

Data Mining with the PDF-4 Databases

FeO Non-stoichiometric Oxides



This is one of three example-based tutorials for using the data mining capabilities of the PDF-4+ database and it covers the following topic:

- FeO Non-stoichiometric Oxides
 - sorting out temperature and stoichiometric effects on cell parameters

Two other similar tutorials for data mining exist and cover the following topics:

- <u>CIGS Photovoltaics</u> (Solid Solution Example)
 - solid solution / cell parameter relationship
- <u>Carbamazepine</u> (Resolving Pharmaceutical Polymorphs)
 - a PDF-4/Organics application
 - investigating polymorphic forms of an active pharmaceutical ingredient (API)



Stoichiometric Factors Affecting the Diffraction Pattern of FeO

- FeO is frequently non-stoichiometric with Fe-site vacancies.
- These defects have crystallographic effects and can cause shifts in the observed powder diffraction peaks.
- Summaries of this effect can be "mined" from the PDF-4+ database and displayed for further study.



Crystal Structure of FeO*



Cubic System Space Group: Fm-3m NaCl type structure

*Structure taken from PDF entry 04-004-7638 calculated from the Linus Pauling File database (MPDS).



Data Mining for FeO Entries: Step 1

Use the Preferences Window to establish what will be displayed in the Search Results table . . .

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Selecting Fields for the Results Table

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Selecting Fields for the Results Table

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Available Fields:

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Selecting Fields for the Results Table



Selected Fields: Use these buttons to move a selected item up or down in the listed order for the results table.

Available Fields:

Use these buttons to move selected items between the 'Available Fields' list of 90 items and the 'Selected Fields' list of items that will be displayed in the results table.



Selecting Fields for Results Table (FeO)

| -Selected Fields <u>Available Fields folder</u> | | | | | | | | | |
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| SPGR | - | Structures | | | | | | | |
| SG # | - | Structures | | | | | | | |
| XtlCell-a | - | Structures | | | | | | | |
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Setting up the fields as shown here will serve the purposes of this example. (Click 'OK' at the bottom of the 'Preferences' screen when finished.)







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| Period 3 | 11 Na 22.990 | 12 Mg 24.305 | V | n Undo | | Not | | u O | Just | @ A | nd 🔘 | Or | 13 AI 26.982 | 14 Si 28.086 | 15 P 30.974 | 16 S 32.065 | 17 CI 35.453 | 18 Ar 39.948 | |
| Period 4 | 19 K 39.098 | 20 Ca 40.078 | 21 Sc 44.956 | 22 Ti 47.867 | 23 V 50.941 | 24 Cr 51.996 | 25 Mr 54.938 | 26 Fe 55.845 | 27 Co 58.993 | 28 Ni 58.693 | 29 Cu | 30 Zn | 31 Ga | 32 Ge | 33 As | 34 Se | ³⁵ Br | ³⁶ Kr | |
| Period 5 | 37 Rb 85.468 | 38 Sr 87.62 | 39 Y 88.906 | 40 Zr 91.224 | 41 Nb 92.906 | 42 Mo 95.94 | 43 Tc [98] | 44 Ru 101.07 | 45 Rh 102.906 | 46 Pd 106.42 | 107.868 | 112.41 | 114.818 | K e | 121.76 | ent 127.6 | SF 126.904 | e ar | nd C |
| Period 6 | 55 Cs 132.905 | 56 Ba 137.327 | | 72 Hf 178.49 | 73 Ta 180.948 | 74 W 183.84 | 75 Re 186.207 | 76 Os 190.23 | 77 Ir 192.217 | 78 Pt 195.078 | 79 Au 196.967 | 80 Hg 200.59 | 81 TI 204.383 | 82 Pb 207.2 | 83 Bi 208.98 | 84 Po [209] | 85 At [210] | 86 Rn [222] | |
| Period | 87 Fr [223] | 88 Ra [226] | | | | | | | | | | | | | | | | | |
| 7 | | | 57 La 138.906 | 58 Ce 140.116 | 59 Pr 140.908 | 60 Nd 144.242 | 61 Pm [145] | 62 Sm 150.36 | 63 Eu 151.964 | 64 Gd 157.25 | 65 Tb 158.925 | 66 Dy 162.5 | 67 Ho 164.93 | 68 Er 167.259 | 69 Tm 168.934 | 70 Yb 173.04 | 71 Lu 174.967 | | |
| 7 LN: | | | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 | 1 | |







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| Period | 19 K 39.098 | 20 Ca 40.078 | 21 Sc 44.956 | 22 Ti 47.867 | 23 V 50.941 | 24 Cr 51.996 | 25 Mr 54.938 | 26 Fe 55.845 | 27 Co 58.993 | 28 Ni 58.693 | 29 Cu 63.546 | 30 Zn 65.409 | 31 Ga 69.723 | 32 Ge 72.64 | 33 As 74.922 | 34 Se 78.96 | 35 Br 79.904 | 36 Kr 83.798 | |
| Period 5 | 37 Rb 85.468 | 38 Sr 87.62 | 39 Y 88.906 | 40 Zr 91.224 | 41 Nb 92.906 | 42 Mo 95.94 | 43 Tc [98] | 44 Ru 101.07 | 45 Rh 102.906 | 46 Pd 106.42 | 47 Ag 107.868 | 48 Cd 112.41 | 49 In 114.818 | 50 Sn 118.71 | 51 Sb 121.76 | 52 Te 127.6 | 53 126.904 | 54 Xe 131.293 | |
| Period 6 | 55 Cs 132.905 | 56 Ba 137.327 | | 72 Hf 178.49 | 73 Ta 180.948 | 74 W 183.84 | 75 Re 186.207 | 76 Os 190.23 | 77 Ir 192.217 | 78 Pt 195.078 | 79 Au 196.967 | 80 Hg 200.59 | 81 TI 204.383 | 82 Pb 207.2 | 83 Bi 208.98 | 84 Po [209] | 85 At [210] | 86 Rn [222] | |
| Period 7 | 87 Fr [223] | 88 Ra [226] | | | | | | | | | | | | | | | | | |
| LN: | | | 57 La 138.906 | 58 Ce 140.116 | 59 Pr 140.908 | 60 Nd 144.242 | 61 Pm [145] | 62 Sm 150.36 | 63 Eu 151.964 | 64 Gd 157.25 | 65 Tb 158.925 | 66 Dy 162.5 | 67 Ho 164.93 | 68 Er 167.259 | 69 Tm 168.934 | 70 Yb 173.04 | 71 Lu 174.967 | | |
| AC: | | | 89 Ac [227] | 90 Th 232.038 | 91 Pa 231.036 | 92 U 238.029 | 93 Np [237] | 94 Pu [244] | 95 Am [243] | 96 Cm [247] | 97 Bk [247] | 98 Cf [251] | 99 Es [252] | 100 Fm [257] | 101 Md [258] | 102 No [259] | 103 Lr [262] | | |
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Structure Criterion for Search: FCC Space Group #225 – 'Fm-3m'

entered on 'Structures' tab of 'Search' window

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Structure Criterion for Search: FCC Space Group #225 – 'Fm-3m'

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A total of 60 entries for Fe_{1-x}O compounds

You will get 66 entries if the 'Include Deleted Patterns' box is checked on the 'Subfiles/ Database Filters' tab of the Search window.

A description of your search_____ criteria is shown here.

Results of PDF-4+ Search for FeO

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| PDF # | QM | Amb. | Chemical For | Atomic | % | SYS | SPGR | SG # | XtlCell a | Dcalc | |
| 00-006-0615 | L | A | Fe O | Fe50.00 O50 | 0.00 | С | Fm-3m | 225 | 4.307 | 5.973 | ٩, |
| 00-046-1312 | В | A | Fe O | Fe50.00 O50 | 0.00 | C | Fm-3m | 225 | 4.293 | 6.032 | I F |
| 01-071-4461 | 1 | Т | Fe O | Fe50.00 O50 | 0.00 | C | Fm-3m | 225 | 4.354 | 5.782 | |
| 01-073-2143 | 1 | A | Fe.974 O | Fe49.34 O50 | .66 | С | Fm-3m | 225 | 4.309 | 5.845 | |
| 01-073-2144 | I. | A | Fe.942 O | Fe48.51 O51 | .49 | С | Fm-3m | 225 | 4.280 | 5.812 | : |
| 01-074-1880 | 1 | A | Fe0.911 O | Fe47.67 O52 | 2.33 | С | Fm-3m | 225 | 4.290 | 5.625 | |
| 01-074-1881 | 1 | A | Fe0.918 O | Fe47.86 O52 | 2.14 | С | Fm-3m | 225 | 4.293 | 5.646 | |
| 01-074-1882 | 1 | A | Fe0.929 O | Fe48.16 O51 | .84 | С | Fm-3m | 225 | 4.300 | 5.672 | |
| 01-074-1883 | 1 | A | Fe0.932 O | Fe48.24 O51 | .76 | С | Fm-3m | 225 | 4.301 | 5.682 | |
| 01-074-1884 | L | A | Fe0.944 O | Fe48.56 O51 | .44 | C | Fm-3m | 225 | 4.308 | 5.707 | |
| 01-074-1885 | 1 | A | Fe0.944 O | Fe48.56 O51 | .44 | C | Fm-3m | 225 | 4.310 | 5.702 | |
| 01-074-1886 | н | A | Fe O | Fe50.00 O50 | 0.00 | С | Fm-3m | 225 | 4.341 | 5.834 | |
| 01-075-1550 | 1% | A | Fe O | Fe50.00 O50 | 0.00 | С | Fm-3m | 225 | 4.303 | 5.99 | |
| 01-077-7980 | В | A | Fe O | Fe50.00 O50 | 0.00 | C | Fm-3m | 225 | 4.312 | 5.952 | |
| 01-079-1969 | 1 | Т | Fe.920 O | Fe47.92 O52 | 2.08 | С | Fm-3m | 225 | 4.361 | 5.396 | |
| 01-079-1971 | I. | Т | Fe.902 O | Fe47.42 O52 | 2.58 | С | Fm-3m | 225 | 4.355 | 5.338 | |
| 01-079-1972 | 1 | Т | Fe.888 O | Fe47.03 O52 | 2.97 | C | Fm-3m | 225 | 4.349 | 5.297 | |
| 01-079-1973 | I. | Т | Fe.880 O | Fe46.81 O53 | 8.19 | C | Fm-3m | 225 | 4.344 | 5.277 | |
| 01-079-2175 | 1 | Т | Fe.928 O | Fe48.13 O51 | .87 | C | Fm-3m | 225 | 4.351 | 5.47 | |
| 01-079-2177 | I | Т | Fe0.92 O | Fe47.92 O52 | 2.08 | С | Fm-3m | 225 | 4.360 | 5.401 | |
| 01-084-0302 | I. | Т | Fe0.909 O | Fe47.62 O52 | 2.38 | С | Fm-3m | 225 | 4.290 | 5.617 | , |
| | | 5 | | | C-1-1-1 | 1000 | | - T - S - S - S - S - S - S - S - S - S | | | |



Analysis of the Resulting Database Entries

Most fields in the results table can be graphically illustrated in either X-Y plot or histogram form.

For the current application, we will use an X-Y plot to illustrate the a-axis cell parameter as a function of atomic % Fe.

To do this, 'Graph Fields...' is first selected from the 'Results' drop down menu of the 'Results' window.

| Results (60 of Search Prefer | 328 renci | S 25 | 'DF Card Imulated Profile Graph Fields | |] | | | | | |
|---------------------------------|--------------|------|--|-----------------|-----|-------|------|-----------|-------|---|
| PDF # | QM | Amb. | Chemical For | Atomic % | SYS | SPGR | SG # | XtlCell a | Dcalc | |
| 00-006-0615 | I | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.307 | 5.973 | |
| 00-046-1312 | в | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.293 | 6.032 | Г |
| 01-071-4461 | 1 | Т | Fe O | Fe50.00 O50.00 | C | Fm-3m | 225 | 4.354 | 5.782 | |
| 01-073-2143 | 1 | A | Fe.974 O | Fe49.34 O50.66 | С | Fm-3m | 225 | 4.309 | 5.845 | |
| 01-073-2144 | 1 | A | Fe.942 O | Fe48.51 O51.49 | С | Fm-3m | 225 | 4.280 | 5.812 | Ξ |
| 01-074-1880 | I. | A | Fe0.911 O | Fe47.67 O52.33 | С | Fm-3m | 225 | 4.290 | 5.625 | |
| 01-074-1881 | 1 | A | Fe0.918 O | Fe47.86 O52.14 | С | Fm-3m | 225 | 4.293 | 5.646 | |
| 01-074-1882 | 1 | A | Fe0.929 O | Fe48.16 O51.84 | С | Fm-3m | 225 | 4.300 | 5.672 | |
| 01-074-1883 | I. | A | Fe0.932 O | Fe48.24 O51.76 | С | Fm-3m | 225 | 4.301 | 5.682 | |
| 01-074-1884 | L | A | Fe0.944 O | Fe48.56 O51.44 | C | Fm-3m | 225 | 4.308 | 5.707 | |
| 01-074-1885 | 1 | A | Fe0.944 O | Fe48.56 O51.44 | C | Fm-3m | 225 | 4.310 | 5.702 | |
| 01-074-1886 | Н | A | Fe O | Fe50.00 O50.00 | C | Fm-3m | 225 | 4.341 | 5.834 | |
| 01-075-1550 | 1 | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.303 | 5.99 | |
| 01-077-7980 | В | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.312 | 5.952 | |
| 01-079-1969 | 1 | Т | Fe.920 O | Fe47.92 O52.08 | C | Fm-3m | 225 | 4.361 | 5.396 | |
| 01-079-1971 | 1 | Т | Fe.902 O | Fe47.42 O52.58 | С | Fm-3m | 225 | 4.355 | 5.338 | |
| 01-079-1972 | 1 | Т | Fe.888 O | Fe47.03 O52.97 | С | Fm-3m | 225 | 4.349 | 5.297 | |
| 01-079-1973 | L | Т | Fe.880 O | Fe46.81 O53.19 | С | Fm-3m | 225 | 4.344 | 5.277 | 6 |
| 01-079-2175 | 1 | Т | Fe.928 O | Fe48.13 O51.87 | C | Fm-3m | 225 | 4.351 | 5.47 | |
| 01-079-2177 | 1 | Т | Fe0.92 O | Fe47.92 O52.08 | C | Fm-3m | 225 | 4.360 | 5.401 | |
| 04 004 000D | 1 | T | Ee0.000 O | Ee 47 62 OE2 38 | 0 | Em_3m | 225 | 4 290 | 5.617 | |



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| Y-Axis | 1 |
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FeO a-axis Cell Parameter vs. Atomic % Fe



This graph shows little apparent correlation between atomic % Fe and a-axis.

Note that entries *reported* as being stoichiometric (1:1) are in a vertical line at right (50 at.% Fe). All others report less than stoichiometric amounts of Fe.

FeO a-axis Cell Parameter vs. Atomic % Fe



Further examination of individual entries separates ambient, high-temperature, and high-pressure determinations of the a-axis.





 Individual entries from this chart may be examined by left-clicking on individual spots. The illustration above shows the point label that appears when the mouse cursor is 'hovered' over this data point.



FeO a-axis Cell Parameter vs. Atomic % Fe



• If you left-click at this point, depending on the proximity of nearby points on the graph, you may directly bring up the 01-074-1883 entry, or bring up a list of the nearby points as shown above. In the latter case, the point of interest is selected from the list and then 'OK' is clicked. This entry is shown on the next slide.



PDF Card for FeO (01-074-1883)

| 🕒 Fe0.932 O - 01-074-1883 | | | | | | | | | | | | | | | | | | | | | | | X |
|-----------------------------------|-----------|----------------|----------|----------|-------|------|-----------------|-------|------|-------|-------------------|-------|--------|-------|---------|-------|--------|-------|------|-----|-------|-----|----|
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| Cu Ka1 1.54056Å 🛛 👻 | 28 | d(Å) | I | h | k | 1 | * | | | 750 | | | | | | | | | | | | | |
| Å | 36.1450 | 2.483010 | 604 | 1 | 1 | 1 | | | _ | 750 | | | | | | | | | | | | | |
| <u>1</u> | 41.9808 | 2.150350 | 999 | 2 | 0 | 0 | | ं | 12 I | | | | | | | | | | | | | | |
| Stick Datterne | 60.8735 | 1.520530 | 463 | 2 | 2 | 0 | | | fe | 500 - | | | | | 1 | | | | | | | | |
| | 72.8865 | 1.296710 | 157 | 3 | 1 | 1 | | | - | | | | | | | | | | | | | | |
| V Fixed Slit Intensity | 76.6963 | 1.241510 | 116 | 2 | 2 | 2 | | | | 250 - | | | | | 1 | | | | | | | | 5 |
| 🥅 Variable Slit Intensity | 91.5193 | 1.075180 | 43 | 4 | 0 | 0 | | 8 | | | | | | | | | | | | | | | |
| Integrated Intensity | 102.6501 | 0.986648 | 48 | 3 | 3 | 1 | _ | | | 0 | | | | - | | | - | | - | - | | 1 | - |
| Diffraction Patterns | 105.4485 | 0.951555 | 109 | 4 | 2 | 0 | _ | | | | | | | | | | | | | | | | _ |
| | 137 0761 | 0.877670 | 04 | 9 | 6 | 2 | | | | | 30 | 40 | 50 | 60 | 70 | 80 | 90 | 100 | 110 | 120 | 130 | 140 | |
| Simulated Profile | 101.0101 | 0.021010 | F | ב | | (| | | | | | | | | | | 20 | | | | | | |
| Raw Diffraction Data (PD3) | | | 1 1 | <u>ر</u> | 93 | 2 | | | | - 0' | 1-074 | -188 | 3 (Fi) | (ed § | Slit In | tensi | ity) — | - 01- | 074- | 188 | 3 (Ca | lc) | |
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| PDF Experimental Physical Crystal | Optical S | tructore Mis | cellanec | us I | Refe | ence | es C | ommen | ts | | | | | | | | | | | | | | |
| PDF #: 01-074-1883 | | | State | us: Pr | imary | (| | | | | | Q | M: Ind | dexe | d (l) b | | |] | | | | | |
| Pressure/Temperature: Ambient | | | | | | > | | | | | | 0.555 | | | | | | | | | | | j |
| Chemical Formula (Fe0.932 O | | | | | | | | | | | | | | | | | | | | | | | |
| Structural Formula: | | | | | | | | | | | | | | | | 1 | | | | | | | |
| Empirical Formula: Fe0.932 O | | The | 'PC |)F' | ta | b | of [·] | this | W | vind | OW | di | spl | lay | /S | | | | | | | | |
| Weight %: Fe76.49 O23.51 | | the | actu | al | fo | rm | ula | a ar | ۱d | stc | oich | nioi | me | etr\ | /. | | | | | | | | |
| Atomic %: Fe48.24 O51.76 | | | | | | | | | | | | | | , | | | | | | | | | |
| ANX: AX | | | | | | | | | | | | | | | | | | | | | | | |
| Compound Name: Iron Oxide | | | | | | | | | | | | | | | | | | | | | | | Ĩ |
| Mineral Name: Wustite, syn | | | | | | | | | | | | | | | | | | | | | | | -1 |
| Common Name: | | | | | | | | | | | | | | | | | | | | | | | |



PDF Card for FeO (01-074-1883)

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| Raw Diffraction Data (PD3) | | | | | [| | -1883 (Fixed Slit Intensity) — 01-074-1883 (Calc) |
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| Primary Reference | Calculated from I | CSD using . | POWD | -12++. | | | |
| Structure | "An x-ray study o | f the wuest | ite (Fe | O) solid s | olution: ". Je | tte, E.R., Foo | ote, F., Ohem. Phys. 1, 29 (1933). |
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| | The 'Rei | ferenc | es' t | ah of | this wi | ndows | shows the source of the |
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| | informat | ion. Al | Jtho | rs, in | this ca | se, are | E. R. Jette and F. Foote. |
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PDF Card for FeO (01-074-1883)

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| Wavelength previous graphical plot of 'a' vs. atomic % Fe Cu Kal 1.54056Å A Å A Stick Patterns 28 d(Å) I h k I * Variable Slit Intensity 1.50030 493 2 0 0 50 | d-Spacings | | | | | | | This w | indc | w r | nay | y be | e cl | ose | ed to | o re | etur | n to | o th | е | |
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| Raw Diffraction Data (PD3) — 01-074-1883 (Fixed Slit Intensity) — 01-074-1883 (Calc) DF Experimental Physical Crystal Optical Structure Miscellaneous References Comments Type Reference Reference Calculated from ICSD using POWD-12++. Reference | 📝 Simulated Profile | 137.0761 | 0.827670 | 40 | 5 | 1 | 1 | | | | | | | | 2 | 20 | | | | | |
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| Structure "An x-ray study of the wuestite (Fe O) solid solutions". Jette, E.R., Foote, F. J. Ohem. Phys. 1, 29 (1933). | Structure | "An x | (-ray study of | f the wu | estite | (Fe | 0) s | d solutions". | Jette, E | .R., F | oote, | F. <i>J</i> . | Chem | . Phys | 9. 1, 29 | 9 (19 | 33). | | | | - |





Examining another nearby point, corresponding to entry 01-074-1882, we note that the reference lists the same authors, E. R. Jette and F. Foote.

There may be other entries across the range of stoichiometries that are based on these authors' work. We can add an author's name to the search criteria to examine just their entries.



Adding an Author to the Search

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Without resetting the previous search criteria, we can add an author to the previous Periodic Table (Only Fe and O) and Structure (Space Group 225) specifications. Adding 'Jette' to the 'Author' box, and clicking 'Search' gives the Results list on the next slide:



Search Result Including 'Jette' as Author

| PDF # | QM | Amb. | Chemical For | Atomic % | SYS | SPGR | SG # | XtlCell a | Dcalc |
|-------------|----|------|--------------|----------------|-----|-------|------|-----------|-------|
| 01-074-1880 | E | A | Fe0.911 O | Fe47.67 O52.33 | С | Fm-3m | 225 | 4.290 | 5.625 |
| 01-074-1881 | I | A | Fe0.918 O | Fe47.86 O52.14 | С | Fm-3m | 225 | 4.293 | 5.646 |
| 01-074-1882 | 1 | A | Fe0.929 O | Fe48.16 O51.84 | С | Fm-3m | 225 | 4.300 | 5.672 |
| 01-074-1883 | 1 | A | Fe0.932 O | Fe48.24 O51.76 | С | Fm-3m | 225 | 4.301 | 5.682 |
| 01-074-1884 | t | A | Fe0.944 O | Fe48.56 O51.44 | С | Fm-3m | 225 | 4.308 | 5.707 |
| 01-074-1885 | 1 | A | Fe0.944 O | Fe48.56 O51.44 | С | Fm-3m | 225 | 4.310 | 5.702 |
| 01-074-1886 | Н | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.341 | 5.834 |

These results can be graphed as before . . .



These represent the results of one systematic study of stoichiometry vs. structure published by Jette & Foote in *J. Chem. Phys.*





The underlying numerical values from this resulting graph can be exported for analysis by other software programs such as Microsoft® Excel®. From the 'File' menu on this graph, 'Save...' is selected.



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The values can be saved to a 'CSV' (comma separated values) file for import into many other software analysis programs. The file name and folder are specified here as well.





An example of a Microsoft® Excel® analysis of the Jette & Foote data. The linear analysis equation can be rearranged to give . . .

This would allow one to calculate the atomic % Fe from a measured aaxis value.

FeO a-axis Cell Parameter vs. Atomic % Fe



Several entries in the 'High Temperature' region of the original results graph come from a single study, "Point Defect Clusters in Wuestite" by Radler, Cohen, & Faber, *J. Phys. Chem. Solids*, 51, 217 (1990). We can again use the author criterion to look at just these entries.



Change Author for Search

| 🗟 Search | |
|--|-------------------------------------|
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| Subfiles/Database Filters Periodic Table Elements Name | References Structures Miscellaneous |
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On the 'References' tab, 'Cohen' has been entered in the 'Author' field to obtain the desired PDF entries. The 'Structures' and 'Periodic Table' tabs contain the previously entered information regarding FeO and space group 225. This search will yield the 10 entries found on the next slide.



PDF Entries from Radler, Cohen, & Faber Study (1990)

| Results (10 o Search Prefe | f 328 renc | F 2015 2015 2015 2015 2015 2015 2015 2015 | PDF Card Simulated Profile Graph Fields. | | •] | | | | | |
|--|-----------------|---|--|-------------------------------|--------------------------------------|-----|-------------------------|--------------------------|-------------------------|---|
| PDF # | QM | Amb. | Chemical For | At | omic % | SYS | SPGR | SG # | XtlCell a | Dcalc |
| 01-079-1969 | I | Т | Fe.920 O | Fe47.92 | O52.08 | С | Fm-3m | 225 | 4.361 | 5.396 |
| 01-079-1971 | L | Т | Fe.902 O | Fe47.42 | O52.58 | С | Fm-3m | 225 | 4.355 | 5.338 |
| 01-079-1972 | 1 | Т | Fe.888 O | Fe47.03 | O52.97 | С | Fm-3m | 225 | 4.349 | 5.297 |
| 01-079-1973 | 1 | т | Fe.880 O | Fe46.81 | O53.19 | С | Fm-3m | 225 | 4.344 | 5.277 |
|)1-079-2175 | | Т | Fe.928 O | Fe48.13 | O51.87 | С | Fm-3m | 225 | 4.351 | 5.47 |
|)1-079-2177 | I. | Т | Fe0.92 O | Fe47.92 | O52.08 | С | Fm-3m | 225 | 4.360 | 5.401 |
| 04-014-4357 | 1 | Т | Fe0.913 O | Fe47.73 | O52.27 | С | Fm-3m | 225 | 4.367 | 5.343 |
|)4-014-4358 | 1 | Т | Fe0.911 O | Fe47.67 | O52.33 | С | Fm-3m | 225 | 4.372 | 5.316 |
|)4-014-4359 | I. | Т | Fe0.950 O | Fe48.72 | O51.28 | С | Fm-3m | 225 | 4.376 | 5.475 |
|)4-014-4360 | L | Т | Fe0.945 O | Fe48.59 | O51.41 | C | Fm-3m | 225 | 4.373 | 5.462 |
| 04-014-4358 04-014-4358 04-014-4359 04-014-4360 | 1 | T T T | Fe0.911 O Fe0.950 O Fe0.945 O | Fe47.67 Fe48.72 Fe48.59 | 052.27 052.33 051.28 051.41 | | Fm-3m Fm-3m Fm-3m | 225 225 225 225 | 4.372 4.376 4.373 | 5.3 ¹ 5.4 ¹ 5.4 |

The a-axis cell parameter for just these resulting 10 entries can now be plotted vs. atomic % Fe and the resulting graph is shown on the following slide.



Graph of Radler, Cohen, and Faber FeO Entries



These points represent two sets of high-temperature X-ray data obtained in the referenced report as follows:

1. Data varying T from 1123 to 1373 C with slightly increasing O content

2. Data varying stoichiometry at 1323 C from $Fe_{0.88}O$ to $Fe_{0.95}O$



Another Look at FeO results - Density

Return to the original list of 63 FeO entries using 'History' ...

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| 5earch #3 | {Only (Fe And O)} And {Author Contains Words 'Jette' Number Exactly '225'} And {Not Status (Deleted)} | } And {International Space Group | 7 | E Belete |
| 5earch #4 | {Only (Fe And O)} And {Author Contains Words 'Coher Number Exactly '225'} And {Not Status (Deleted)} | n'} And {International Space Group | 10 | Telete All |
| ombined Searches Name | Description | | ¥ Hits | Operation |
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Another Look at FeO results - Density

Return to the original list of 60 FeO entries using 'History' ...





Another way to analyze this data is to look at the density as a function of cell parameter. This is performed by using the 'Results' drop down menu to access 'Graph Fields...'

Another Look at FeO results - Density

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| PDF # | QM | Amb. | Chemical For | Atomic % | SYS | SPGR | SG # | XtlCell a | Dcalc | | |
| 00-006-0615 | L | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.307 | 5.973 | | |
| 00-046-1312 | В | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.293 | 6.032 | | |
| 01-071-4461 | 1 | Т | Fe O | Fe50.00 O50.00 | C | Fm-3m | 225 | 4.354 | 5.782 | | |
| 01-073-2143 | I. | A | Fe.974 O | Fe49.34 O50.66 | С | Fm-3m | 225 | 4.309 | 5.845 | | |
| 01-073-2144 | 1 | A | Fe.942 O | Fe48.51 O51.49 | С | Fm-3m | 225 | 4.280 | 5.812 | E | |
| 01-074-1880 | 1× | A | Fe0.911 O | Fe47.67 O52.33 | С | Fm-3m | 225 | 4.290 | 5.625 | | |
| 01-074-1881 | I. | A | Fe0.918 O | Fe47.86 O52.14 | С | Fm-3m | 225 | 4.293 | 5.646 | | |
| 01-074-1882 | 1 | A | Fe0.929 O | Fe48.16 O51.84 | C | Fm-3m | 225 | 4.300 | 5.672 | | |
| 01-074-1883 | 1 | A | Fe0.932 O | Fe48.24 O51.76 | С | Fm-3m | 225 | 4.301 | 5.682 | | |
| 01-074-1884 | L | A | Fe0.944 O | Fe48.56 O51.44 | С | Fm-3m | 225 | 4.308 | 5.707 | 8 | |
| 01-074-1885 | 1 | A | Fe0.944 O | Fe48.56 O51.44 | C | Fm-3m | 225 | 4.310 | 5.702 | | |
| 01-074-1886 | Н | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.341 | 5.834 | | |
| 01-075-1550 | 1 | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.303 | 5.99 | | |
| 01-077-7980 | В | A | Fe O | Fe50.00 O50.00 | С | Fm-3m | 225 | 4.312 | 5.952 | | |
| 01-079-1969 | I | Т | Fe.920 O | Fe47.92 O52.08 | С | Fm-3m | 225 | 4.361 | 5.396 | | |
| 01-079-1971 | 1 | Т | Fe.902 O | Fe47.42 O52.58 | C | Fm-3m | 225 | 4.355 | 5.338 | | |
| 01-079-1972 | 1 | Т | Fe.888 O | Fe47.03 O52.97 | С | Fm-3m | 225 | 4.349 | 5.297 | | |
| 01-079-1973 | 1 | Т | Fe.880 O | Fe46.81 O53.19 | C | Fm-3m | 225 | 4.344 | 5.277 | | |
| 01-079-2175 | 1 | Т | Fe.928 O | Fe48.13 O51.87 | C | Fm-3m | 225 | 4.351 | 5.47 | | |
| 01-079-2177 | 1 | T | Fe0.92 O | Fe47.92 O52.08 | C | Fm-3m | 225 | 4.360 | 5.401 | | |
| 01-084-0302 | I | Т | Fe0.909 O | Fe47.62 O52.38 | С | Fm-3m | 225 | 4.290 | 5.617 | - | |

Search Description

Calculations

{Only (Fe And O)} And {International Space Group Number Exactly '225'} And {Not Status (Deleted)}

Mean:

ES

Median:

ESD:



Another Look at FeO results - Density

For this graph, we will plot the calculated density as a function of the cubic cell parameter.

| Graph Fields | | X |
|---------------------|---------------------|----|
| Help | | |
| Rows: All X-Axis | • | |
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Results: density vs. a-axis cell parameter for reported FeO structures





Illustration of correllations within this graph of density verses cell parameter for Fe_{1-x}O data





Summary for Data Mining Non-stoichiometric Cubic FeO

- Multiple explanations exist for unit cell parameter variations in non-stoichiometric FeO in the PDF
- Systematic studies regarding stoichiometry and/or temperature can be "mined" from the database
- No single relationship describes all the data, thus different "defect" arrangements must exist for these materials
- Ability to access PDF entries directly from graphs' facilitates obtaining other data and references



Thank you for viewing our tutorial. Additional tutorials are available at the ICDD website. <u>www.icdd.com</u>

International Centre for Diffraction Data

12 Campus Boulevard

Newtown Square, PA 19073

Phone: 610.325.9814

Toll Free Number in US & Canada: 866.378.0331

Fax: 610.325.9823

