NON-AMBIENT DATA CALCULATING THERMAL EXPANSION

A REVIEW OF CAPABILITIES

INTRODUCTION

The purpose of this PowerPoint presentation is to demonstrate how to calculate thermal expansion and thermal expansion coefficients using the functions embedded in the Powder Diffraction File.

There are two advantages to using this method versus conventional methods

1) The user can combine data from several different authors and publications, including single point temperature measurements, and combine them in a temperature series

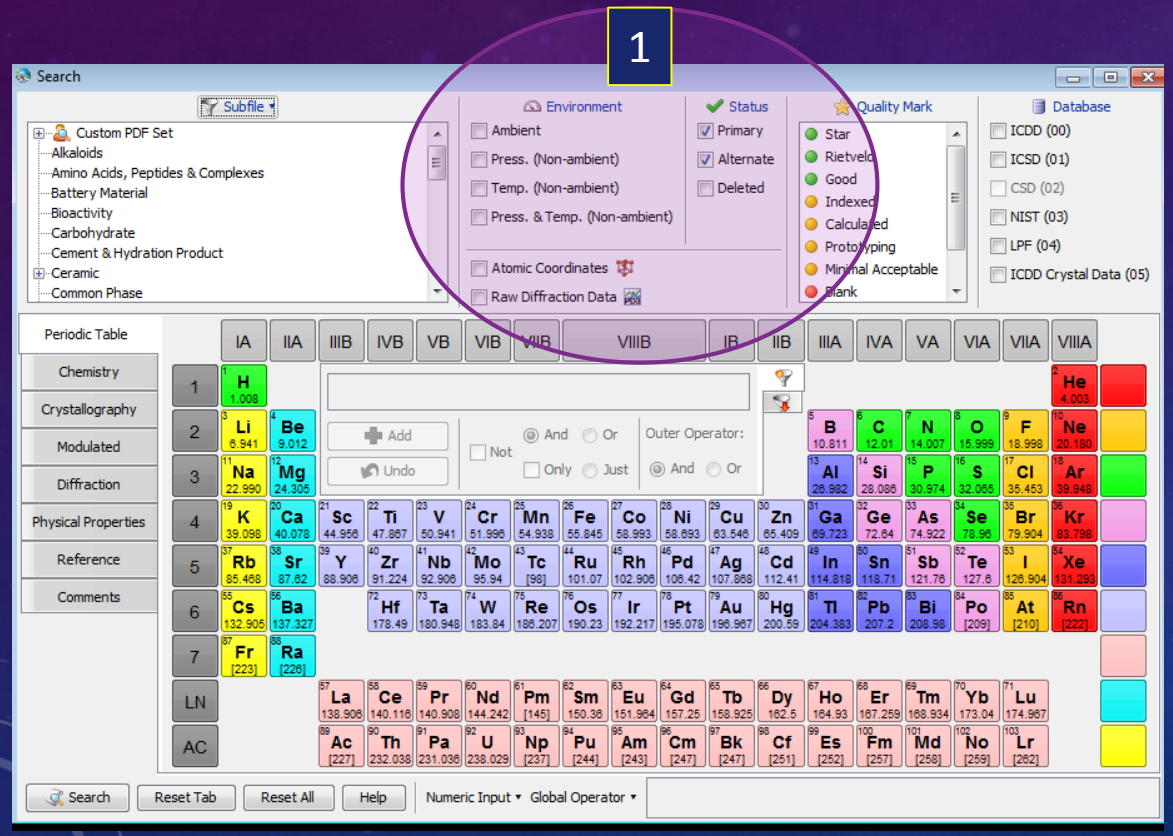
2) The user can incorporate the quality review analysis performed by the ICDD to select the most precise and accurate data for the analysis.

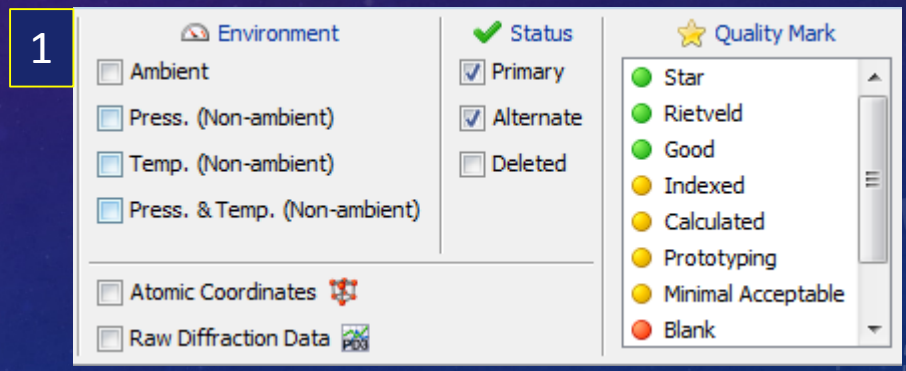
For both points 1 & 2 the ICDD has created software and index tables to facilitate the measurements. There are temperature series for over 10,000 materials in the PDF-4+ database. The software and index tables are incorporated into all PDF-2 and PDF-4+ products. The software features and applications shown in this presentation were developed in Releases 2013 through 2015.

For future releases we are working on pressure series.

FIRST STEP. USE THE SEARCH MENU FROM THE PDF-4 DATABASE TO SELECT MATERIALS

Ambient is defined as data taken within a range of room temperature. At the ICDD we define ambient as 290 – 310 Kelvin. Non-ambient can be temperatures above or below this range.



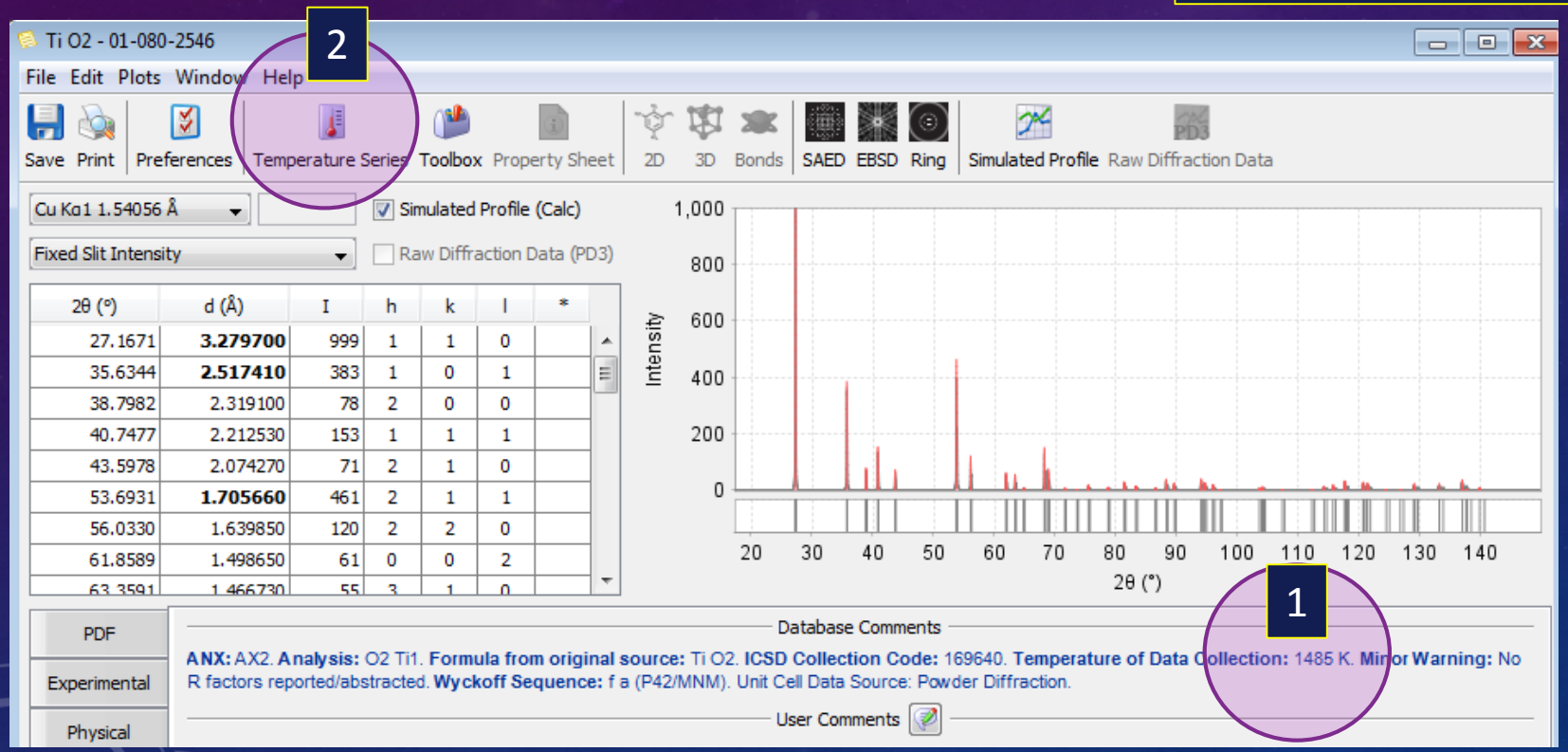


The “Environment selection allow the user to choose either pressure data, temperature data or pressure *and* temperature data. The user can also select materials based on their quality evaluation (i.e. Quality Mark)

NON-AMBIENT DATA

Entries that are non-ambient always have the temperature or pressure specified in the editor comment section of a data entry. 1

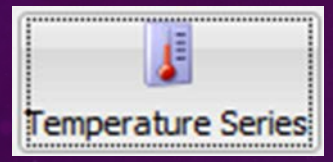
ICDD editors have flagged identical compounds contained in a temperature series. *If* an entry is part of A temperature series the “Temperature Series” icon will be activated. Activated icons are in bold colors. 2



1 Temperature of Data Collection

2 Part of a Temperature Series (3 entries at 3 temperatures)

Select



Temp (K)	PDF #	QM	Chemical Fo...	Compound Name	RedCell Vol (Å³)	Author - PR	Journal - PR	Year - PR	Dcalc (g/cm³)	Dstruc (g/cm³)
15.0	01-084-1284	S	Ti O2	Titanium Oxide	62.15	Burdett, J.K., Hughbanks, T., Miller, ...	J. Am. Chem. Soc.	1987	4.27	4.27
100.0	04-004-4337	S	Ti O2	Titanium Oxide	62.00	Restori R., Schwarzenbach D., Sch...	Acta Crystallogr., Sec. B: Struct. Sci.	1987	4.28	4.28
273.0	04-002-9135	P	Ti O2	Titanium Oxide	62.38	Siratori K., Iida S.	J. Phys. Soc. Jpn.	1962	4.254	4.25
293.0	04-006-2653	P	Ti O2	Titanium Oxide	62.42	Shannon R.D.	J. Appl. Phys.	1964	4.251	4.25
293.0	04-006-2654	P	Ti O2	Titanium Oxide	62.42	Shannon R.D.	J. Appl. Phys.	1964	4.251	4.25
295.0	01-084-1283	S	Ti O2	Titanium Oxide	62.42	Burdett, J.K., Hughbanks, T., Miller, ...	J. Am. Chem. Soc.	1987	4.251	4.25
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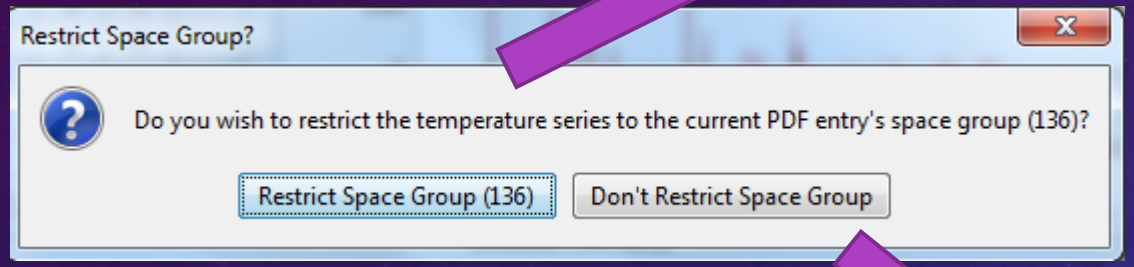
296.0	01-080-2528	I	Ti O2	Titanium Oxide	62.37	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.254	4.25
298.0	00-001-1292	B	Ti O2	Titanium Oxide	61.88	Hanawalt, J., et al.	Anal. Chem.	1938	4.288	
298.0	00-002-0494	O	Ti O2	Titanium Oxide	61.88	Kerr.	Econ. Geol.	1932	4.288	
298.0	01-072-7374	S	Ti O2	Titanium Oxide	63.78	Theisinger, H., Baier, M., Brummer, ...	Am. Mineral.	2003	4.161	4.16
298.0	01-071-4809	I	Ti O2	Titanium Oxide	60.13	Vegard, L.	Philos. Mag.	1916	4.413	4.41
298.0	04-016-0561	B	Ti O2	Titanium Oxide	62.30	Greenwood G.	Philos. Mag.	1924	4.259	4.26
298.0	04-014-1641	H	Ti O2	Titanium Oxide	64.00	Le Bacq O., Salinas E., Pisch A., Be...	Philos. Mag.	2006	4.146	4.15
298.0	01-076-1938	S	Ti O2	Titanium Oxide	62.42	Meagher, E.P., Lager, G.A.	Can. Mineral.	1979	4.251	4.25
298.0	04-015-7316	B	Ti O2	Titanium Oxide	62.73	Rasmussen S.E.	Powder Diffr.	2003	4.23	4.23
298.0	04-006-2536	P	Ti O2	Titanium Oxide	61.88	Bond W.L.	J. Appl. Phys.	1965	4.288	4.29
298.0	04-006-3570	P	Ti O2	Titanium Oxide	62.46	Armenise M.N., Canall C., De Sario ...	J. Appl. Phys.	1983	4.249	4.25
298.0	04-005-4625	I	Ti O2	Titanium Oxide	62.43	Abrahams S.C., Bernstein J.L.	J. Chem. Phys.	1971	4.25	4.25
298.0	04-005-4857	I	Ti O2	Titanium Oxide	62.45	Gonschorek W.	Z. Kristallogr.	1982	4.249	4.25
298.0	04-005-4858	I	Ti O2	Titanium Oxide	62.46	Gonschorek W., Feld R.	Z. Kristallogr.	1982	4.248	4.25
298.0	04-005-4859	I	Ti O2	Titanium Oxide	62.45	Gonschorek W., Feld R.	Z. Kristallogr.			4.25

170 Entries



2

Once the space group is selected a listing of all entries In the series will be shown to the user

275 Entries

Temperature Series (Ti O2 - 01-080-2546)

File Edit Fields Similarity Index Help

Preferences | Open PDF Card | Simulated Profile

Temp (K)	PDF #	QM	Chemical Fo...	Compound Name	RedCell Vol (Å³)	Author - PR	Journal - PR	Year - PR	Dcalc (g/cm³)	Dstruc (g/cm³)
15.0	01-084-1284	S	Ti O2	Titanium Oxide	62.15	Burdett, J.K., Hughbanks, T., Miller, ...	J. Am. Chem. Soc.	1987	4.27	4.27
15.0	01-084-1286	B	Ti O2	Titanium Oxide	67.96	Burdett, J.K., Hughbanks, T., Miller, ...	J. Am. Chem. Soc.	1987	3.904	3.9
100.0	04-004-4337	S	Ti O2	Titanium Oxide	62.00	Restori R., Schwarzenbach D., Sch...	Acta Crystallogr., Sec. B: Struct. Sci.	1987	4.28	4.28
133.0	04-014-5365	S	Ti O2	Titanium Oxide	122.16	Filatov S.K., Bendeliani N.A., Albert ...	Dokl. Phys.	2007	4.344	4.34
223.0	04-014-5354	S	Ti O2	Titanium Oxide	122.20	Filatov S.K., Bendeliani N.A., Albert ...	Dokl. Phys.	2007	4.343	4.34
273.0	04-002-9135	P	Ti O2	Titanium Oxide	62.38	Siratori K., Iida S.	J. Phys. Soc. Jpn.	1962	4.254	4.25
290.0	04-007-6246	B	Ti O2	Titanium Oxide	142.11	Feist T.P., Davies P.K.	J. Solid State Chem.	1992	3.734	3.73
290.15	03-065-6429	I	Ti O2	Titanium Oxide	284.23	Feist, T. P., Davies, P. K.	J. Solid State Chem.	1992	1.867	1.87
293.0	04-014-5353	S	Ti O2	Titanium Oxide	121.95	Filatov S.K., Bendeliani N.A., Albert ...	Dokl. Phys.	2007	4.352	4.35
293.0	04-006-2653	P	Ti O2	Titanium Oxide	62.42	Shannon R.D.	J. Appl. Phys.	1964	4.251	4.25
293.0	04-006-2654	P	Ti O2	Titanium Oxide	62.42	Shannon R.D.	J. Appl. Phys.	1964	4.251	4.25
293.0	04-012-6345	I	Ti O2	Titanium Oxide	104.20	Swamy V., Dubrovinsky L.S., Dubro...	Solid State Commun.	2005	5.093	5.09
293.0	04-012-6346	I	Ti O2	Titanium Oxide	100.60	Swamy V., Dubrovinsky L.S., Dubro...	Solid State Commun.	2005	5.275	5.27
293.0	04-007-6487	I	Ti O2	Titanium Oxide	137.19	Akimoto J., Gotoh Y., Oosawa Y., N...	J. Solid State Chem.	1994	3.868	3.87
293.0	04-007-6488	P	Ti O2	Titanium Oxide	266.66	Akimoto J., Gotoh Y., Oosawa Y., N...	J. Solid State Chem.	1994	4.135	4.13
293.0	04-014-5762	S	Ti O2	Titanium Oxide	68.13	Leinekugel Le Cocq Errien A.Y., De...	J. Solid State Chem.	2007	3.895	3.89
293.0	04-014-5764	S	Ti O2	Titanium Oxide	68.14	Leinekugel Le Cocq Errien A.Y., De...	J. Solid State Chem.	2007	3.894	3.89
295.0	01-070-3463	I	(Ti , Cr , Fe ,...	Titanium Chromium Iron ...	708.51	Wang, L.-P., Rouse, R.C., Essene, ...	Am. Mineral.	2000		4.11
295.0	01-084-1283	S	Ti O2	Titanium Oxide	62.42	Burdett, J.K., Hughbanks, T., Miller, ...	J. Am. Chem. Soc.	1987	4.251	4.25
295.0	01-084-1285	S	Ti O2	Titanium Oxide	68.13	Burdett, J.K., Hughbanks, T., Miller, ...	J. Am. Chem. Soc.	1987	3.895	3.89
295.0	01-081-9508	I	Ti O2	Titanium Oxide	552.50	Mamiya, M., Kataoka, K., Kikuchi, S....	J. Phys. Chem. Solids	2012	3.842	3.84
295.0	04-004-4338	S	Ti O2	Titanium Oxide	62.38	Restori R., Schwarzenbach D., Sch...	Acta Crystallogr., Sec. B: Struct. Sci.	1987	4.254	4.25
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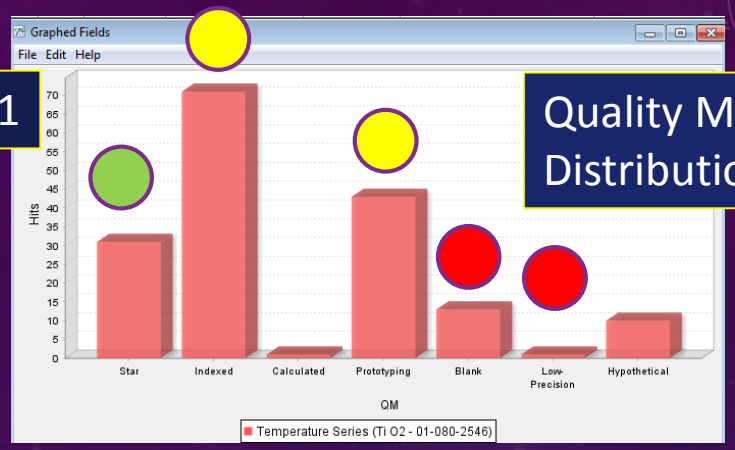
298.0	00-033-1381	I	Ti O2	Titanium Oxide	418.53	Liu, L.	Science	1978	5.072	
298.0	04-007-3644	P	Ti O2	Titanium Oxide	104.87	Sato H., Endo S., Sugiyama M., Kike...	Science	1991	5.061	5.06
298.0	00-048-1278	B	Ti O2	Titanium Oxide	104.87	Sato, H., Endo, S., Sugiyama, M., Ki...	Science	1991	5.061	

1

Selection of the icon will then ask the user if they want to restrict the space group. In this particular case we are looking at TiO_2 Restriction of the space group limits the series to the mineral rutile. Unrestricted space groups would include the TiO_2 polymorphic minerals - rutile, anatase, brookite and akaogiite.

1



Quality Mark Distribution

1

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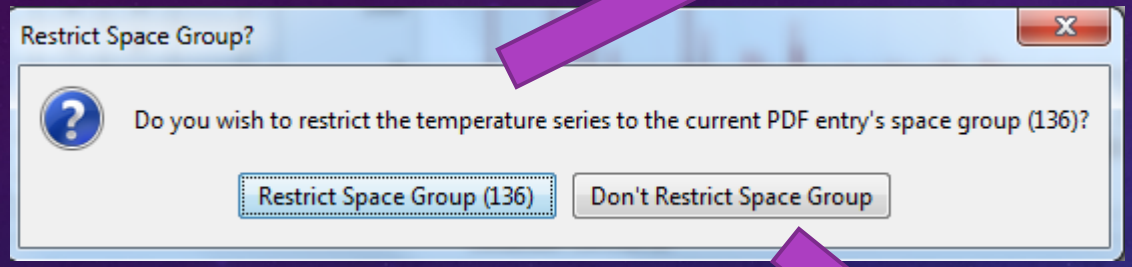
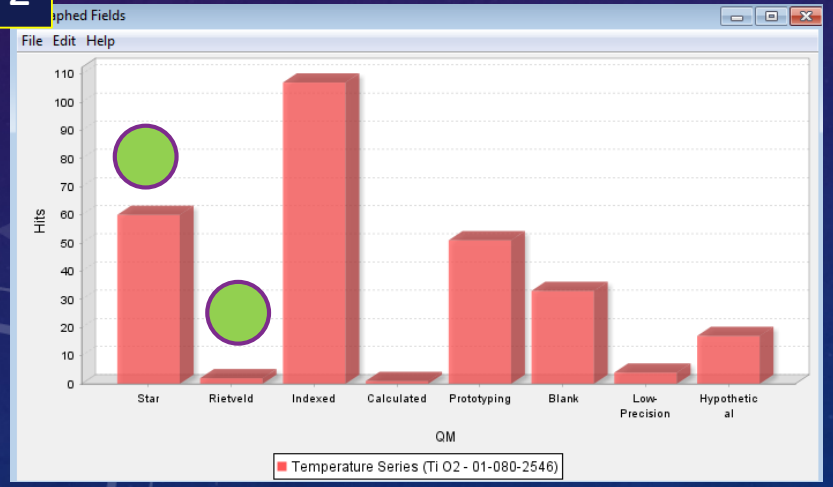


Once the entries are tabulated in a preference data any column can be plotted. For example, 1 and 2 show the table and quality distributions plotted for each collection.

2



2

Temperature Series (Ti O2 - 01-080-2546)

Edit Fields Similarity Index Help

References | Open PDF Card | Simulated Profile

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100.0	04-004-4337	S	Ti O2	Titanium Oxide	62.00	Restori R., Schwarzenbach D., Sch...	Acta Crystallogr., Sec. B: Struct. Sci.	1987	4.28	4.28
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293.0	04-014-5764	S	Ti O2	Titanium Oxide	68.14	Leinekugel Le Cocq Errien A.Y., De...	J. Solid State Chem.	2007	3.894	3.89
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298.0	04-048-1278	B	Ti O2	Titanium Oxide	104.87	Sato, H., Endo, S., Sugiyama, M., Ki...	Science	1991	5.061	

275 Entries

PDF DATABASES

ICDD databases contain a substantial amount of non-ambient data. New data are added every year from the world literature sources. New temperature data series are added each year.

Release 2015: PDF-4+

- 327,085 Ambient
- 5,491 Pressure Data
- 32,566 Temperature Data
  - **>300 K** **11,785 Entries**
  - 280 K < 20,569 Entries

Release 2016: PDF-4/Organics

- 312,068 Ambient
- 1,096 Pressure Data
- 188,581 Temperature Data
  - >300 K 2,519
  - **280 K <** **185,531**

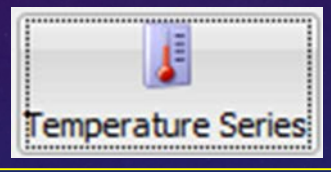
DATA MINING

Compound Name
(Common, Mineral, Zeolite)

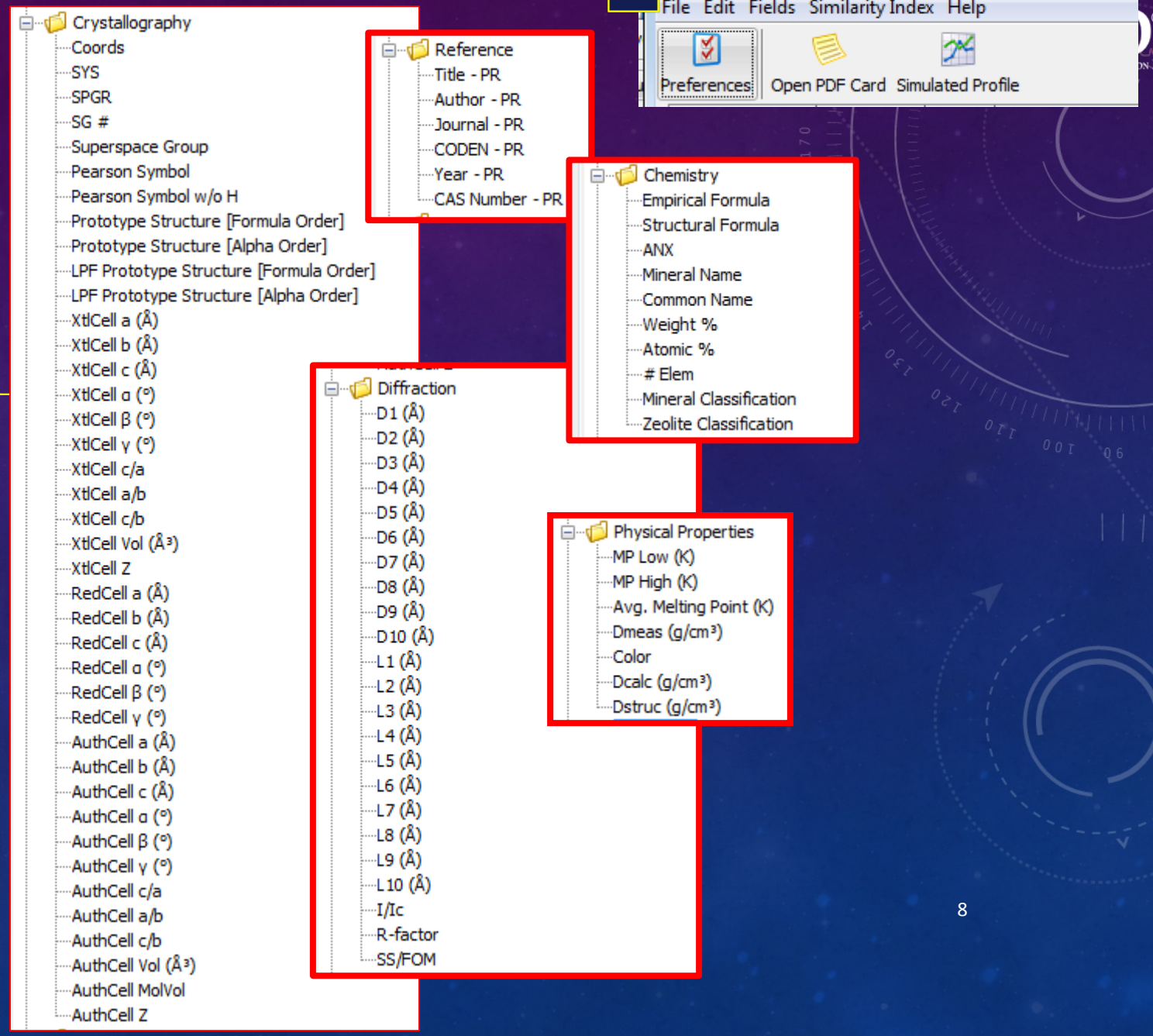
Temperature of Data Collection

Quality Mark

Space Group



Once the temperature series icon is selected
A table will be presented to the user. The user has already selected a material and the space group. By using the Preferences icon at the top of the temperature series display 1 the user can select a large number of data types that they wish to display in a temperature series table.



PREFERENCE TABLE

With PDF-4+ the user has a choice of 116 display fields, for PDF-2 the user has a choice of 48 display fields, and for PDF/Organics the user has a choice of 95 display fields. Which fields should you select ?

Formula and Space Group

To have a measurement of thermal volume expansion, the user should limit themselves to a single material. This is usually done by selecting a specific chemical formula and space group. The space group typically, *but not always*, separates out polymorphic forms (materials of different structure, same formula). To be safe the user may also want to check common and mineral names for polymorphism, where the materials would have different names or designations.

Reduced Cell Volume, Temperature

To calculate a thermal volume expansion a volumetric measurement is required as a function of temperature.
We prefer reduced cell volumes since they are standardized, but crystal cell volumes and author cell volumes can also be user selected. If the user wants to check thermal anisotropy (different expansion in different directions) then they can select a unit cell edge (9 choices – 3 axes for 3 systems) , or a specific indexed d-spacing (20 choices). Temperatures are available in Fahrenheit, Celsius or Kelvin.

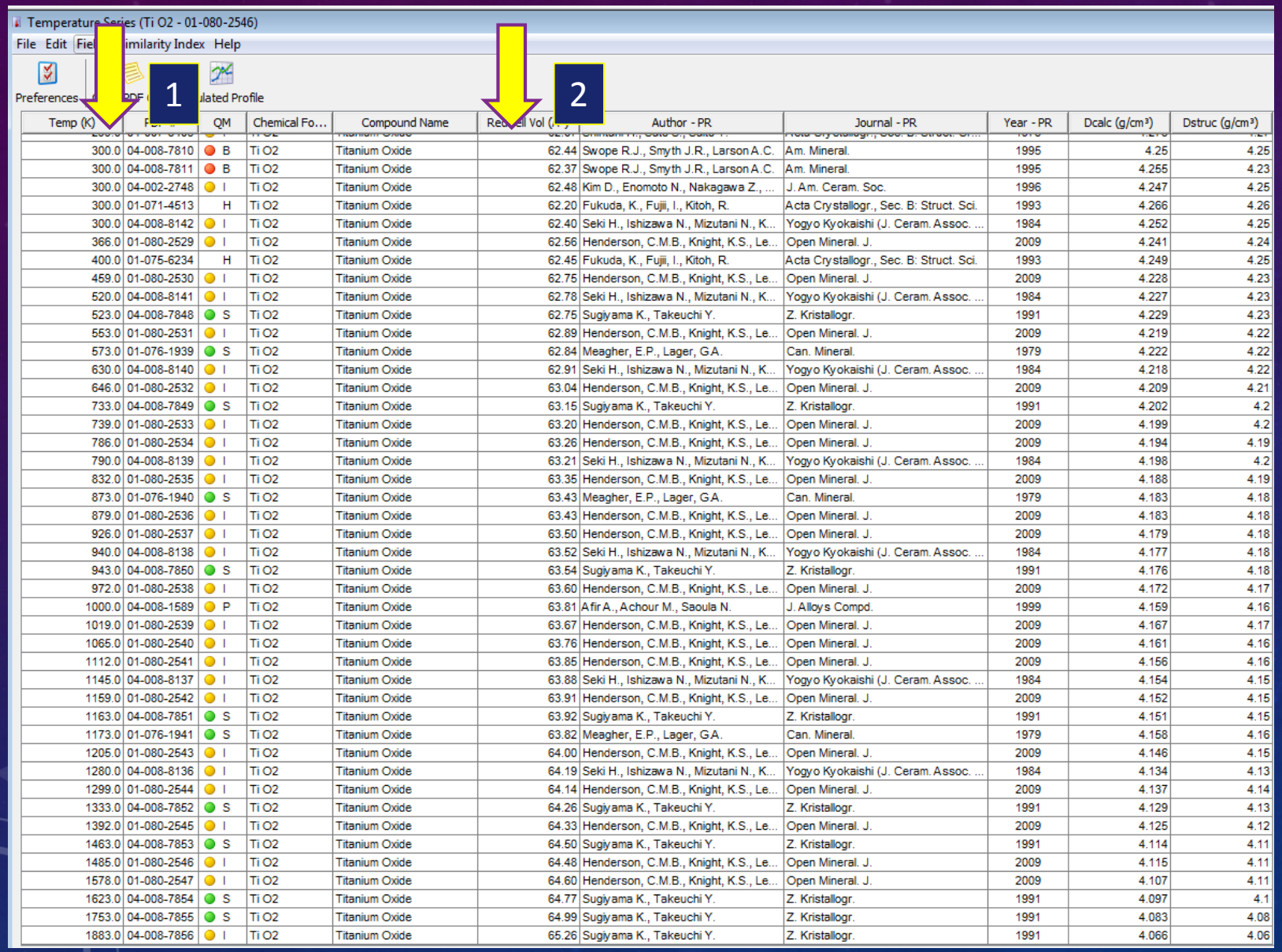
Quality Mark

The ICDD editors perform over 100 quality checks and summarize the output in the quality mark. The highest quality marks are also coded green. The user may want to delete low quality data and/or hypothetical data from an analysis. Older data typically have lower quality marks since the available equipment were not as precise and international calibration standards were not commonly available before the 1980's.

Author and Reference

Selection of author and reference lets the user know how many publications are used in the analysis and which data entries are associated with the same series of measurements.

PREFERENCES TABLE FOR TEMPERATURE SERIES



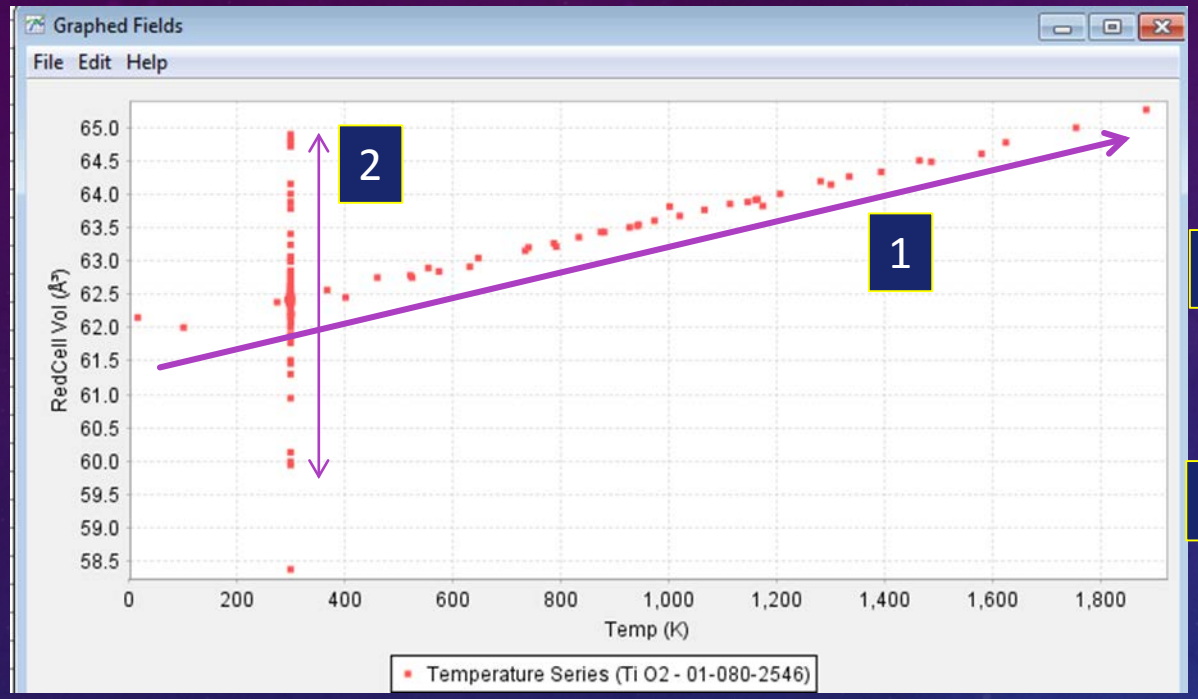
Temp (K)	Fi	QM	Chemical Fo...	Compound Name	Red ell Vol (A	Author - PR	Journal - PR	Year - PR	Dcalc (g/cm³)	Dstruc (g/cm³)
300.0	04-008-7810	B	Ti O2	Titanium Oxide	62.44	Swope R.J., Smyth J.R., Larson A.C.	Am. Mineral.	1995	4.25	4.25
300.0	04-008-7811	B	Ti O2	Titanium Oxide	62.37	Swope R.J., Smyth J.R., Larson A.C.	Am. Mineral.	1995	4.255	4.23
300.0	04-002-2748	I	Ti O2	Titanium Oxide	62.48	Kim D., Enomoto N., Nakagawa Z., ...	J. Am. Ceram. Soc.	1996	4.247	4.25
300.0	01-071-4513	H	Ti O2	Titanium Oxide	62.20	Fukuda, K., Fujii, I., Kitoh, R.	Acta Crystallogr., Sec. B: Struct. Sci.	1993	4.266	4.26
300.0	04-008-8142	I	Ti O2	Titanium Oxide	62.40	Seki H., Ishizawa N., Mizutani N., K...	Yogyo Kyokaishi (J. Ceram. Assoc. ...	1984	4.252	4.25
366.0	01-080-2529	I	Ti O2	Titanium Oxide	62.56	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.241	4.24
400.0	01-075-6234	H	Ti O2	Titanium Oxide	62.45	Fukuda, K., Fujii, I., Kitoh, R.	Acta Crystallogr., Sec. B: Struct. Sci.	1993	4.249	4.25
459.0	01-080-2530	I	Ti O2	Titanium Oxide	62.75	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.228	4.23
520.0	04-008-8141	I	Ti O2	Titanium Oxide	62.78	Seki H., Ishizawa N., Mizutani N., K...	Yogyo Kyokaishi (J. Ceram. Assoc. ...	1984	4.227	4.23
523.0	04-008-7848	S	Ti O2	Titanium Oxide	62.75	Sugiyama K., Takeuchi Y.	Z. Kristallogr.	1991	4.229	4.23
553.0	01-080-2531	I	Ti O2	Titanium Oxide	62.89	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.219	4.22
573.0	01-076-1939	S	Ti O2	Titanium Oxide	62.84	Meagher, E.P., Lager, G.A.	Can. Mineral.	1979	4.222	4.22
630.0	04-008-8140	I	Ti O2	Titanium Oxide	62.91	Seki H., Ishizawa N., Mizutani N., K...	Yogyo Kyokaishi (J. Ceram. Assoc. ...	1984	4.218	4.22
646.0	01-080-2532	I	Ti O2	Titanium Oxide	63.04	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.209	4.21
733.0	04-008-7849	S	Ti O2	Titanium Oxide	63.15	Sugiyama K., Takeuchi Y.	Z. Kristallogr.	1991	4.202	4.2
739.0	01-080-2533	I	Ti O2	Titanium Oxide	63.20	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.199	4.2
786.0	01-080-2534	I	Ti O2	Titanium Oxide	63.26	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.194	4.19
790.0	04-008-8139	I	Ti O2	Titanium Oxide	63.21	Seki H., Ishizawa N., Mizutani N., K...	Yogyo Kyokaishi (J. Ceram. Assoc. ...	1984	4.198	4.2
832.0	01-080-2535	I	Ti O2	Titanium Oxide	63.35	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.188	4.19
873.0	01-076-1940	S	Ti O2	Titanium Oxide	63.43	Meagher, E.P., Lager, G.A.	Can. Mineral.	1979	4.183	4.18
879.0	01-080-2536	I	Ti O2	Titanium Oxide	63.43	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.183	4.18
926.0	01-080-2537	I	Ti O2	Titanium Oxide	63.50	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.179	4.18
940.0	04-008-8138	I	Ti O2	Titanium Oxide	63.52	Seki H., Ishizawa N., Mizutani N., K...	Yogyo Kyokaishi (J. Ceram. Assoc. ...	1984	4.177	4.18
943.0	04-008-7850	S	Ti O2	Titanium Oxide	63.54	Sugiyama K., Takeuchi Y.	Z. Kristallogr.	1991	4.176	4.18
972.0	01-080-2538	I	Ti O2	Titanium Oxide	63.60	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.172	4.17
1000.0	04-008-1589	P	Ti O2	Titanium Oxide	63.81	Afir A., Achour M., Saoula N.	J. Alloys Compd.	1999	4.159	4.16
1019.0	01-080-2539	I	Ti O2	Titanium Oxide	63.67	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.167	4.17
1065.0	01-080-2540	I	Ti O2	Titanium Oxide	63.76	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.161	4.16
1112.0	01-080-2541	I	Ti O2	Titanium Oxide	63.85	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.156	4.16
1145.0	04-008-8137	I	Ti O2	Titanium Oxide	63.88	Seki H., Ishizawa N., Mizutani N., K...	Yogyo Kyokaishi (J. Ceram. Assoc. ...	1984	4.154	4.15
1159.0	01-080-2542	I	Ti O2	Titanium Oxide	63.91	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.152	4.15
1163.0	04-008-7851	S	Ti O2	Titanium Oxide	63.92	Sugiyama K., Takeuchi Y.	Z. Kristallogr.	1991	4.151	4.15
1173.0	01-076-1941	S	Ti O2	Titanium Oxide	63.82	Meagher, E.P., Lager, G.A.	Can. Mineral.	1979	4.158	4.16
1205.0	01-080-2543	I	Ti O2	Titanium Oxide	64.00	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.146	4.15
1280.0	04-008-8136	I	Ti O2	Titanium Oxide	64.19	Seki H., Ishizawa N., Mizutani N., K...	Yogyo Kyokaishi (J. Ceram. Assoc. ...	1984	4.134	4.13
1299.0	01-080-2544	I	Ti O2	Titanium Oxide	64.14	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.137	4.14
1333.0	04-008-7852	S	Ti O2	Titanium Oxide	64.26	Sugiyama K., Takeuchi Y.	Z. Kristallogr.	1991	4.129	4.13
1392.0	01-080-2545	I	Ti O2	Titanium Oxide	64.33	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.125	4.12
1463.0	04-008-7853	S	Ti O2	Titanium Oxide	64.50	Sugiyama K., Takeuchi Y.	Z. Kristallogr.	1991	4.114	4.11
1485.0	01-080-2546	I	Ti O2	Titanium Oxide	64.48	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.115	4.11
1578.0	01-080-2547	I	Ti O2	Titanium Oxide	64.60	Henderson, C.M.B., Knight, K.S., Le...	Open Mineral. J.	2009	4.107	4.11
1623.0	04-008-7854	S	Ti O2	Titanium Oxide	64.77	Sugiyama K., Takeuchi Y.	Z. Kristallogr.	1991	4.097	4.1
1753.0	04-008-7855	S	Ti O2	Titanium Oxide	64.99	Sugiyama K., Takeuchi Y.	Z. Kristallogr.	1991	4.083	4.08
1883.0	04-008-7856	I	Ti O2	Titanium Oxide	65.26	Sugiyama K., Takeuchi Y.	Z. Kristallogr.	1991	4.066	4.06

Rutile
Space Group 136
Temperature of Data Collection
> 300 K

Results
Variable Quality Data
T range 300-1883 K
Publications 1984 to 2009
8 publications

Anything on this form can be plotted.
In this case we plot temperature 1
versus reduced cell volume 2

PLOTS



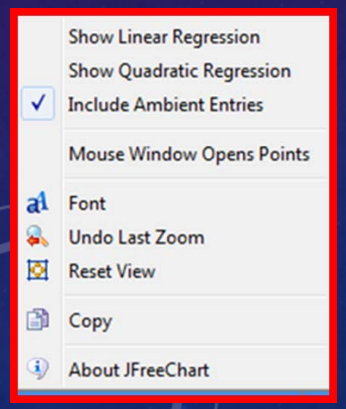
With common materials, such as rutile, there is often a large amount of data because of the engineering applications of the material and this plot can exhibit complex behavior because of multiple variables. In addition the number of ambient determinations may overwhelm non-ambient determinations In this graph there appears to be two groups of data.

1

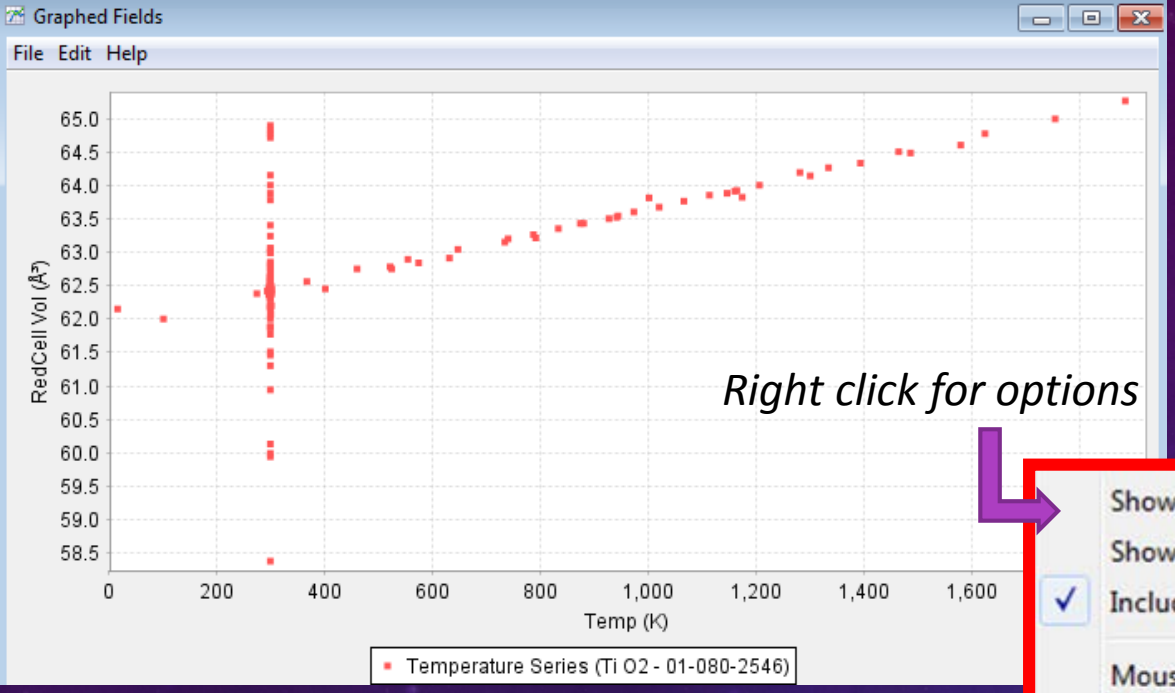
This appear to be the temperature series we are interested in where volume is changing as a function of temperature.

2

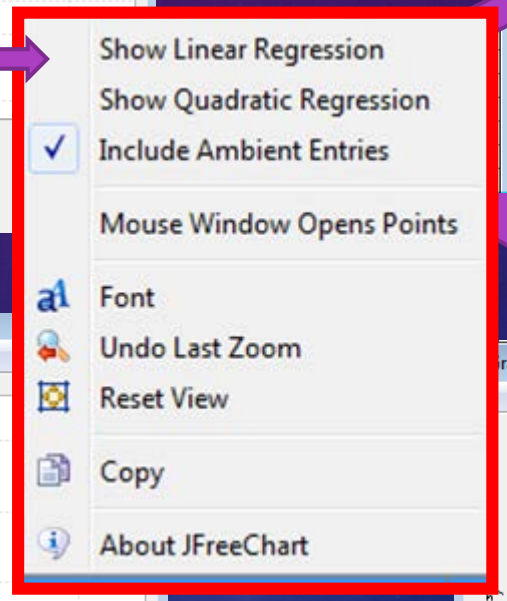
There is a large number of ambient determinations where the volume is changing. By clicking on any point the data entry can be viewed . The Editors comment shows that some of these data are from a pressure series. Additional data points represent samples that were annealed for a long period of time, cooled, and then measured at room temperature.

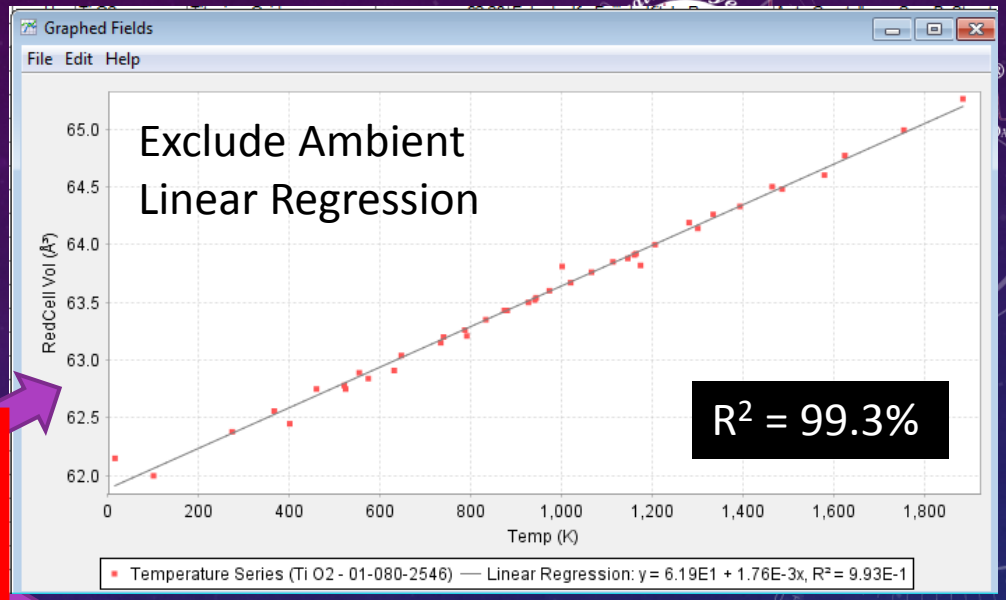


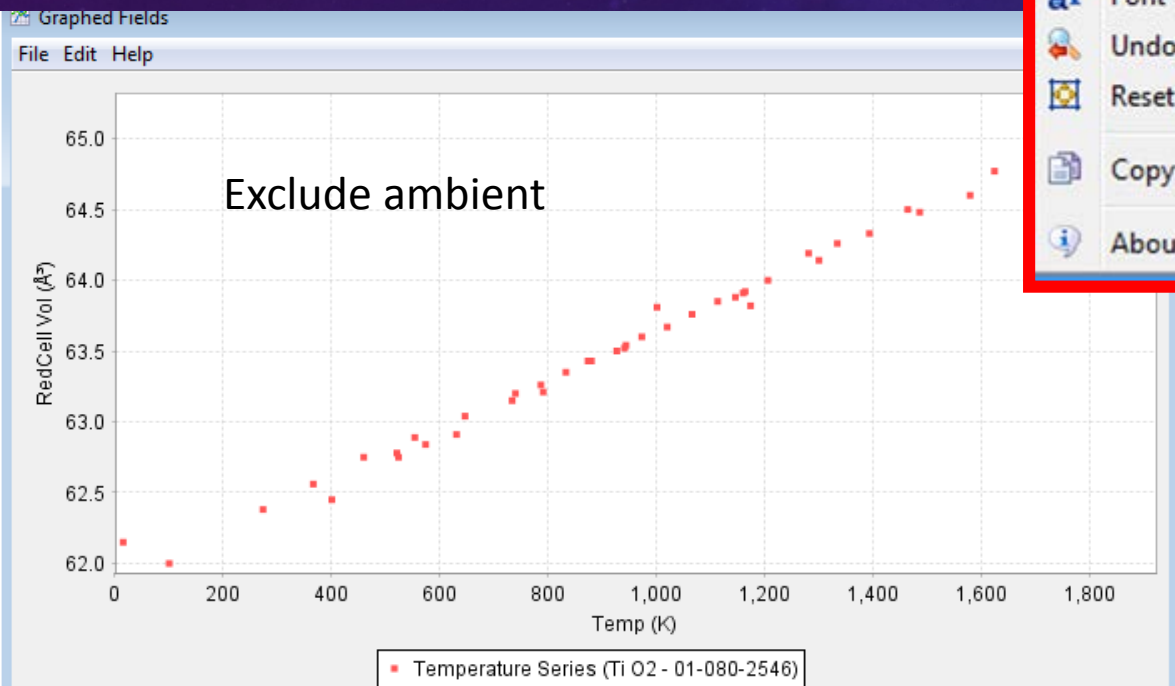
To separate the two groups of data, there is an options menu, activated by a right mouse click on the graph that allows the user to remove or include all ambient data. Individual entries can be Removed by removing rows in the preference table.

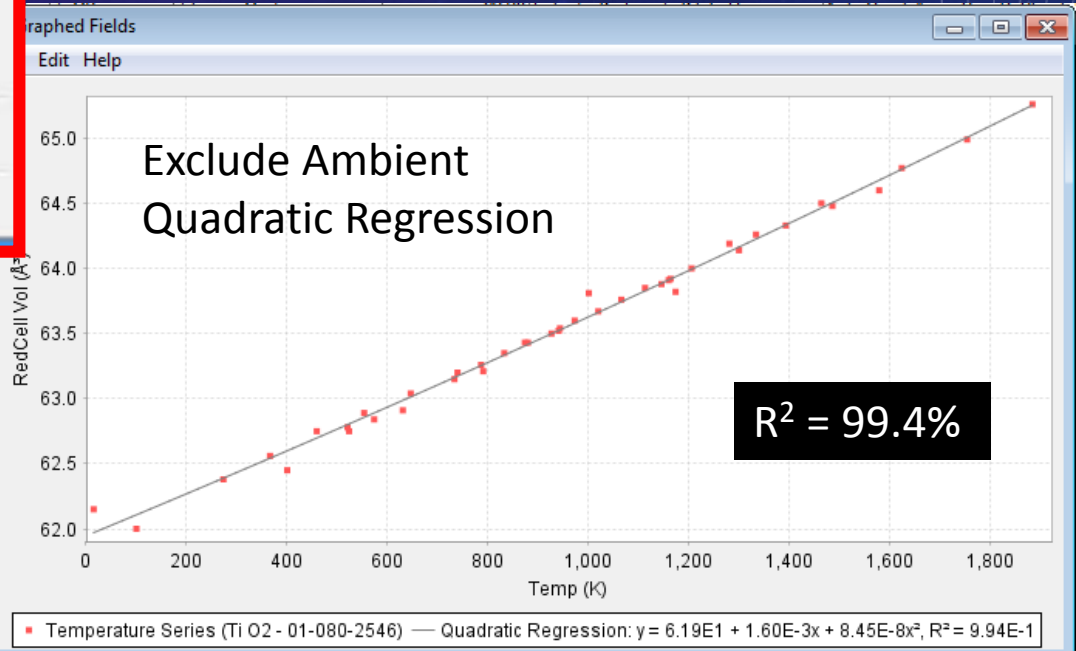


Right click for options









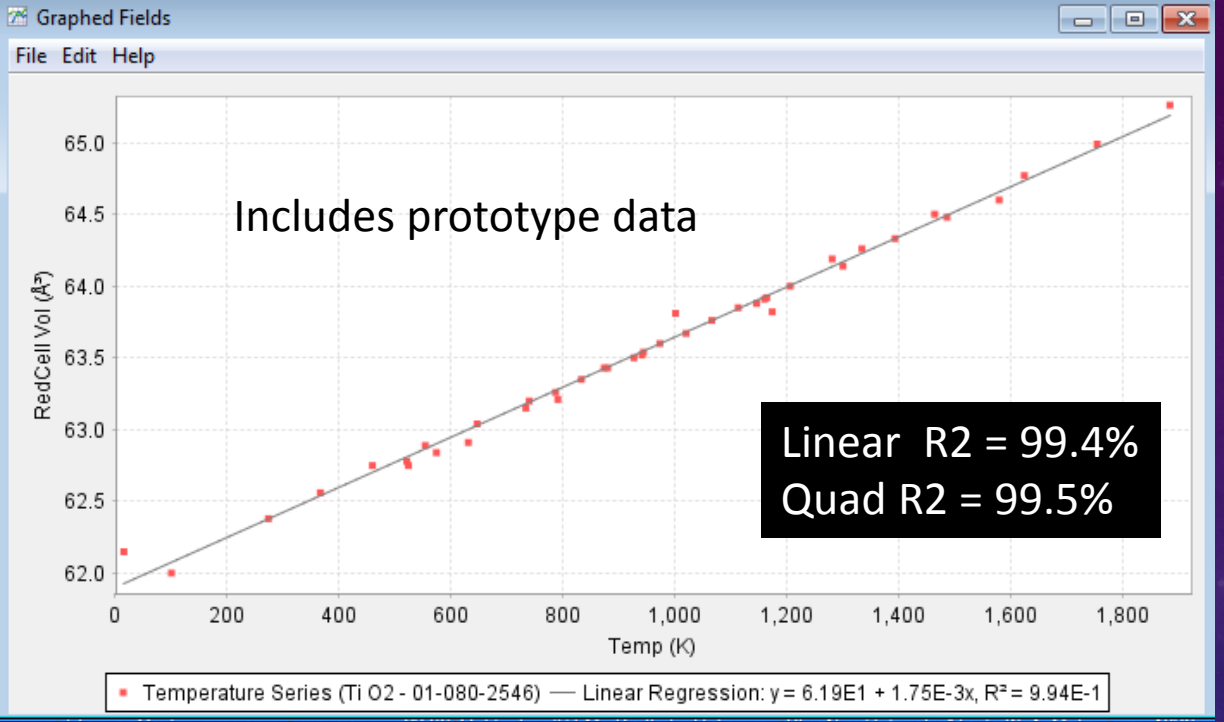
What about poor quality data ?

Sort preferences by quality mark

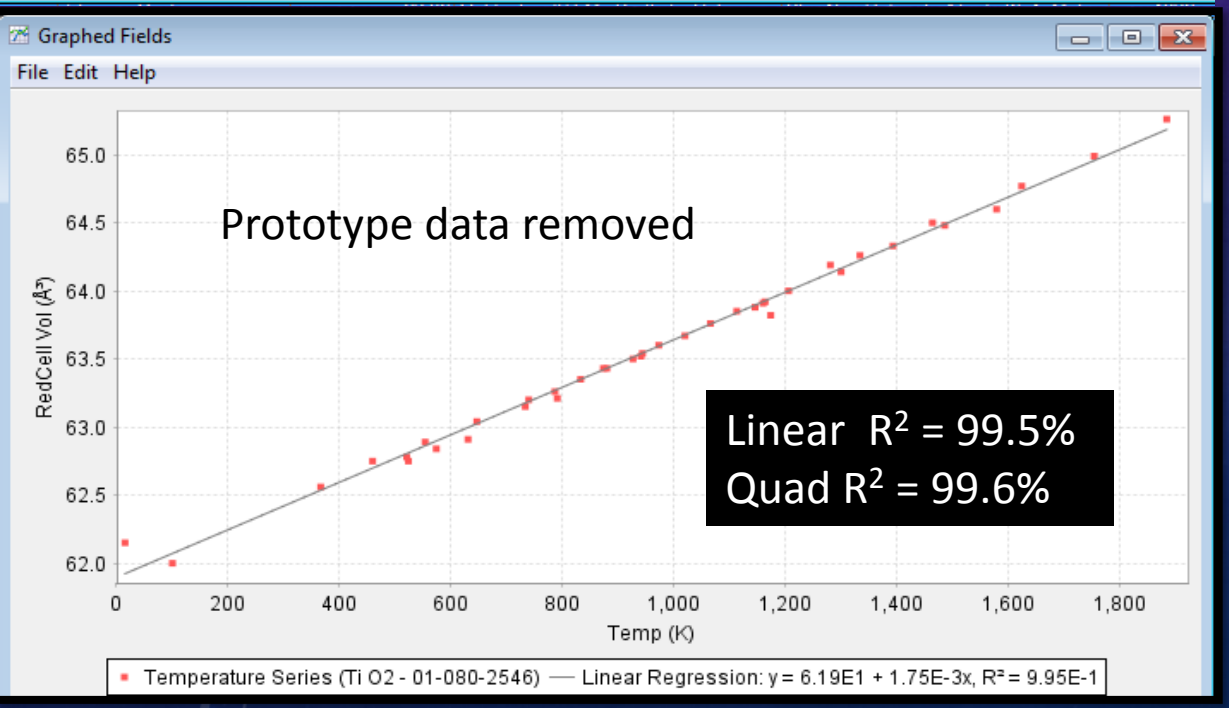
Highlight only high quality data

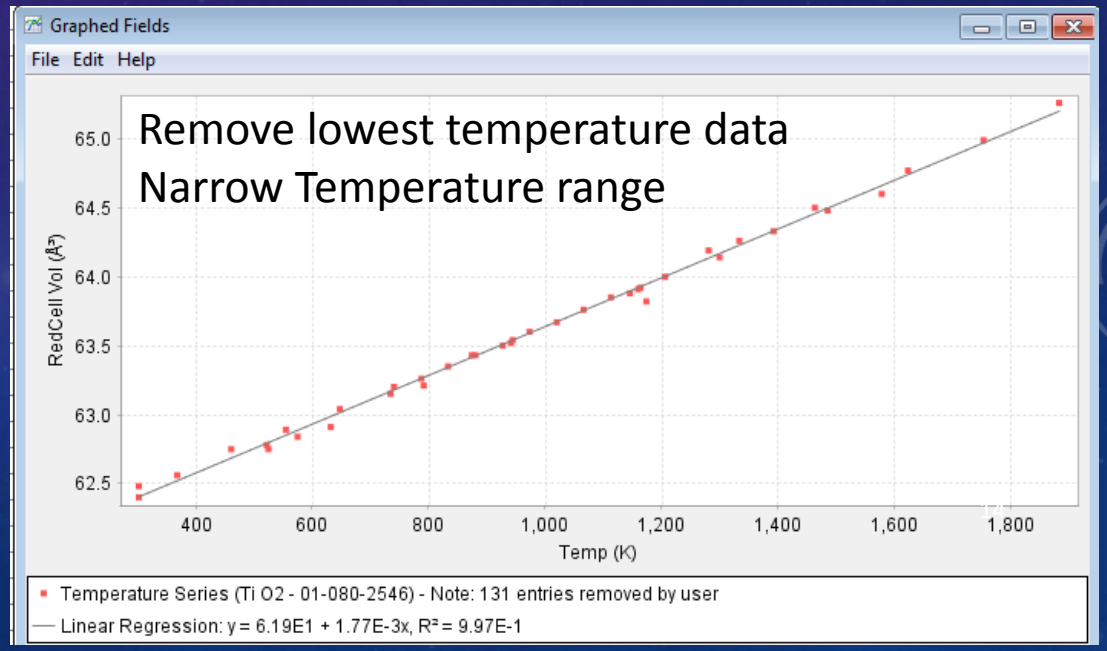
Use menu to remove ambient entries

Graph temperature vs reduced cell volume

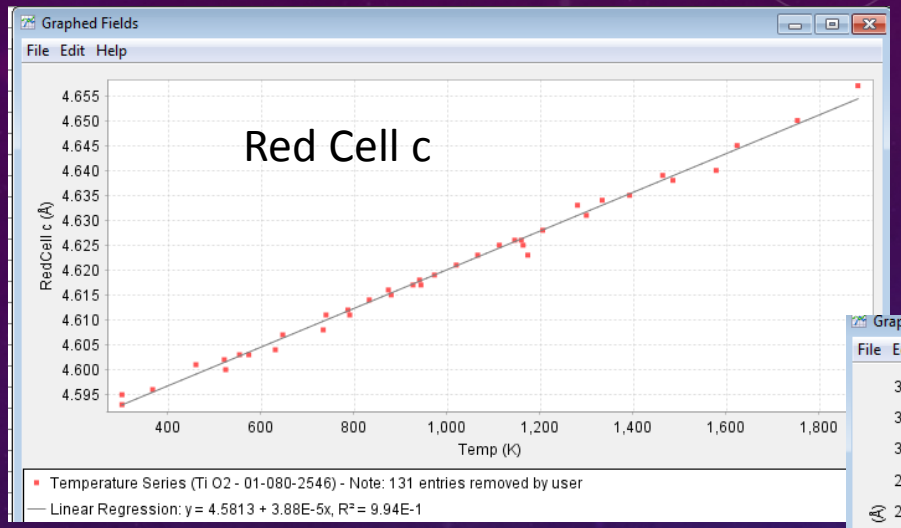


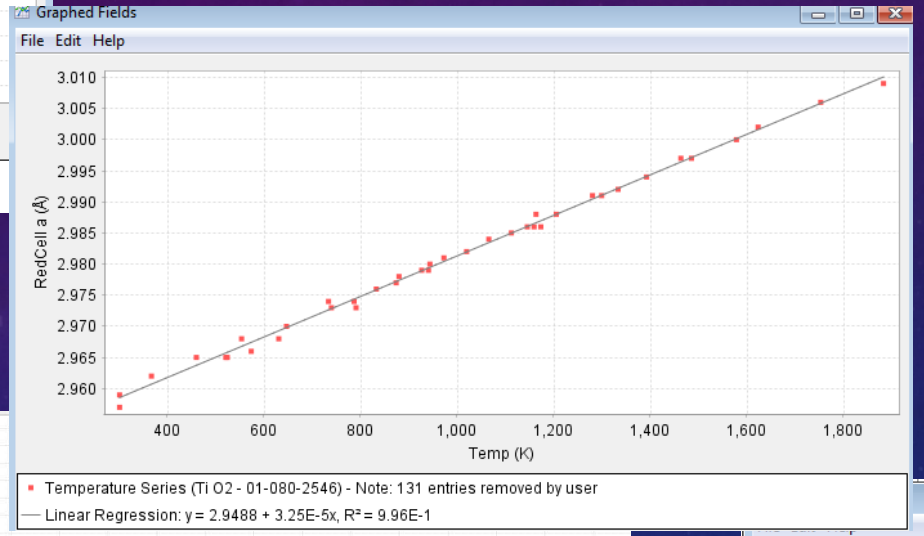
Data Sets	Determinations	R^2	Range
All data	170 points		
Remove Ambient (8 publications)	47 points	99.3	0-1883
Remove Poor Quality (7 publications)	43 points	99.4	0-1883
Remove Prototype (6 publications)	41 points	99.5	0-1883
Remove lowest temps (5 publications)	39 points	99.7	300-1883



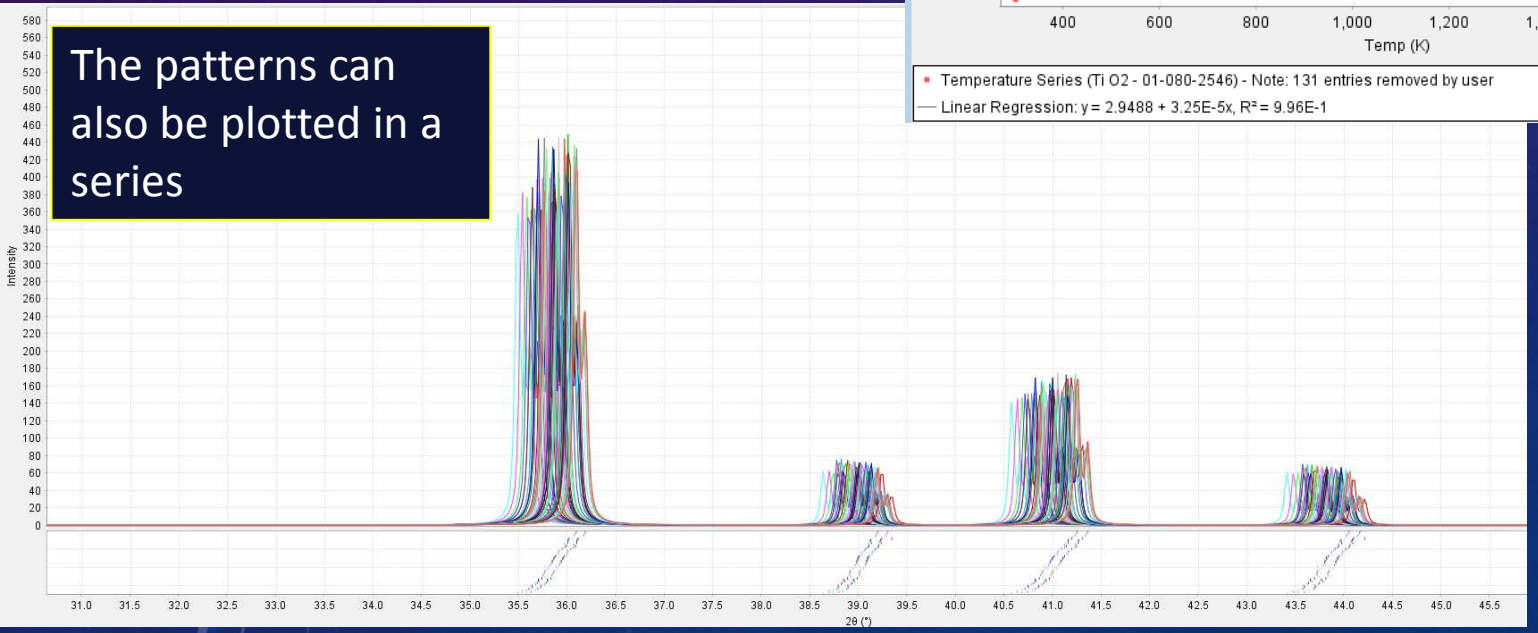


Once a set of data have been reviewed for the analysis and placed in the Preferences Table, we can also add additional display elements and plot directional thermal expansion along a lattice plane or cell axis.





The patterns can also be plotted in a series



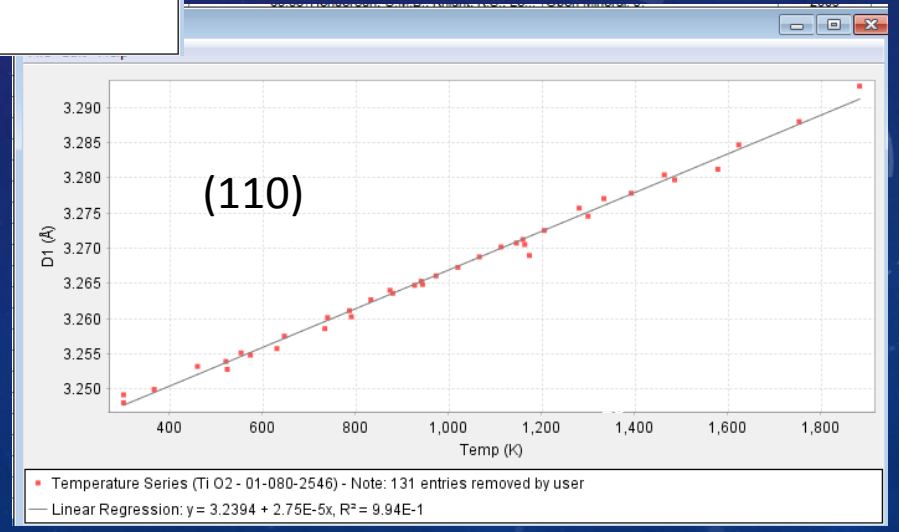


Table 4. Thermal Expansion Coefficients (Units 10^{-6}/Degree) for Unit Cell Parameters and T-O Bondlengths for Rutile and Geikielite (this work) and Published Data for Rutile

	α_a	α_c	α_V	$\alpha_{Ti\text{-}O1a}$	$\alpha_{Ti\text{-}O1b}$	$\alpha_{Mg\text{-}O1a}$	$\alpha_{Mg\text{-}O1b}$
Rutile							
This work	8.25	10.86	27.35	2.36	19.3		
Meagher & Lager [13]	7.4	10.4	25.2	8.7	7.4		
Burdett *et al.* [14]				4.9	5.7		
Sugiyama & Takeuchi [15]	8.9	11.1	28.9	8.4(3)	11.5(3)		
Seki *et al.* [16]	8.64	11.63	28.9				
Rao *et al.* [18]	7.25	8.82	23.3				
Merz *et al.* [19]	8.34	10.77	27.5				
Taylor [20]	7.61	9.87	25.1				
Geikielite				$\alpha_{Ti\text{-}O1}$	$\alpha_{Ti\text{-}O7}$	$\alpha_{Mg\text{-}O1}$	$\alpha_{Mg\text{-}O4}$
This work	10.6	13.6	34.8	10.90	12.7	-8.2	26.0

Published values for the thermal expansion.
Are there really 7 values or just 1 ?

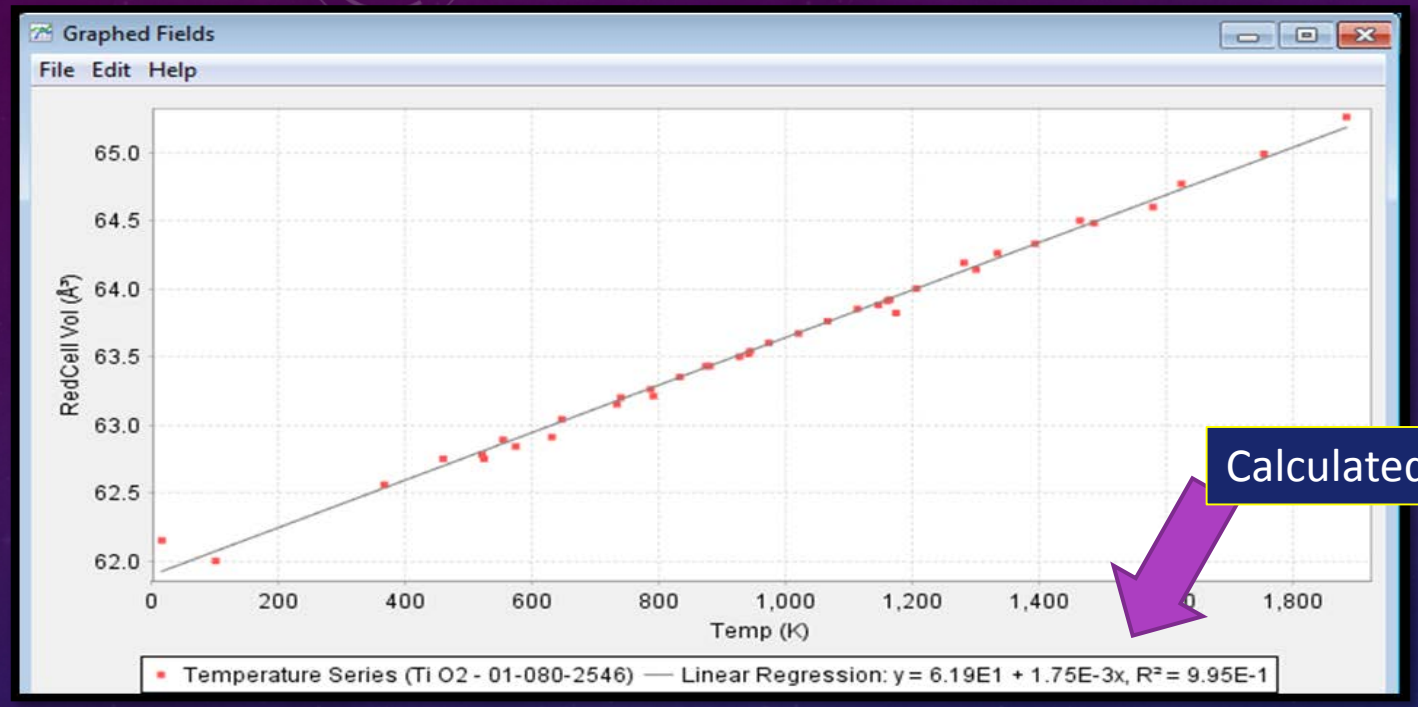
The Open Mineralogy Journal, 2009, *3*, 1-11 1

Open Access

Temperature Dependence of Rutile (TiO_2) and Geikielite ($MgTiO_3$) Structures Determined Using Neutron Powder Diffraction

C.M.B. Henderson[1,2,*], K.S. Knight[3] and A.R. Lennie[2]

[1]*STFC Daresbury Laboratory, Warrington, WA4 4AD;* [2]*School of Earth, Atmospheric and Environmental Science, University of Manchester, Manchester M13 9PL and* [3]*ISIS, STFC Rutherford-Appleton Laboratory, Didcot, Oxford OX11 0QX, UK*



Calculated slope

For a solid, we can ignore the effects of pressure on the material, and the volumetric thermal expansion coefficient can be written:

$$\alpha_V = \frac{1}{V}\frac{dV}{dT}$$

where V is the volume of the material, and dV/dT is the rate of change of that volume with temperature.

Rutile

High quality experimental data used exclusively

α_v = 28.0 ppm

Single value representing five publications and 39 entries

Table 4. Thermal Expansion Coefficients (Units 10^{-6}/Degree) for Unit Cell Parameters and T-O Bondlengths for Rutile and Geikielite (this work) and Published Data for Rutile

	α_a	α_c	α_V	$\alpha_{Ti\text{-}O1a}$	$\alpha_{Ti\text{-}O1b}$	$\alpha_{Mg\text{-}O1a}$	$\alpha_{Mg\text{-}O1b}$
Rutile							
This work	8.25	10.86	27.35	2.36	19.3		
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Sugiyama & Takeuchi [15]	8.9	11.1	28.9	8.4(3)	11.5(3)		
Seki *et al.* [16]	8.64	11.63	28.9				
Rao *et al.* [18]	7.25	8.82	23.3				
Merz *et al.* [19]	8.34	10.77	27.5				
Taylor [20]	7.61	9.87	25.1				
Geikielite				$\alpha_{Ti\text{-}O1}$	$\alpha_{Ti\text{-}O7}$	$\alpha_{Mg\text{-}O1}$	$\alpha_{Mg\text{-}O4}$
This work	10.6	13.6	34.8	10.90	12.7	-8.2	26.0

High quality data used in the ICDD analysis

The Open Mineralogy Journal, 2009, *3*, 1-11 1

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Temperature Dependence of Rutile (TiO_2) and Geikielite ($MgTiO_3$) Structures Determined Using Neutron Powder Diffraction

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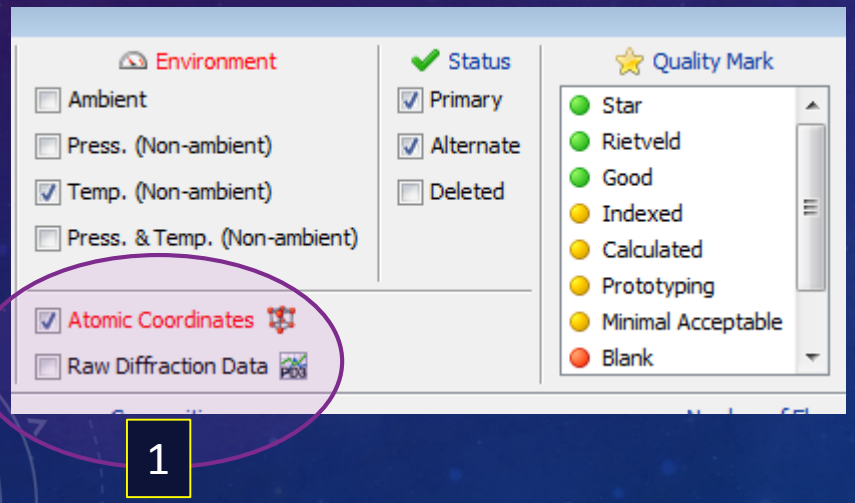
THERMAL EXPANSION OF CHEMICAL BONDS

In order to understand the nature of chemical bonding and phase transitions some scientists like to examine the thermal expansion of specific covalent and ionic bonds.

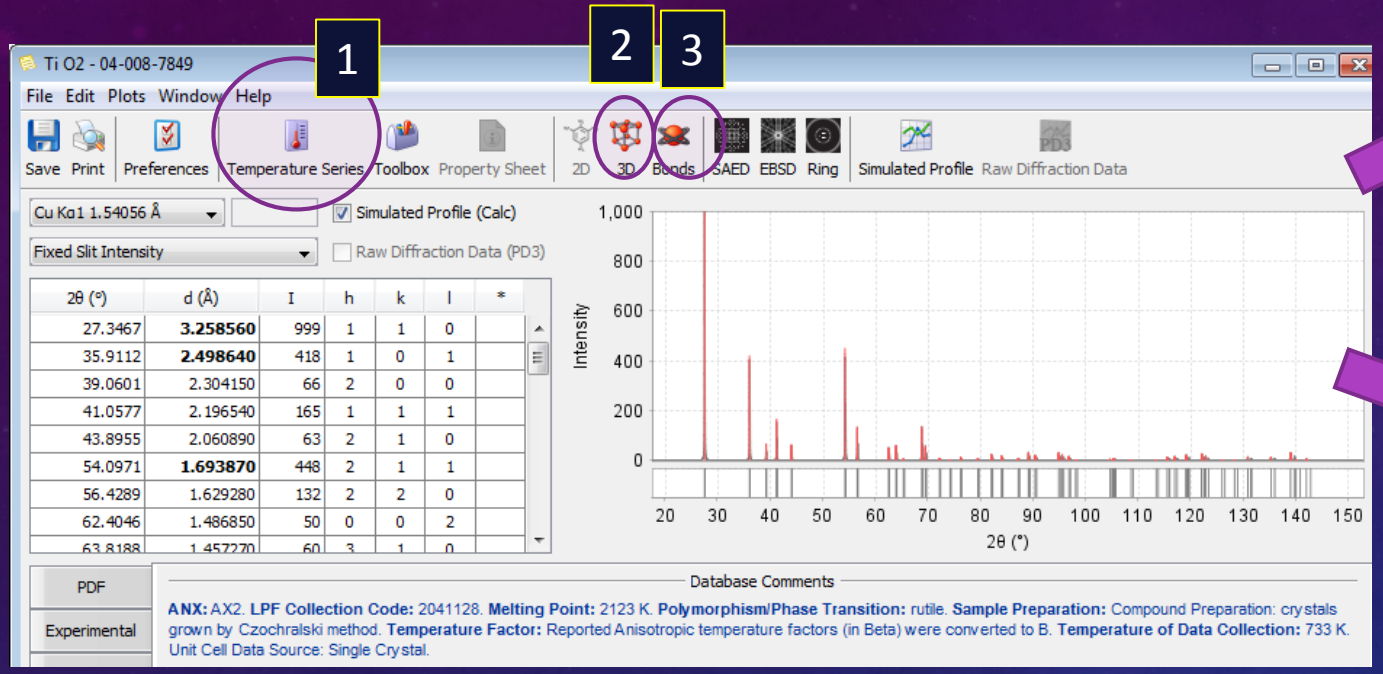
This is possible in PDF-4+, PDF-4/Minerals and PDF-4/Organics because these databases also have substantial populations of single crystal structures with calculated bond distances. However we have not automated the process with embedded software applications or index tables so more steps are required.

The user needs to select entries with atomic coordinates 1 and then look at the bond distances in the individual entries.



In the specific case for rutile, *most* of the 39 entries previously selected contain atomic coordinates.

For any entries with atomic coordinates

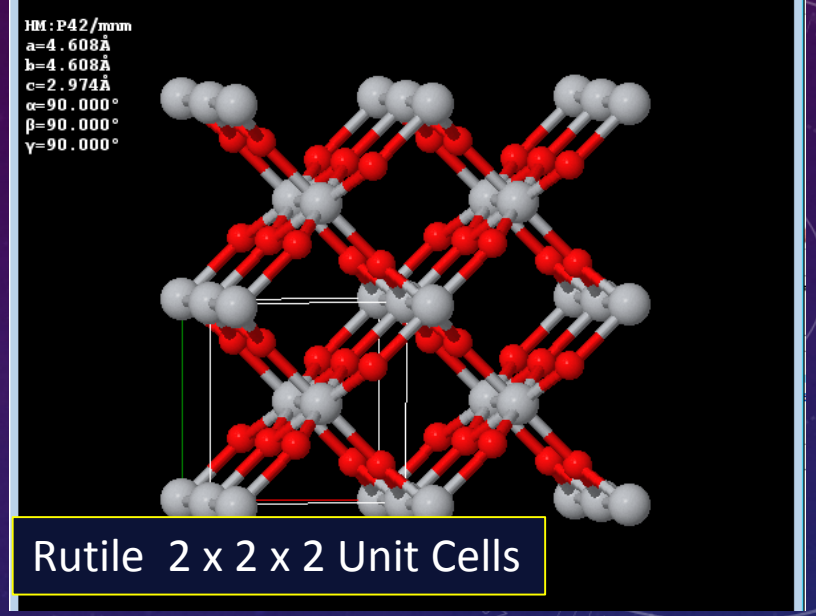


1

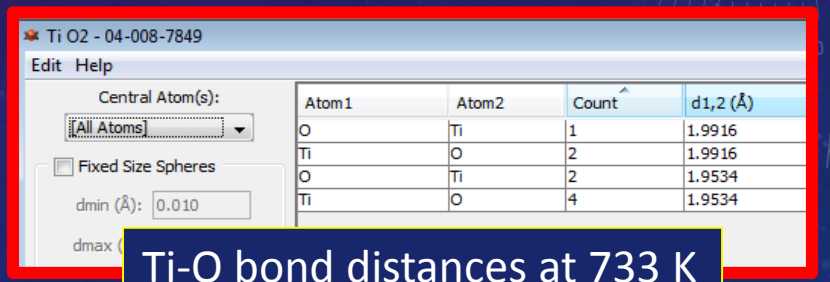
2 3

2

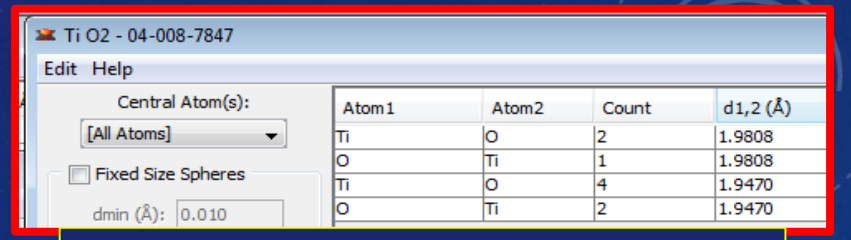
3



Rutile 2 x 2 x 2 Unit Cells



Ti-O bond distances at 733 K



For reference, same authors work, Ti-O bond distances at room temp.

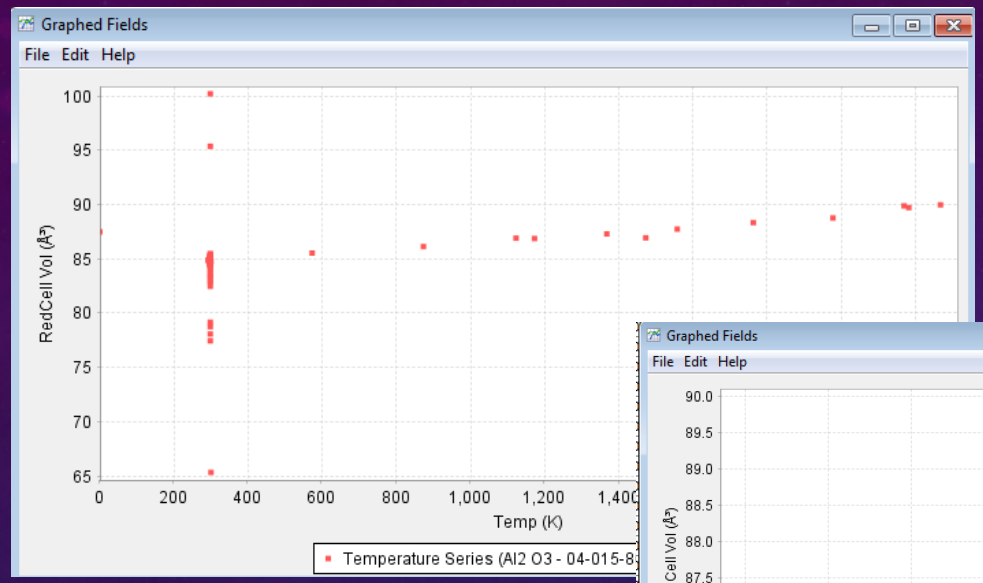
1 The above entry is part of the rutile temperature series Where the temperature series icon is activated and the temperature of data collection was 733 K.

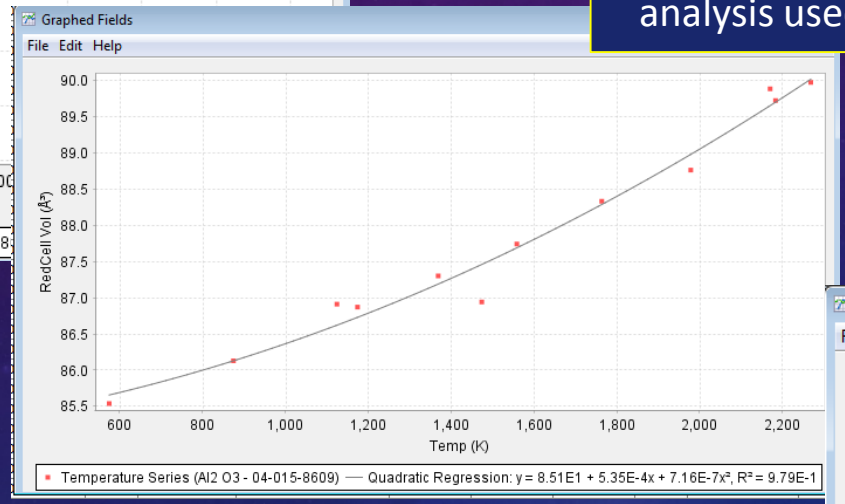
2 3 The entry also has an activated 3D icon and a bonds icon

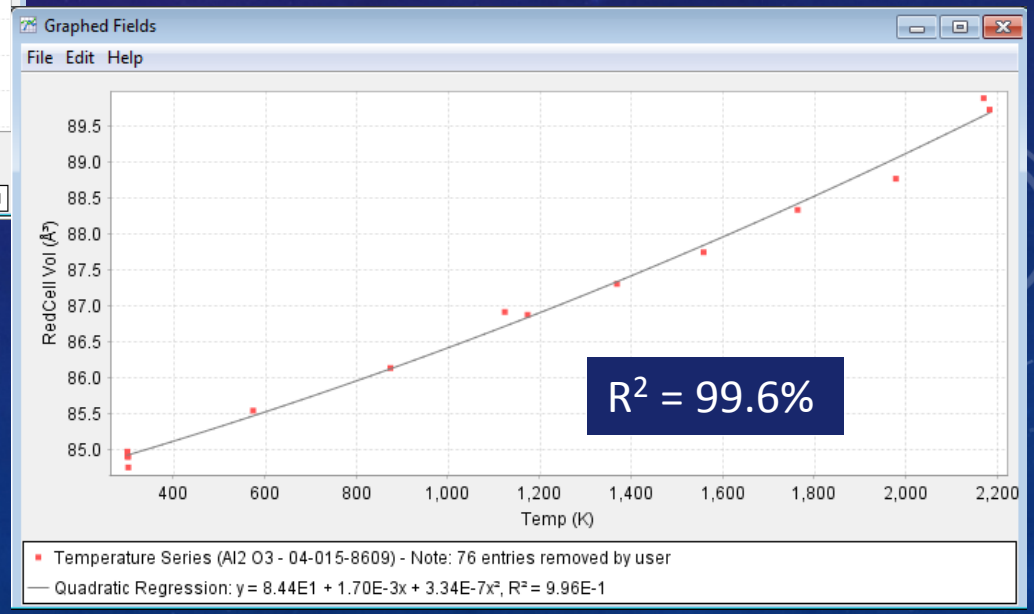
From the bond distances we can create a table of distances versus temperatures (not automated)

CORUNDUM

This series of data plots was generated in about 5 minutes total time.
Top left: All data from corundum in the temperature series, 96 entries
Middle: All ambient temperature data removed, 13 entries.
Bottom right: All low quality, hypothetical and prototype data removed. Ambient data from NIST SRM 674, 674a added as well as data from NBS Monograph 539 and NBS special publications. These were all high purity materials and the measurement were calibrated. Quality marks and editors comments were used in the selection. All remaining data are from S and I quality references. The analysis used 9 reference publications and 20 entries.







SUMMARY – THERMAL EXPANSION

In this presentation we demonstrated how numerous physical constants can be calculated from temperature series data – this includes lattice expansion, volume expansions, lattice plane expansion and bond expansions.

Applications and index tables have been used assist the user and facilitate the calculations

A suite of graphics programs enable the data to be graphed and plotted

The methods described are unique because they embed the unique quality review system developed by the ICDD, enabling the best data to be used in the analysis.

As part of ICDD's editorial processes the data employed by the method are continuously updated and new materials are added every year.