

# Quantitative Analysis

## Reference Intensity Ratio (RIR)

# Reference Intensity Ratio (RIR)

## What is it?

The Reference Intensity Ratio (RIR) is a method used for Quantitative Analysis by Powder Diffraction.

The RIR method is based upon scaling all diffraction data to the diffraction of standard reference materials.

# Reference Intensity Ratio (RIR)

## Why?

The intensity of a diffraction peak profile is a convolution of many factors, only one of which is the concentration of the analyte (species being measured).

By using the RIR method, ratios scaled to a common reference, are used in the experiment. The assumption is that all the factors, except concentration, of the analyte are ratioed and reduced to a constant.

By using ratios and measuring peak areas, the RIR method can be used to determine concentrations.

# Reference Intensity Ratio (RIR)

## How ?

The RIR method scales all diffraction data to a standard. By convention, corundum is used as the international reference and the scale factor is defined by:

$$\text{Intensity Analyte} / \text{Intensity Corundum} = I / I_c$$

$I/I_c$  can be experimentally derived by adding a known weight fraction of corundum to a pure specimen of the analyte of interest.

$I/I_c$  can also be calculated if the atomic parameters of analyte are known because the atomic parameters of corundum have been determined.

In PDF-4+,  $I/I_c$  has been experimentally determined for close to 10,000 materials and has been calculated for >170,000 materials.

# Overview of the Method

To understand how to use  $I/I_c$  values for quantitative analysis with the PDF-4+ database, a short description of the method is provided in the following slides.

RIR  
Method

# Reference Intensity Ratio (RIR)

## What?

### RIR Method

- RIR, as used in the Powder Diffraction File, is  $I/I_c$  (reference to corundum).
- $I/I_c$  can be determined, experimentally or calculated, from a crystal structure, both methods are used in the PDF-4+ database.
- Experimentally,  $I/I_c$  can be determined by taking the ratio of the strongest line of the pattern to the intensity of the strongest line of corundum in a 50/50 weight mixture.
- If we know the crystal structure, we can calculate  $I/I_c$  as shown in the following slide.

# Reference Intensity Ratio (RIR)

RIR  
Method

All calculated patterns have  $I/I_c$ .

$$I/I_c = \mu \gamma \rho_c / \mu_c \gamma_c \rho$$

$\mu$  = Linear attenuation coefficient

$\gamma$  = Absolute scale factor

$\rho$  = Density

(Subscript “c” corresponds to corundum)

Single crystal determinations have all the data necessary to calculate the variables in the above equation from atomic parameters and the unit cell parameters with the use of atomic scattering factors and published constants. These are used by the ICDD to calculate  $I/I_c$  for these entries.

# Reference Intensity Ratio (RIR)

## RIR Method

Calculated  $I/I_c$  values often significantly differ from experimental  $I/I_c$  values.

Natural products, minerals, and biomaterials often contain trace impurities, anion/cation substitution in the lattice, or naturally produced vacancies, and/or defects in the crystalline state. These physical phenomena are well known to influence peak intensities and peak profiles that will change the  $I/I_c$  value. This value can be significantly different from one calculated from a perfect crystalline pure material.

If you are using  $I/I_c$  to quantitate a synthetic mixture, you may want to use a calculated value. If you are using  $I/I_c$  to quantitate a natural product or mineral sample, you may prefer experimental values.

# Quantitative Analysis

RIR  
Method

## Main equation for quantitative analysis

$K_{ia}$  contains structure factor, multiplicity, Lorentz-polarization factor, temperature factor + scale factor for reflection  $i$  of phase  $a$

$I_{ia}$  = intensity of reflection  $i$  of phase  $a$

$$I_{ia} = \frac{K_{ia} X_a}{\rho_a \mu}$$

$X_a$  = wt fraction of phase  $a$  **(want this!!)**

$\rho_a$  is density of phase  $a$

$\mu$  = Linear attenuation coefficient

# Quantitative Analysis

RIR  
Method

Measure  
this!!

$$I_{ia} = \frac{K_{ia} X_a}{\rho_a \mu}$$

$X_a$  = wt fraction of  
phase a **(want this!!)**

# Quantitative Analysis

## Reference Intensity Ratios

For  
analyte

$$I_a = \frac{K_a X_a}{\rho_a \mu}$$

For  
corundum

$$I_c = \frac{K_c X_c}{\rho_c \mu}$$

$$\frac{I_a = \frac{K_a X_a}{\rho_a \mu}}{I_c = \frac{K_c X_c}{\rho_c \mu}} \longrightarrow \frac{I_a}{I_c} = \frac{K_a X_a \rho_c}{K_c X_c \rho_a} = K \frac{X_a}{X_c}$$

For 50-50 mixture of analyte with corundum

$$\frac{I_a}{I_c} = K \dots \text{denoted } (I/I_c)_a$$

RIR  
Method

# Quantitative Analysis

## Reference Intensity Ratios

RIR  
Method

$$\frac{I_a}{I_c} = \frac{K_a X_a \rho_c}{K_c X_c \rho_a} = K \frac{X_a}{X_c}$$

For any a + b mixture

$$\frac{(I_a/I_c)}{(I_b/I_c)} = \frac{\frac{K_a \rho_c}{K_c \rho_a}}{\frac{K_b \rho_c}{K_c \rho_b}} = \frac{K_a}{K_b} \frac{\rho_b}{\rho_a} = \frac{K_a}{K_b} \frac{X_b}{X_a}$$

$$\frac{I_a}{I_b} = \frac{\rho_a}{K_b} \frac{X_a}{X_b} = \frac{(I/I_c)_a}{(I/I_c)_b} \frac{X_a}{X_b}$$



# Reference Intensity Ratio (RIR)

## Practical Considerations

### RIR Method

The RIR method uses simultaneous equations to solve analyte concentrations in a multicomponent mixture.

Many vendor programs interface to PDF-4+ to automatically extract  $I/I_c$  and peak areas from the experimental data for automated quantitative analysis.

Automated programs assume that the combination of all phases identified account for all observed scattering and 100% of the specimen. Significant errors can occur, if there are non-crystalline phases or unidentified materials present in the specimen.

# Finding I/Ic Search

Global Operator Numeric Input Help

Subfiles/Database Filters Periodic Table Elements Names References Structures Miscellaneous

Database

Not ICDD (00)  Or  Not Primary  Or  Not Ambient/Non-ambient

Not ICSD-FIZ (01)  Or  Not Alternate  Or  Not Pressure (Non-ambient)

Not Cambridge (02)  Or  Not Deleted  Or  Not Temperature (Non-ambient)

Not NIST (03)  Or  Not Pressure & Temperature (Non-ambient)

Not LPF (04)  Or

Quality Mark (QM)

Not Star (S)  Or

Not Indexed (I)  Or

Not Blank (B)  Or

Not Low-Precision (O)  Or

Not Calculated (C)  Or

Not Prototyping (P)  Or

Not Rietveld (R)  Or

Not Hypothetical (H)  Or

Subfile/Subclass

Not Battery Material  And

Not Cement Material  Or

Not Ceramics  Or

Not Common Phase  Or

Not Education  Or

Not Excipient  Or

Not Explosive  Or

Not Forensic  Or

Not Giant Magneto Resistance  Or

Not Inorganic  Or

Not Intercalate  Or

Not Ionic Conductor  Or

Not Metals & Alloys  Or

Not Metal Related  Or

Not Polymers  Or

Not Pharmaceuticals  Or

Not Pigments  Or

Not Plastics  Or

Not Semiconductors  Or

Not Superconducting Materials  Or

Not Textiles  Or

Not Thin Films  Or

Not Vitreous Solids  Or

Not Wood  Or

Not Zeolites  Or

Not Other  Or

Start at the main Search Page

I/I-corundum (I/Ic)

Not  ESD:

Global Operator Numeric Input Help

Subfiles/Database Filters Periodic Table Elements Names References Structures Miscellaneous

Long Line

Not  Å ESD:  Å

Not  Å ESD:  Å

Density

Not  g/cm<sup>3</sup> ESD:  g/cm<sup>3</sup>

Not  g/cm<sup>3</sup> ESD:  g/cm<sup>3</sup>

Melting Point

Not  ESD:  °C  °K  °F

Not  ESD:

Color

Not Black  And

Not Blue  Or

Not Brown  Or

Not Color Missing  Or

Not Colorless  Or

Not Gray  Or

Not Green  Or

Not Metallic  Or

Not Orange  Or

Not Pink  Or

Not Red  Or

Not Violet  Or

Not White  Or

Not Yellow  Or

Organic Functional Group

Not >4\_Hetero\_Atoms\_in\_Ring(s)  And

Not >5\_Fused\_Rings  Or

Not >9\_Membered\_Ring  Or

Not 1\_Hetero\_atom\_in\_ring(s)  Or

Not 1,2\_dione\_\_O=C=C=O  Or

Not 2\_Fused\_Rings  Or

Not 2\_Hetero\_Atoms\_in\_Ring(s)  Or

Not 3\_Fused\_Rings  Or

Not 3\_Hetero\_Atoms\_in\_Ring(s)  Or

Not 3\_Membered\_Ring  Or

Not 4\_Fused\_Rings  Or

Not 4\_Hetero\_Atoms\_in\_Ring(s)  Or

Not 4\_Membered\_Ring  Or

Not 5\_Fused\_Rings  Or

Smith-Snyder Figure Of Merit (SS/FOM)

Not  ESD:

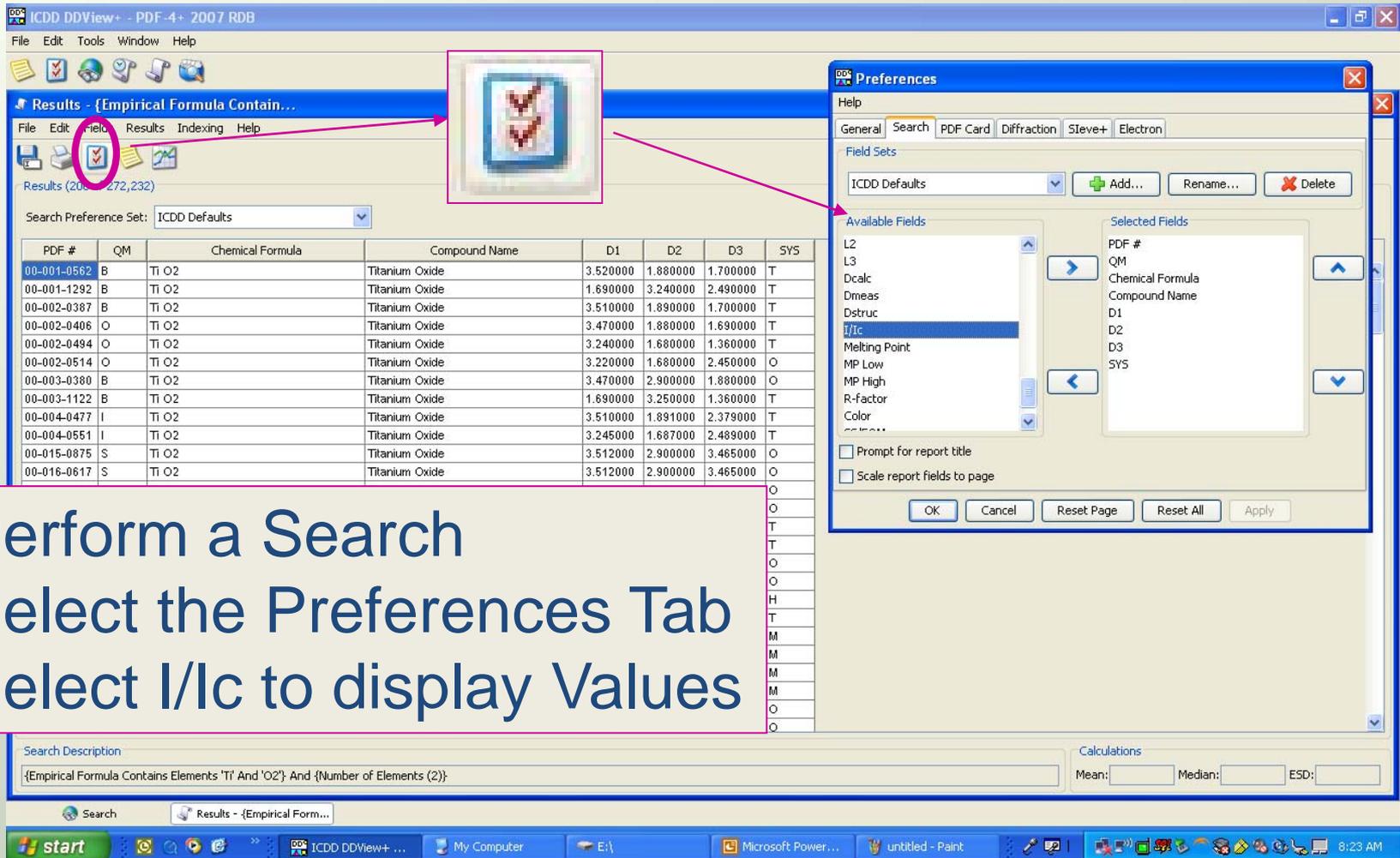
Database Comments

Not  Contains Words  Contains Phrase

Search Show Results Undock Page Reset Page Reset All

Go to the Miscellaneous Tab

# Finding I/Ic for a Material



The screenshot shows the ICDD DDView+ interface. The main window displays search results for Titanium Oxide. A table lists various PDF #s and their corresponding QM, Chemical Formula, Compound Name, and D1, D2, D3, and SYS values. The 'I/Ic' field is highlighted in the 'Available Fields' list in the Preferences dialog box.

**Search Results Table:**

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
00-001-0562	B	Ti O2	Titanium Oxide	3.520000	1.880000	1.700000	T
00-001-1292	B	Ti O2	Titanium Oxide	1.690000	3.240000	2.490000	T
00-002-0387	B	Ti O2	Titanium Oxide	3.510000	1.890000	1.700000	T
00-002-0406	O	Ti O2	Titanium Oxide	3.470000	1.880000	1.690000	T
00-002-0494	O	Ti O2	Titanium Oxide	3.240000	1.680000	1.360000	T
00-002-0514	O	Ti O2	Titanium Oxide	3.220000	1.680000	2.450000	O
00-003-0380	B	Ti O2	Titanium Oxide	3.470000	2.900000	1.880000	O
00-003-1122	B	Ti O2	Titanium Oxide	1.690000	3.250000	1.360000	T
00-004-0477	I	Ti O2	Titanium Oxide	3.510000	1.891000	2.379000	T
00-004-0551	I	Ti O2	Titanium Oxide	3.245000	1.687000	2.489000	T
00-015-0875	S	Ti O2	Titanium Oxide	3.512000	2.900000	3.465000	O
00-016-0617	S	Ti O2	Titanium Oxide	3.512000	2.900000	3.465000	O

**Preferences Dialog Box:**

- Field Sets: ICDD Defaults
- Available Fields: L2, L3, Dcalc, Dmeas, Dstruc, **I/Ic**, Melting Point, MP Low, MP High, R-factor, Color, ...
- Selected Fields: PDF #, QM, Chemical Formula, Compound Name, D1, D2, D3, SYS

**Search Description:** {Empirical Formula Contains Elements 'Ti' And 'O2'} And {Number of Elements (2)}

**Calculations:** Mean: [ ] Median: [ ] ESD: [ ]

- 1) Perform a Search
- 2) Select the Preferences Tab
- 3) Select I/Ic to display Values

# Finding I/Ic for a Material

File Edit Fields Results Indexing Help

Results (206 of 272,232)

Search Preference Set: ICDD Defaults

PDF #	QM	Chemical F...	Compound Name	SYS	I/Ic	D1	D2	D3
01-072-4814	I	Ti O2	Titanium Oxide	T	3.5	3.251060	1.688030	2.486680
01-072-4815	I	Ti O2	Titanium Oxide	T	3.51	3.248800	1.687260	2.486230
01-072-4816	I	Ti O2	Titanium Oxide	T	3.52	3.248100	1.687030	2.486130
01-072-4817	I	Ti O2	Titanium Oxide	T	3.52	3.247810	1.686970	2.486190
01-072-4818	I	Ti O2	Titanium Oxide	T	3.53	3.247390	1.686930	2.486460
01-072-4819	I	Ti O2	Titanium Oxide	T	3.53	3.247110	1.686830	2.486390
01-072-4820	I	Ti O2	Titanium Oxide	T	3.53	3.247440	1.687010	2.486660
01-072-4821	I	Ti O2	Titanium Oxide	T	3.57	3.247370	1.687020	2.486740
01-072-7058	I	Ti O2	Titanium Oxide	T	4.88	3.518310	1.893350	2.378730
01-072-7119	I	Ti O2	Titanium Oxide	A	18.43	12.932000	6.466000	4.310670
01-072-7374	S	Ti O2	Titanium Oxide	T	3.27	3.270860	2.505510	1.699460
01-073-1764	I	Ti O2	Titanium Oxide	T	4.89	3.508270	1.888000	2.371500
01-073-1765	I	Ti O2	Titanium Oxide	T	3.45	3.244910	2.483870	1.685430
01-073-1774	I	{Ti O.716	Titanium Oxide	C	3.78	2.098300	2.422910	1.483720
01-075-1537	I	Ti O2	Titanium Oxide	T	5.2	3.474540	1.870000	2.347500
01-075-1582	I	Ti O2	Titanium Oxide	O	1.62	3.510870	2.900010	3.464020
01-076-1935	S	Ti O2	Titanium Oxide	O	1.62	3.512060	2.901400	3.467840
01-076-1936	S	Ti O2	Titanium Oxide	O	1.63	3.516710	2.905450	3.472170
01-076-1937	S	Ti O2	Titanium Oxide	O	1.61	3.523590	2.911840	3.479830
01-076-1938	S	Ti O2	Titanium Oxide	T	3.64	3.247740	1.687350	2.487480
01-076-1939	S	Ti O2	Titanium Oxide	T	3.55	3.254810	1.691130	2.493230
01-076-1940	S	Ti O2	Titanium Oxide	T	3.47	3.264000	1.696390	2.501830
01-076-1941	S	Ti O2	Titanium Oxide	T	3.44	3.268950	2.508280	1.699790
01-079-1640	H	Ti O2	Titanium Oxide	T	3.57	3.290170	1.703270	2.500480
01-082-0514	H	Ti O2	Titanium Oxide	T	3.43	3.187640	2.513030	1.677950
01-083-2242	B	Ti O2	Titanium Oxide	T	4.14	3.245620	1.686790	2.487600

Search Description

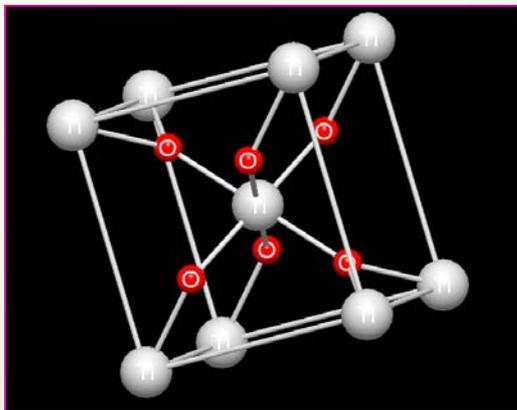
{Empirical Formula Contains Elements 'Ti' And 'O2'} And {Number of Elements (2)}

TiO2's  
and I/Ic  
Displayed

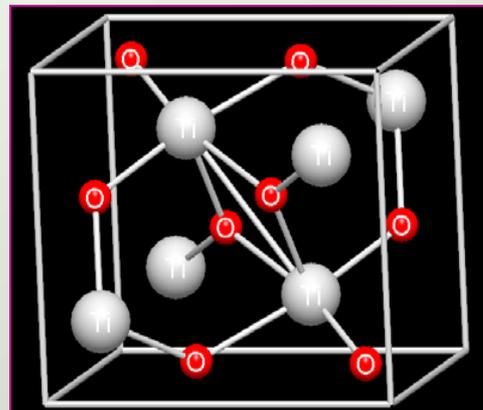
# Selecting Appropriate I/Ic Values

- Choose the appropriate structure.  
Many materials have polymorphs that have the same chemical formula, but different structures. These have different I/Ic's.
- Match the reference to the specimen as closely as possible.
- Use quality marks and indicators to select the best quality reference.

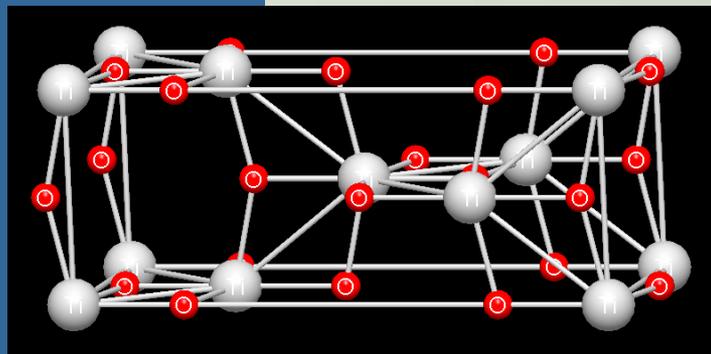
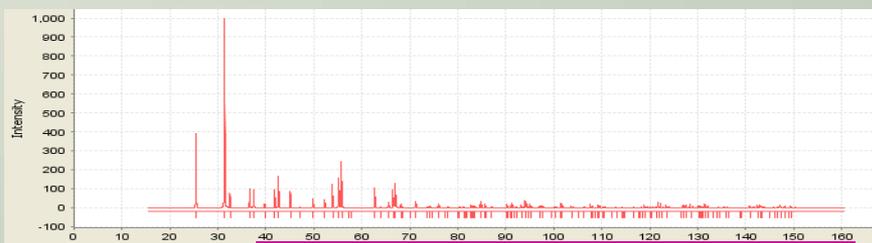
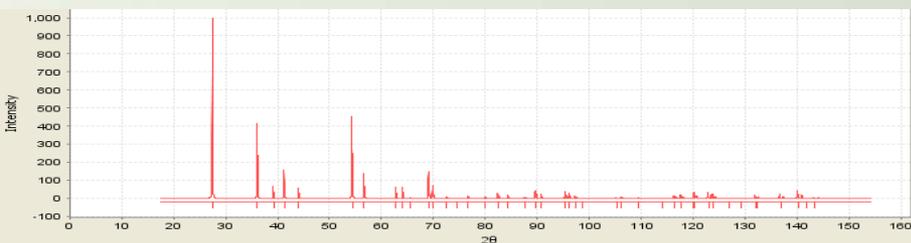
# Selecting I/Ic - Structure



TiO<sub>2</sub>  
Rutile  
I/Ic = 3.54

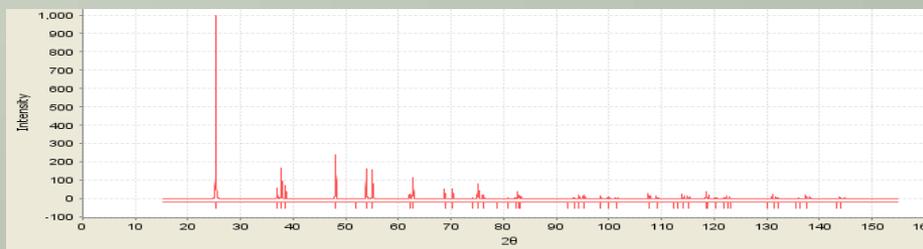


TiO<sub>2</sub>  
Brookite  
I/Ic = 3.06



TiO<sub>2</sub>  
Anatase  
I/Ic = 5.04

Formulae are the same,  
pattern, structure and I/Ic  
are distinctly different



# Structure

From Search Results  
use the Preferences Tab  
to select fields



Help

General Search PDF Card Diffraction Sieve+ Electron

Field Sets

ICDD Defaults + Add... Rename... ✗ Delete

Available Fields

- Common Name
- Author
- Coden
- Journal
- Title
- CAS
- Year
- Pearson w/o H
- AuthCell-a
- AuthCell-b
- AuthCell-c

Selected Fields

- QM
- Chemical Formula
- Mineral Name
- Compound Name
- SYS
- SG #
- I/Ic
- SPGR
- Prototype Structure
- LPF Prototype Structure
- Pearson

Prompt for report title

Scale report fields to page

OK Cancel Reset Page Reset All Apply

You can select many fields that help you determine the structure by matching these data to the experimental data.

These include:

Chemical Name, Mineral Name

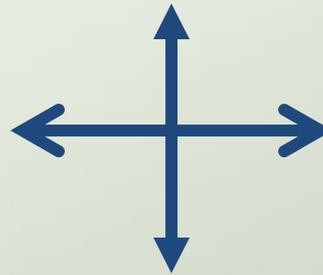
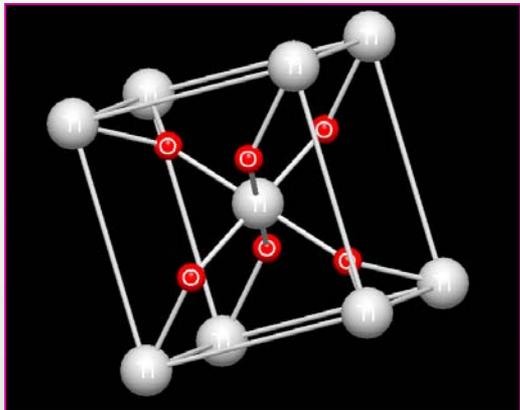
System and Space Group Number (SG#)

Pearson, Prototype Structure and LPF Prototype Structure

Reduced Cell, Author Cell and Crystal Cell

Strong Line (D1, D2, D3) and Long Line (L1, L2, L3)

# Match Reference to Experiment



Temperature can expand or contract the unit cell – and change  $I/I_c$ .

All the known factors that can alter a structure: temperature, pressure, anion or cation substitution, synthesis conditions, vacancies, stress, strain, etc. will change atom positions, electron density distribution, and therefore alter peak intensities and the  $I/I_c$  ratio.

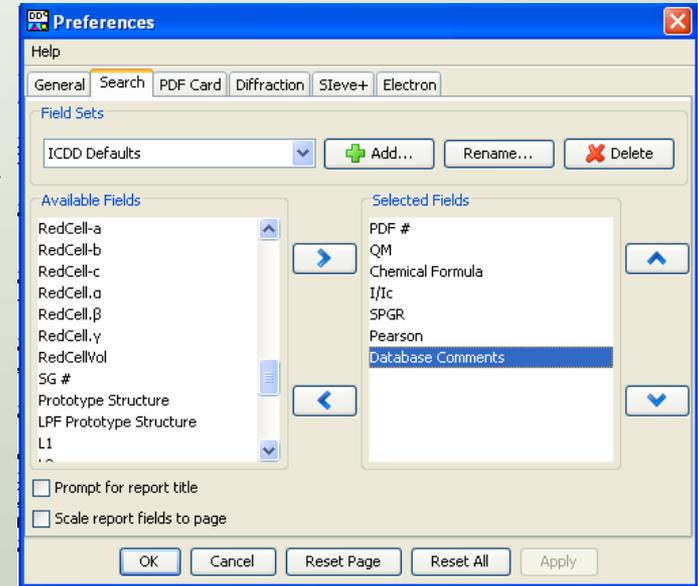
The above factors are changes in the **Kia factor** in the equation for quantitative analysis.

*Select a reference that most closely matches your experiment!*

# Matching References



From the Results Form,  
select Preferences,  
add Database Comments



04-007-5987	P	Ti O2	3.54	P42/mnm	tP6.00	LPF Collection Code: 1403121. Sample Preparation: STARTING MATERIALS:TiO2. Compound Preparation: heated at 1173-1273 K for several hours. Temperature of Data Collection: 298 K. Unit Cell Data Source: Powder Diffraction.
04-007-6246	B	Ti O2	1.82	C2/m	mC24.00	LPF Collection Code: 1403721. Polymorphism/Phase Transition: B. Temperature of Data Collection: 290 K. Significant Warning: Reported temperature factors on non H atoms are outside the range 0.001<U<0.1. Reported temperature factors were ignored and U=0.012 was used in the calculation. Unit Cell Data Source: Powder Diffraction.
04-007-6487	I	Ti O2	3.05	Pbnm	oP12.00	Color: colorless. LPF Collection Code: 1404320. Sample Preparation: STARTING MATERIALS:TiO2. Compound Preparation: heated at 1473 K. Temperature Factor: Reported Anisotropic temperature factors (in Beta) were converted to B. Temperature of Data Collection: 293 K. Minor Warning: LPF Editor Comment: unit for isotropic displacement parameters omitted, assumed to be angstrom 2. Unit Cell Data Source: Single Crystal.

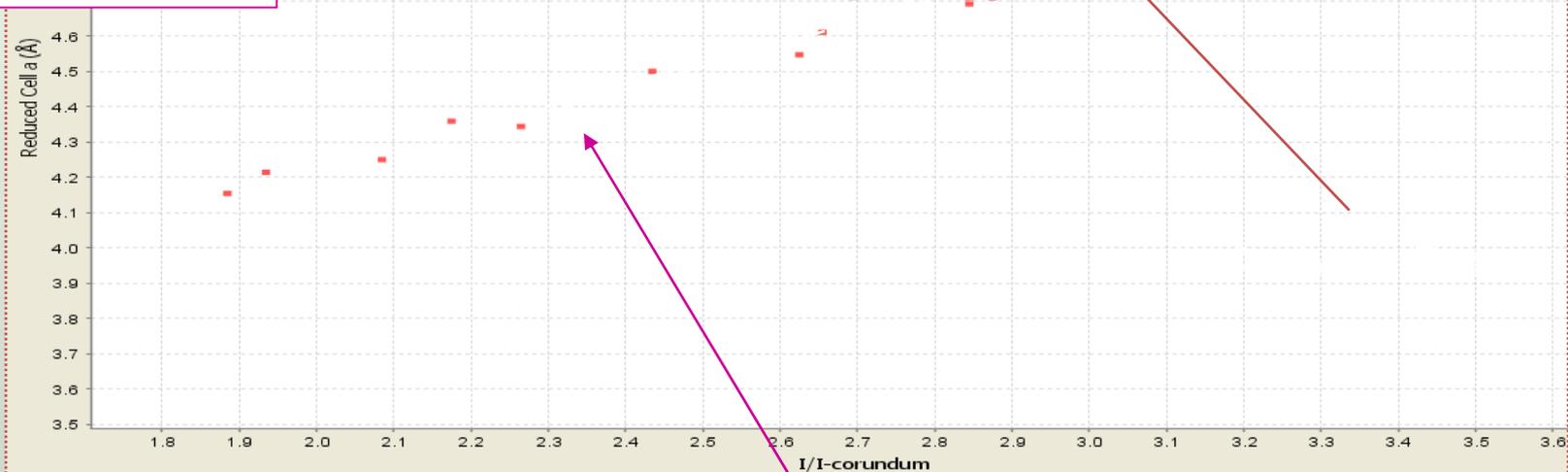
Editor comments contain information on specimen preparation, impurities, temperature of data collection and other factors that can change I/Ic. They can guide you to the appropriate choice.

# I/Ic for Quartz

## Space Group P3221

### 75 Determinations

Data plotted from PDF-4+ Search Form of I/Ic versus reduced cell a, *editor comments describe T, P conditions*

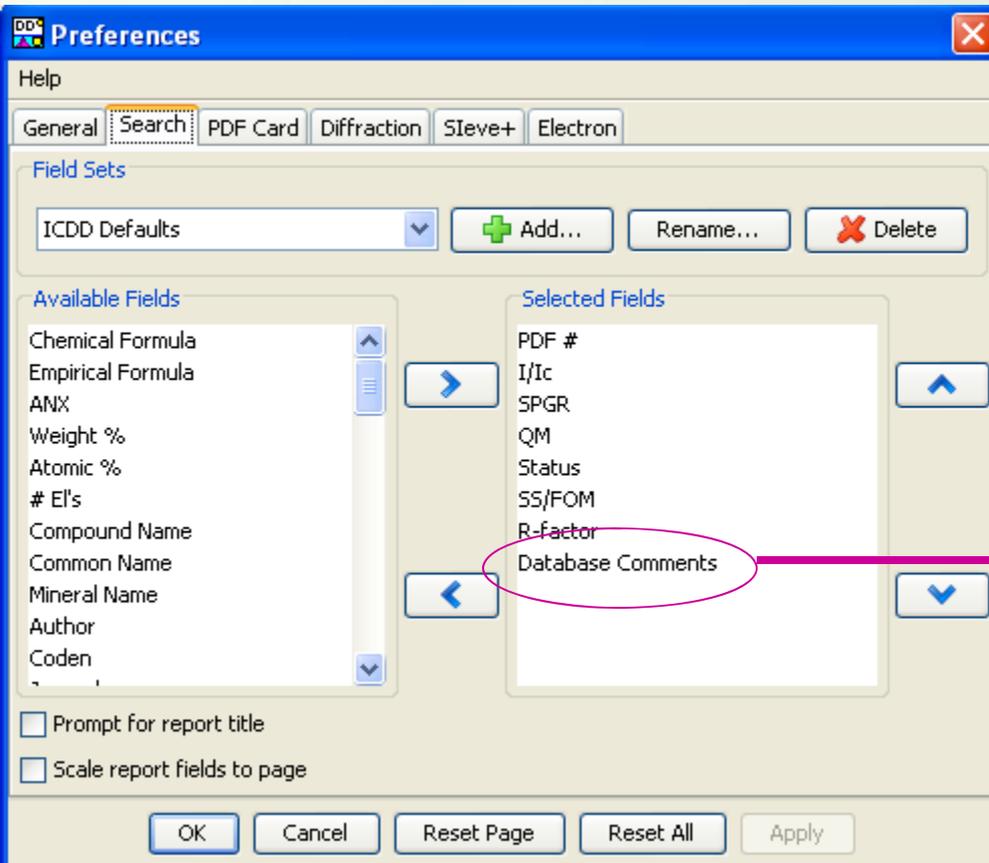


High Temp Series

Effect of Temp and Pressure for Quartz I/Ic

High Pressure Series Synthetic Materials

# Using Quality Marks and Indicators



The database contains many quality Indicators. These include:

<u>Indicator</u>	<u>High Quality Value</u>
Quality Mark	S
Status	Primary
SS/FOM	Highest Number
R-Factor	Lowest Number

**Database Comments:** This includes comments from editors and statistical analyses conducted on the data.

The indicators are defined in the Help documentation in the database.

Use “Preferences” to display quality marks and indicators.

# Using Quality Marks and Indicators

## Poor Quality

Low Quality Marks are designations B and O  
Low Quality Status would be a “Deleted” pattern  
R-factors  $>0.10$  (i.e., 10%) and SS/FOM's below 10 are indications of poor quality

In general, any data meeting the above criteria should not be used in a quantitative analysis calculation as the ICDD's editorial analysis and review would indicate that the calculation may result in large errors.

The data are included because there may not be better alternative choices for a particular material or the entry may contain other types of unique data (i.e., measured physical properties, novel synthesis, etc.).

# Using Cross References

What if a Search/Match program identified an entry with a poor quality mark or poor quality indicator?

*- Check the Cross References*

In this example, a Search/Match program identified entry PDF 04-08-7810, which has an I/Ic of 3.6 and a “B” Quality Mark. The editors’ comments mention that the atomic parameters were derived (not experimentally determined or calculated) from the original publication. This results in low precision for the cell parameters and I/Ic values.

PDF Card - 04-008-7810

File Edit d-Spacings Tools Window Help

Wavelength: Cu Kα1 1.54056Å

Intensity: Fixed Slit

2θ	d(Å)	I	h	k	l
27.4335	<b>3.248450</b>	999	1	1	0
36.079	<b>2.487400</b>	440	1	0	1
39.1866	2.297000	65	2	0	0
41.238	2.187350	171	1	1	1
44.0391	2.054500	60	2	1	0
54.3171	<b>1.687530</b>	483	2	1	1
56.6205	1.624220	138	2	2	0
62.7592	1.479300	66	0	0	2

Former PDF's #: 01-086-0147

Cross-Ref PDF #'s (1)

**04-003-0648 (Primary)**

Mineral Classification: TiO<sub>2</sub>, TP6, 136

Entry Date: 01/05/2005

**Solution:** The entry contains cross-references identified in the “Miscellaneous Tab” of the entry. The primary (high quality) entry is highlighted and is an active link in the database. The primary entry has an I/Ic of 3.61 and is an “S” quality entry.

# Application Examples

- Using ICDD's Slevé and Slevé+ programs, materials are identified, peak intensities of each phase are calculated and  $I/I_c$  values are displayed – allowing the user to calculate concentrations by the RIR method.
- Many software distributors have RIR calculation modules, which can perform multiple, simultaneous calculations for complex mixtures, use integrated intensities and correct for absorption – all in a matter of seconds!

Examples are shown for the above.

# Sleve+

Input experimental data.

GOM	PDF #	Compound Name ▲	Chemical Formula	D1	D2	D3	D4	D5	D6	D7	D8
1254	04-007-6692	Cerium Titanium Oxide	Ce <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub>	2.976300	2.982970	4.186270	3.215220	2.699360	2.757500	2.707670	2.777650
624	01-071-7093	Cerium Yttrium	(Ce <sub>0.98</sub> Y <sub>0.02</sub> )	2.979130	2.580000	1.555800	1.824340	1.183790	1.153810	1.489560	0.872199
662	04-006-7962	Cerium Zirconium Oxide	Ce <sub>0.15</sub> Zr <sub>0.85</sub> O <sub>2</sub>	2.983250	1.832240	1.551350	1.816240	2.568560	1.571400	2.614390	1.188360
768	04-006-7961	Cerium Zirconium Oxide	Ce <sub>0.12</sub> Zr <sub>0.88</sub> O <sub>2</sub>	2.980390	1.830300	1.550080	1.814850	2.566590	1.569450	2.610850	1.187120
580	04-006-7959	Cerium Zirconium Oxide	Ce <sub>0.1</sub> Zr <sub>0.9</sub> O <sub>2</sub>	2.978710	1.828770	1.549810	1.814800	2.566510	1.567310	2.606500	1.186180
542	01-071-3203	Cesium Ammine Phosphide	(Cs <sub>3</sub> P <sub>11</sub> ) (N H <sub>3</sub> ) <sub>3</sub>	2.989480	8.007960	3.130050	3.366560	4.097300	4.639240	4.156330	3.538360
1223	04-009-5795	Cesium Antimony Iodide	Cs <sub>3</sub> Sb <sub>2</sub> I <sub>9</sub>	2.983960	3.440150	3.462000	2.105000	2.114990	5.967910	1.798620	1.795530

Experiment

Search Line(s): 2.98220 Å      D1 Range: 2.968 - 2.997 Å      Rotation: 1 of 3

Preferences

Search Window: 0.15 °      Match Window: 0.15 °

Search Method: Hanawalt      Lowest Allowable GOM: 500

Wavelength: Cu Kα1 1.54056 Å

Phases (2)

# ▲	Accepted	PDF #	Compound Name	Int. Ratio	Int. %	I/Ic	Time
1	<input checked="" type="checkbox"/>	01-089-1487	Magnesium Aluminum Silicate	1.11	78	1.41	47.6s
2	<input type="checkbox"/>	04-006-7962	Cerium Zirconium Oxide	0.311	22	10.88	68.3s

Two phase identification in the analysis of an unknown.

Lines (14 of 20)

Ex d(Å) ▼	Ex I	P1 d(Å)	P1 I	P2 d(Å)	P2 I
11.30794	2				
8.44311	100	8.438780	100		
5.16004	9				
4.90437	15	4.904160	18		
4.85981	8	4.856350	9		
4.66904	11	4.665900	9		
4.08603	38	4.083300	38		
3.52993	6				
3.43370	6				
3.38019	27	3.380380	26		
3.34271	5				
3.14912	13	3.146490	14		
3.13282	33	3.129540	35		
3.09371	4				
3.03184	39	3.029500	26		
3.01178	40	3.010620	23		
2.98220	29			2.983250	100
2.64354	11	2.640670	11		
2.33576	5	2.332950	7		
1.83616	12	1.838080	1	1.832240	32

$$\frac{I_a}{I_b} = \frac{\left(\frac{I}{I_c}\right)_a X_a}{\left(\frac{I}{I_c}\right)_b X_b}$$

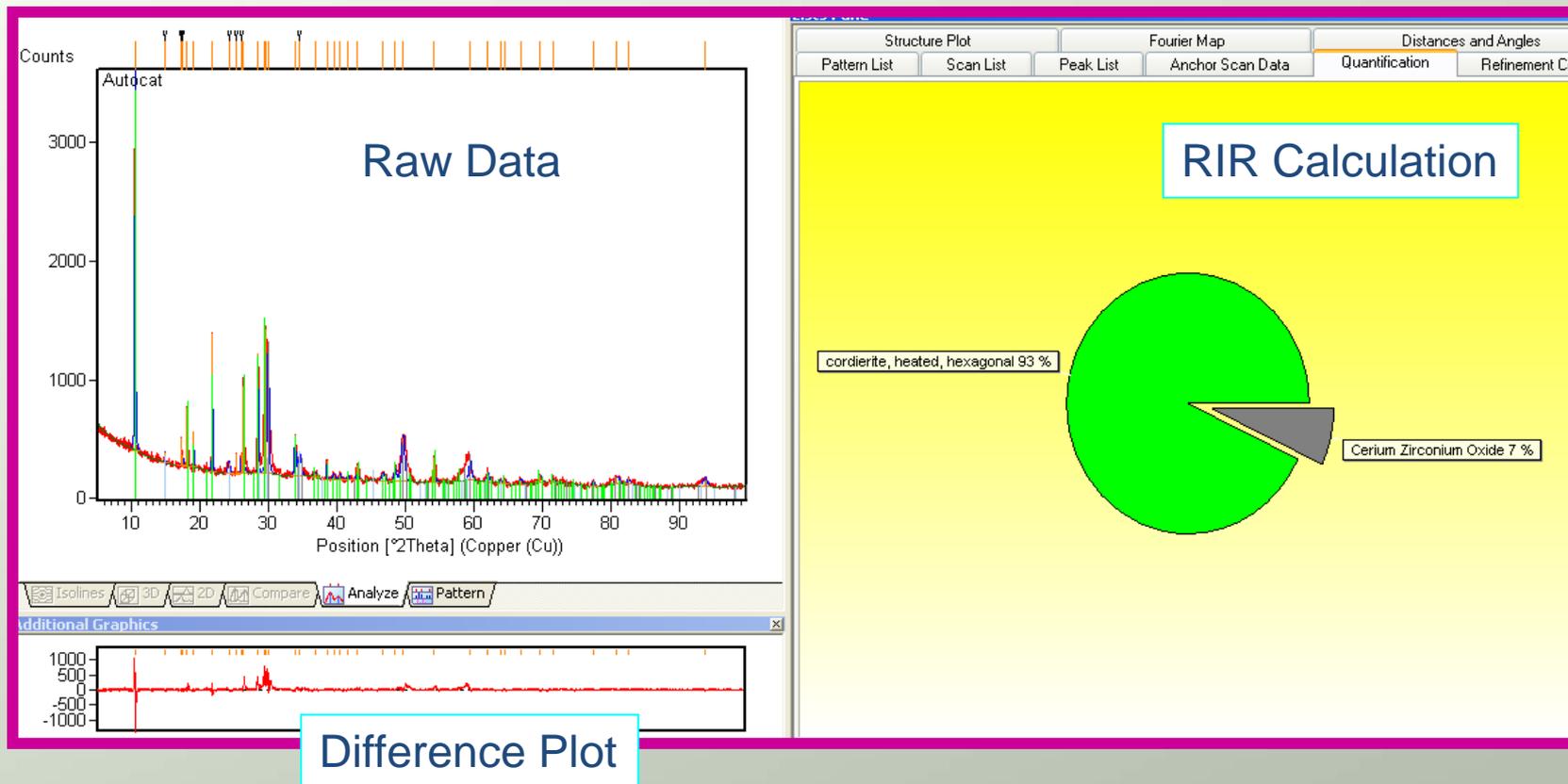
Results summary

Compound Name	Int. Ratio	Int. %	I/Ic
Magnesium Aluminum Silicate	1.11	78	1.41
Cerium Zirconium Oxide	0.311	22	10.88

This results in 96% magnesium aluminum silicate and 4% cerium zirconium oxide and uses peak intensities.

# Automated RIR Analysis

## Vendor Software – Same Example



This software calculated 92% magnesium aluminum silicate and 7% cerium zirconium oxide using integrated intensities.



Thank you for viewing our tutorial.  
Additional tutorials are available at the ICDD website  
([www.icdd.com](http://www.icdd.com)).

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