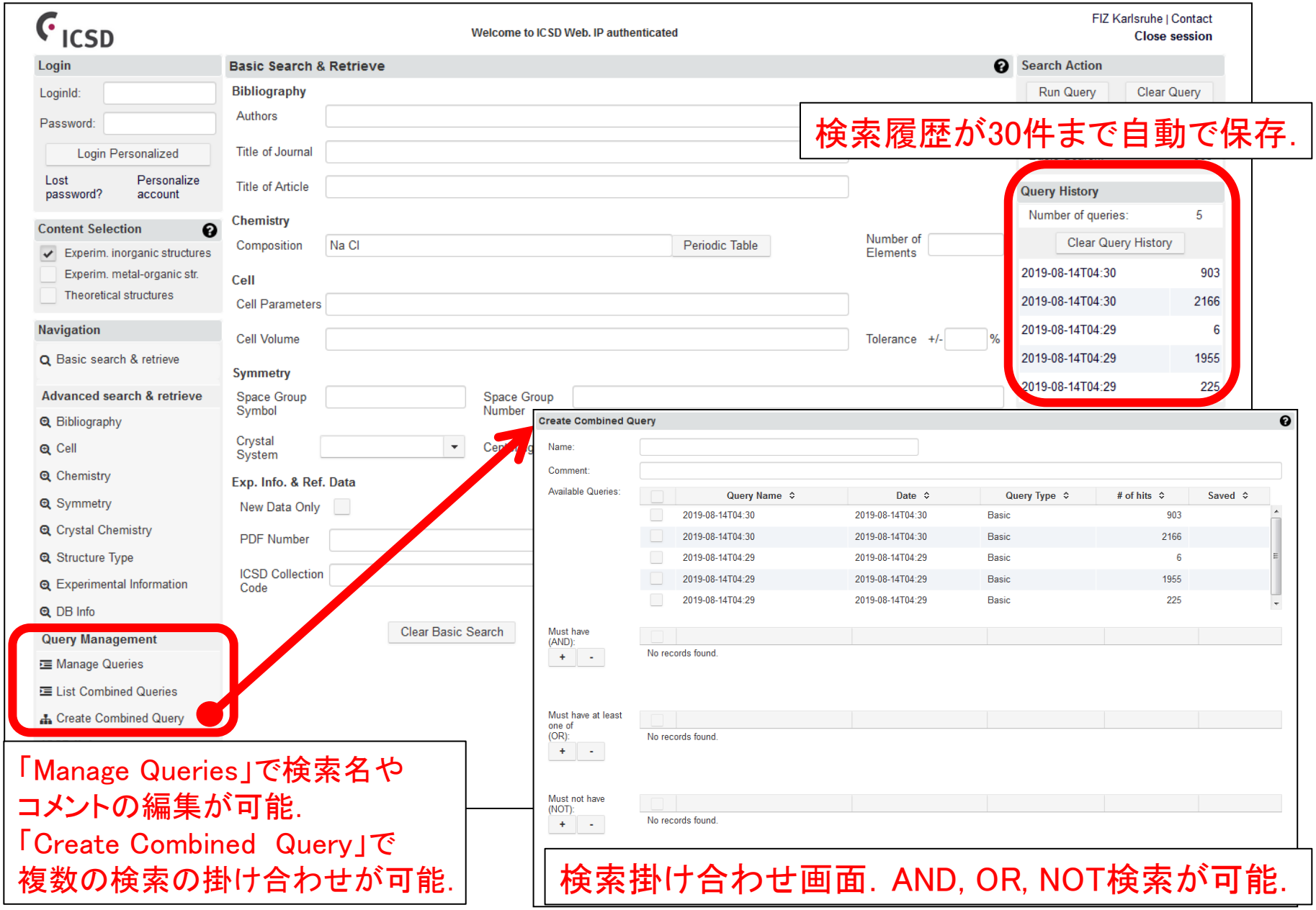
■詳細検索画面例(アドバンスサーチ画面)

格子定数からの検索画面



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



検索履歴が30件まで自動で保存.

「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.

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次に検索結果画面を紹介します.

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■レコード画面例1

CIFファイルの出力やプリンターでの印刷

ICSD

Welcome to ICSD Web. IP authenticated

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 Se2		
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
Temperature	293 [K]	Pressure	atmospheric
Data quality	High quality	R-value	0.0329
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

レコードのサマリー

Details Expand all | Collapse all

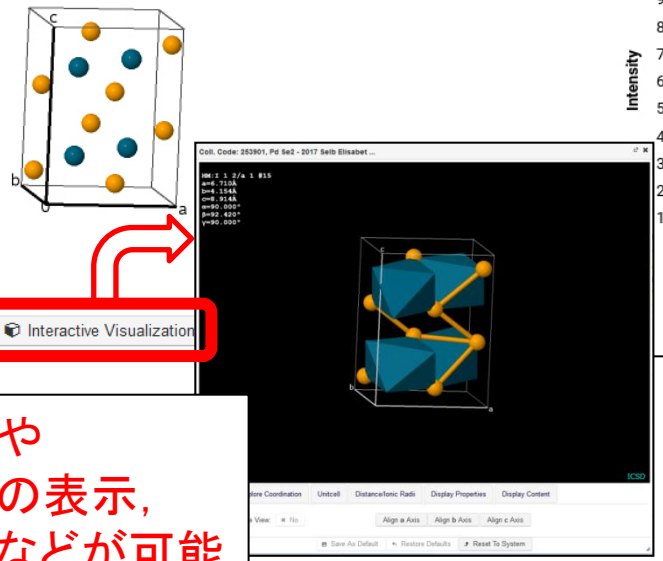
Visualization

↓ここからレコードの詳細.
次ページにも続く.

Published Crystal Structure

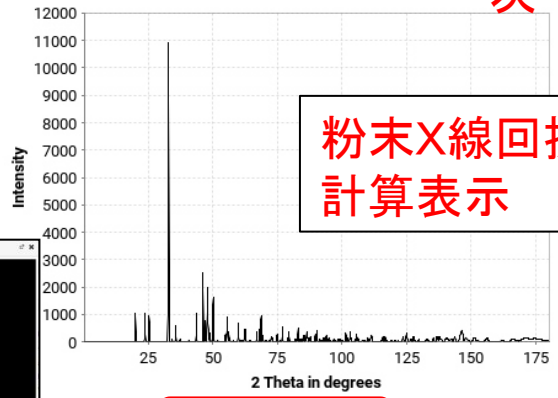
HM:I 1 2/a 1
a=6.710Å
b=4.154Å
c=8.914Å
α=90.000°
β=92.420°
γ=90.000°

3次元構造の表示



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

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: 1.6152, b/c: 0.4661, c/a: 1.3284
Calc. density	7.07 [g/cm³]		

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: 2.6306, b/c: 0.6191, c/a: 0.6140
Transformation info	REMARK Transformed from setting I 1 2/a 1.--> C 2/c TRANS -a-c,b,a		

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

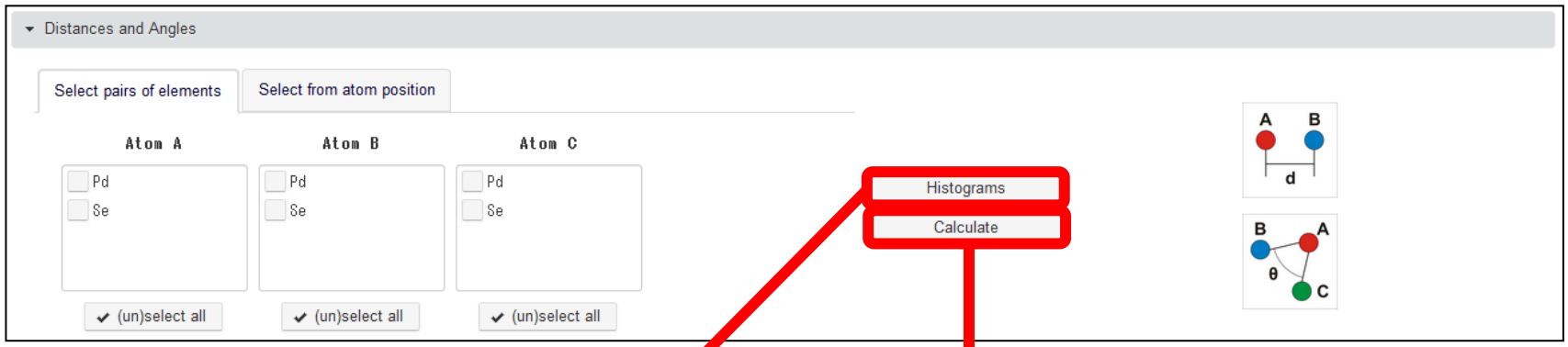
EL	Lbl	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Se	1	0.014300	0.018400	0.014700	0.000300	0.001300	-0.000900
Pd	1	0.011300	0.019800	0.013400	0.001000	0.000600	-0.000700

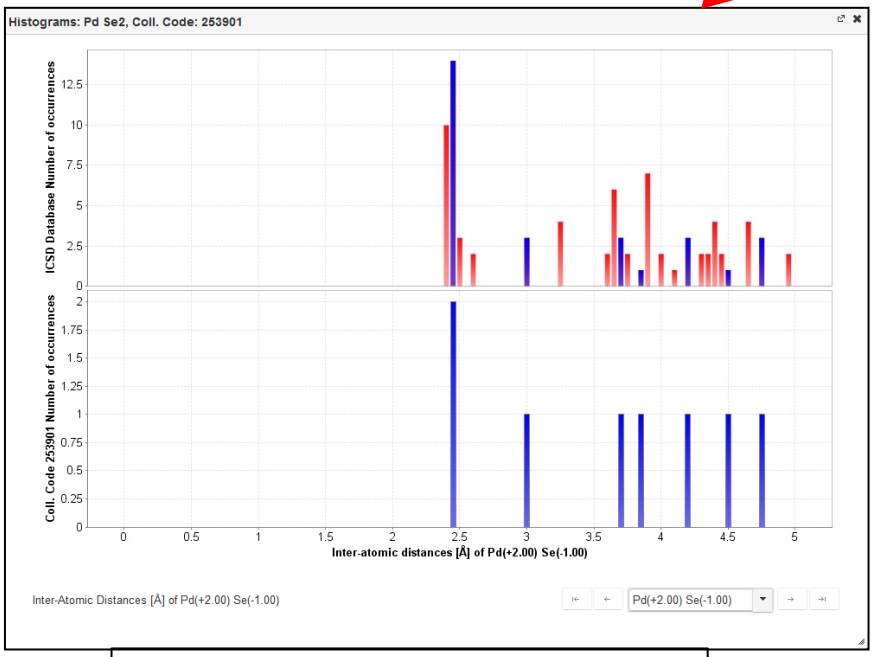
化合物情報，分子式タイプ，鉱物名など

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

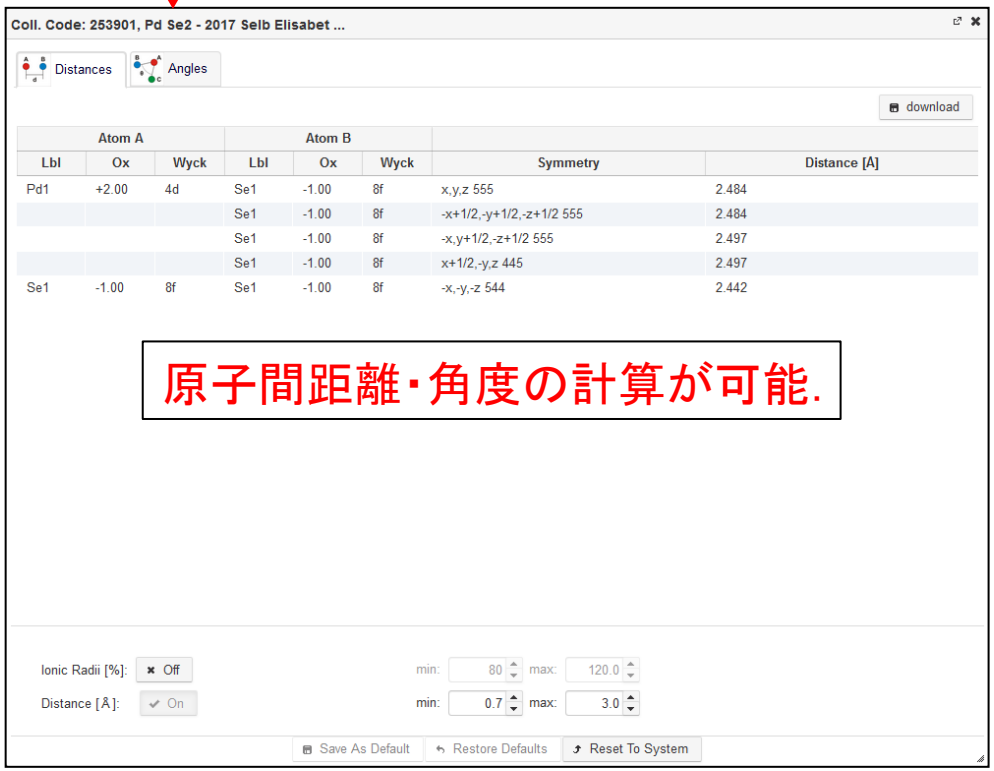
既約格子に変換した場合の格子定数，空間群，原子座標などの結晶学データ

■レコード画面例3





特定の原子間距離の分布のプロットが可能.
（例：Pd^{2+} – Se^{-} 間の距離）



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．Abstructも収録．

Bibliography

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

実験情報

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

Additional information

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

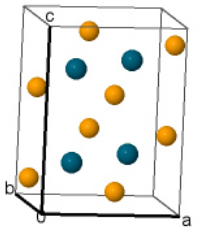
Keywords	Polymorphism	Keywords	Verbeekite type
Keywords	HT-HP synthesis		
Comments	The deposited CIF at Fiz Karlsruhe (CSD-no. 432630) contains data in space group C2/c and are therefore regarded not to contain a final state	Comments	R = R(_refine_ls_R_factor_gt)

Compare Published and Standardized Structure

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

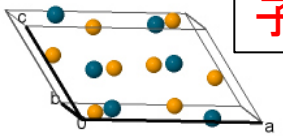
Published Crystal Structure

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



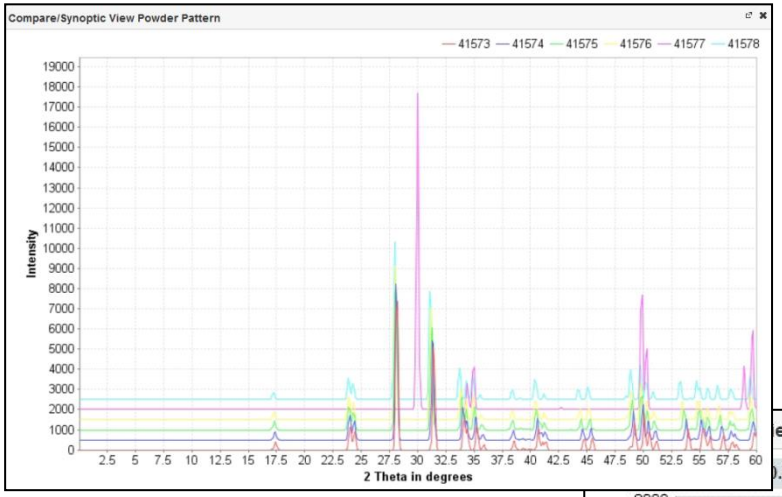
Standardized Crystal Structure

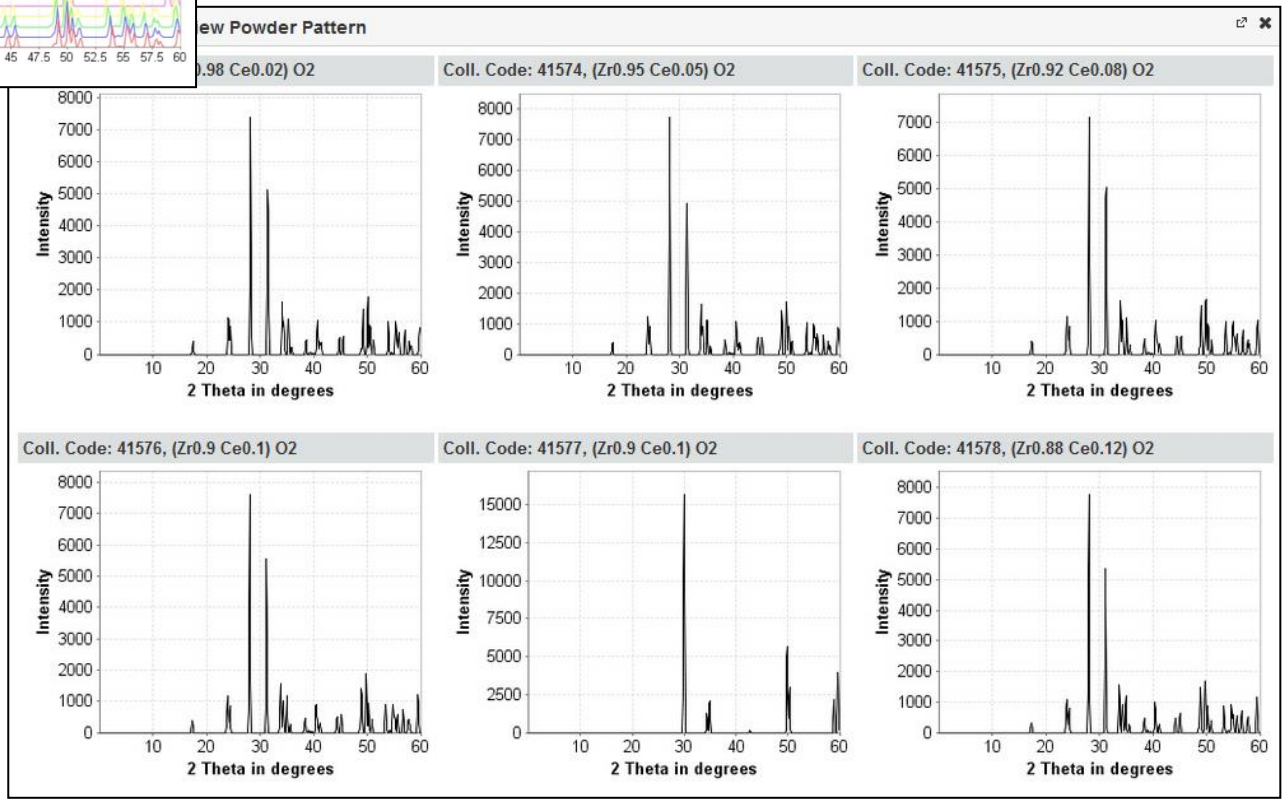
HM:C 1 2/c 1
a=10.928Å
b=4.154Å
c=6.710Å
α=90.000°
β=125.420°
γ=90.000°



★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．

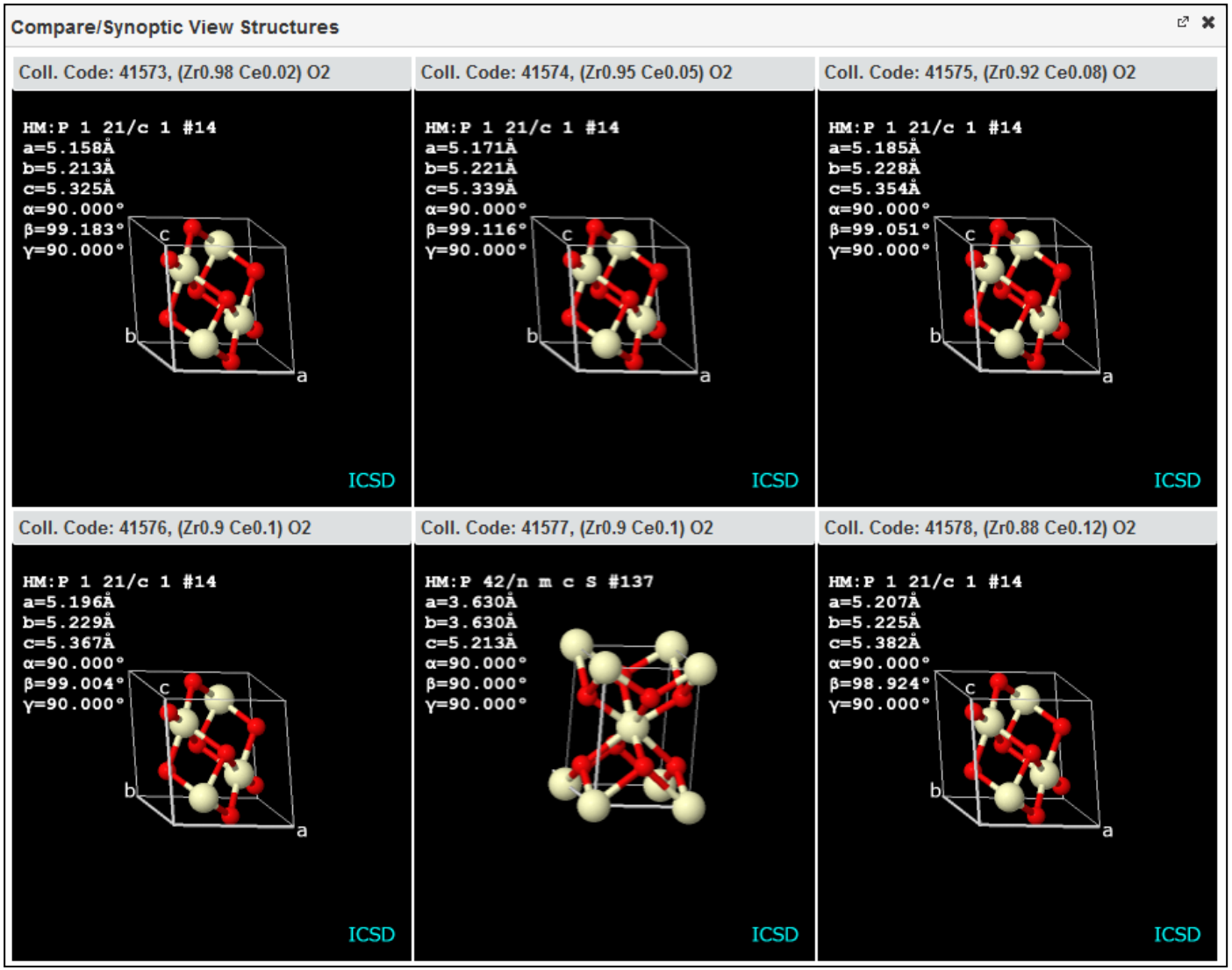
■その他の機能1





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



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 >までお問い合わせください.

以上