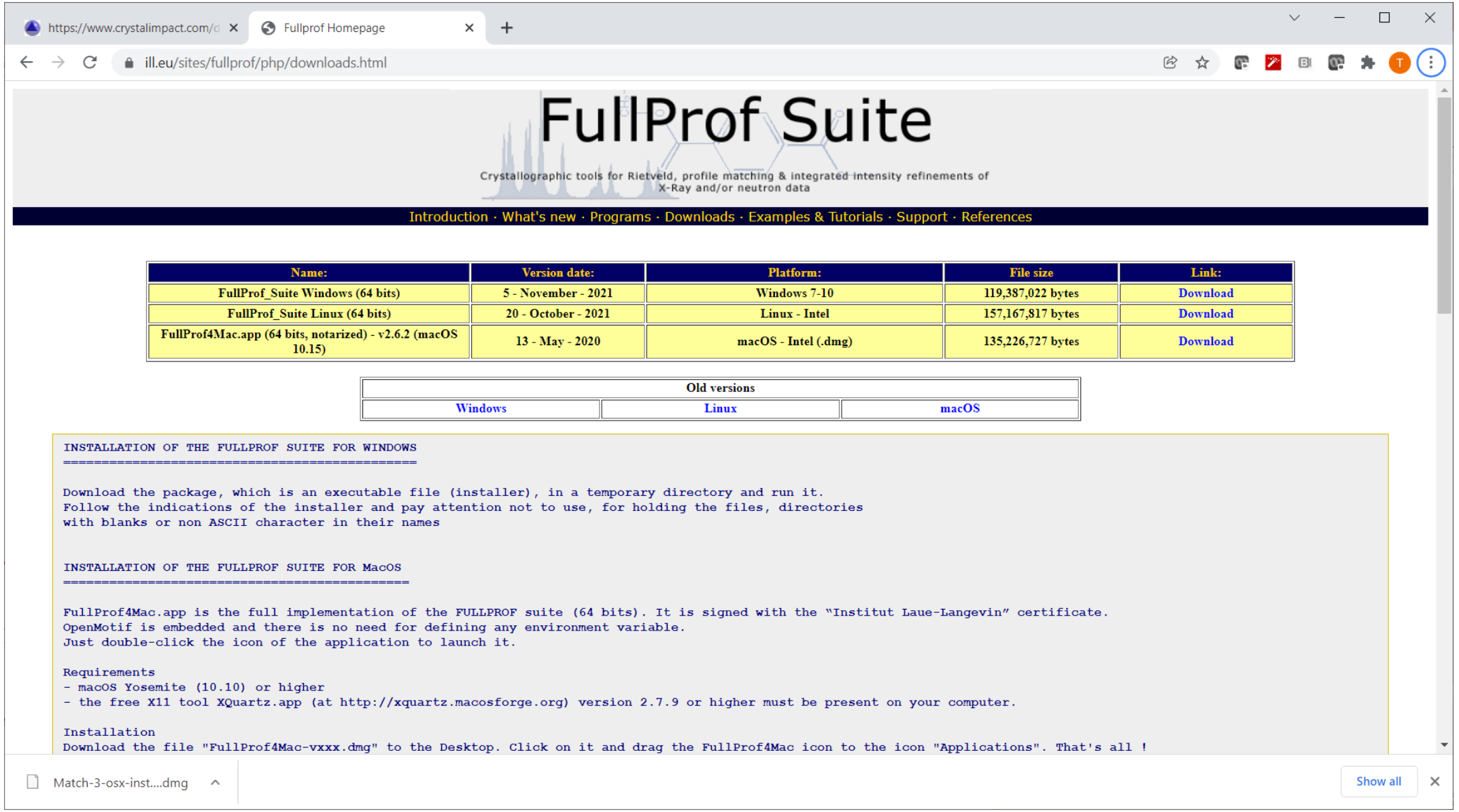
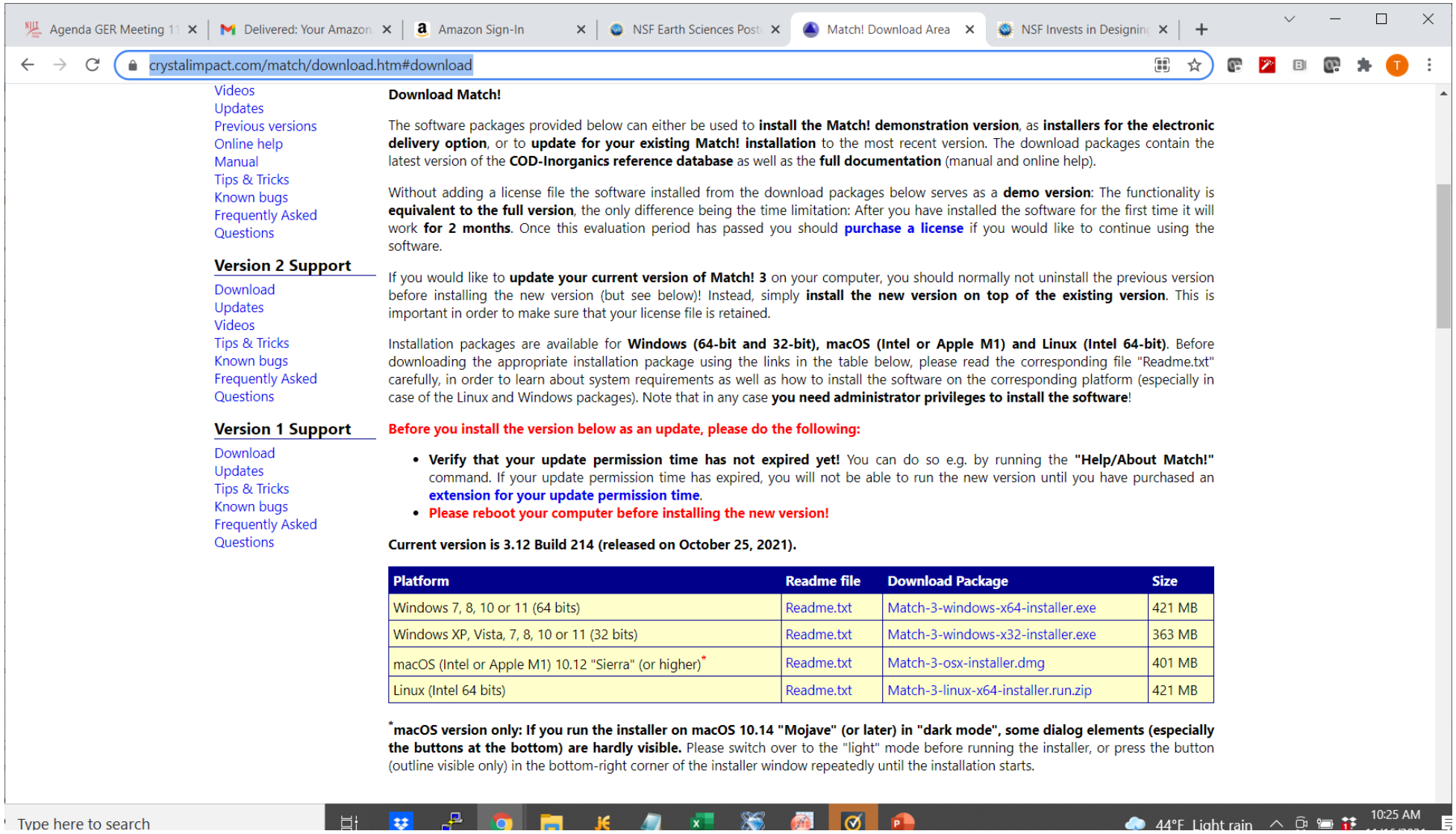
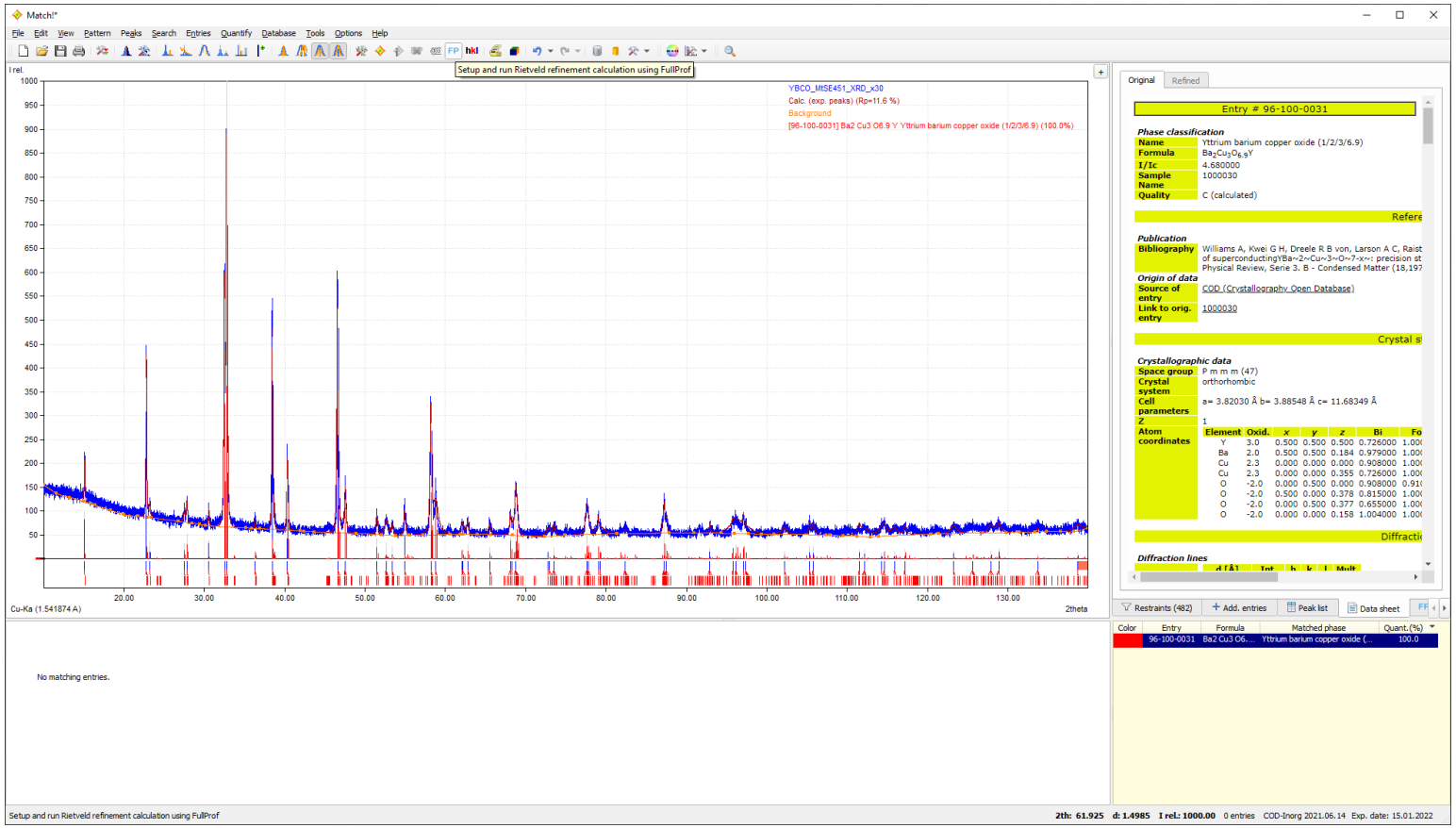
# Install FullProf



https://www.crystalimpact.com/match/download.htm#download



https://www.youtube.com/watch?v=jCD8nYdL-hY


Match!
File Edit View Pattern Peaks Search Entries Quantify Database Tools Options Help
Setup and run Rietveld refinement calculation using FullProf
I rel.
YBCO_MtSE451_XRD_x30
Calc. (exp. peaks) (Rp=11.6 %)
Background
[96-100-0031] Ba2 Cu3 O6.9 Y Yttrium barium copper oxide (1/2/3/6.9) (100.0%)
Cu-Ka (1.541874 A)
2theta
Original
Refined
Entry # 96-100-0031
Phase classification
Name
Formula
I/Ic
Sample Name
Quality
Yttrium barium copper oxide (1/2/3/6.9)
4.680000
1000030
C (calculated)
Publication
Bibliography
Origin of data
Source of entry
Link to orig. entry
COD (Crystallography Open Database)
1000030
Crystallographic data
Space group
Crystal system
Cell parameters
Z
Atom coordinates
P m m m (47)
orthorhombic
a= 3.82030 Å b= 3.88548 Å c= 11.68349 Å
1
Element Oxid. x y z Bi Fe
Y 3.0 0.500 0.500 0.500 0.726000 1.00
Ba 2.0 0.500 0.500 0.184 0.979000 1.00
Cu 2.3 0.000 0.000 0.000 0.908000 1.00
Cu 2.3 0.000 0.000 0.355 0.726000 1.00
O -2.0 0.000 0.500 0.000 0.908000 0.91
O -2.0 0.500 0.000 0.378 0.815000 1.00
O -2.0 0.500 0.000 0.377 0.655000 1.00
O -2.0 0.000 0.000 0.158 1.004000 1.00
Diffraction lines
Restraints (482)
Add. entries
Peak list
Data sheet
Color Entry Formula Matched phase Quant.(%)
96-100-0031 Ba2 Cu3 O6.... Yttrium barium copper oxide (... 100.0
No matching entries.
Setup and run Rietveld refinement calculation using FullProf
2th: 61.925 d: 1.4985 I rel.: 1000.00 0 entries COD-Inorg 2021.06.14 Exp. date: 15.01.2022

FP button

(1.54060*4+1.54443*2)/6

All Maps Shopping Images Videos More Tools

About 3,710 results (0.78 seconds)

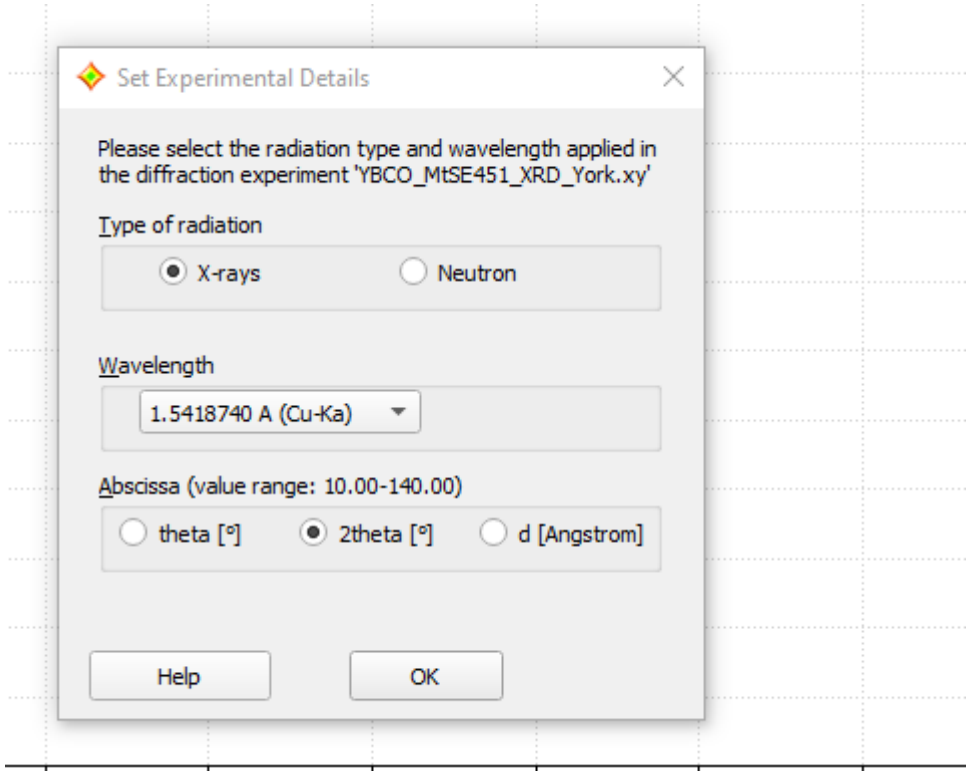
((1.54060 * 4) + (1.54443 * 2)) / 6 =

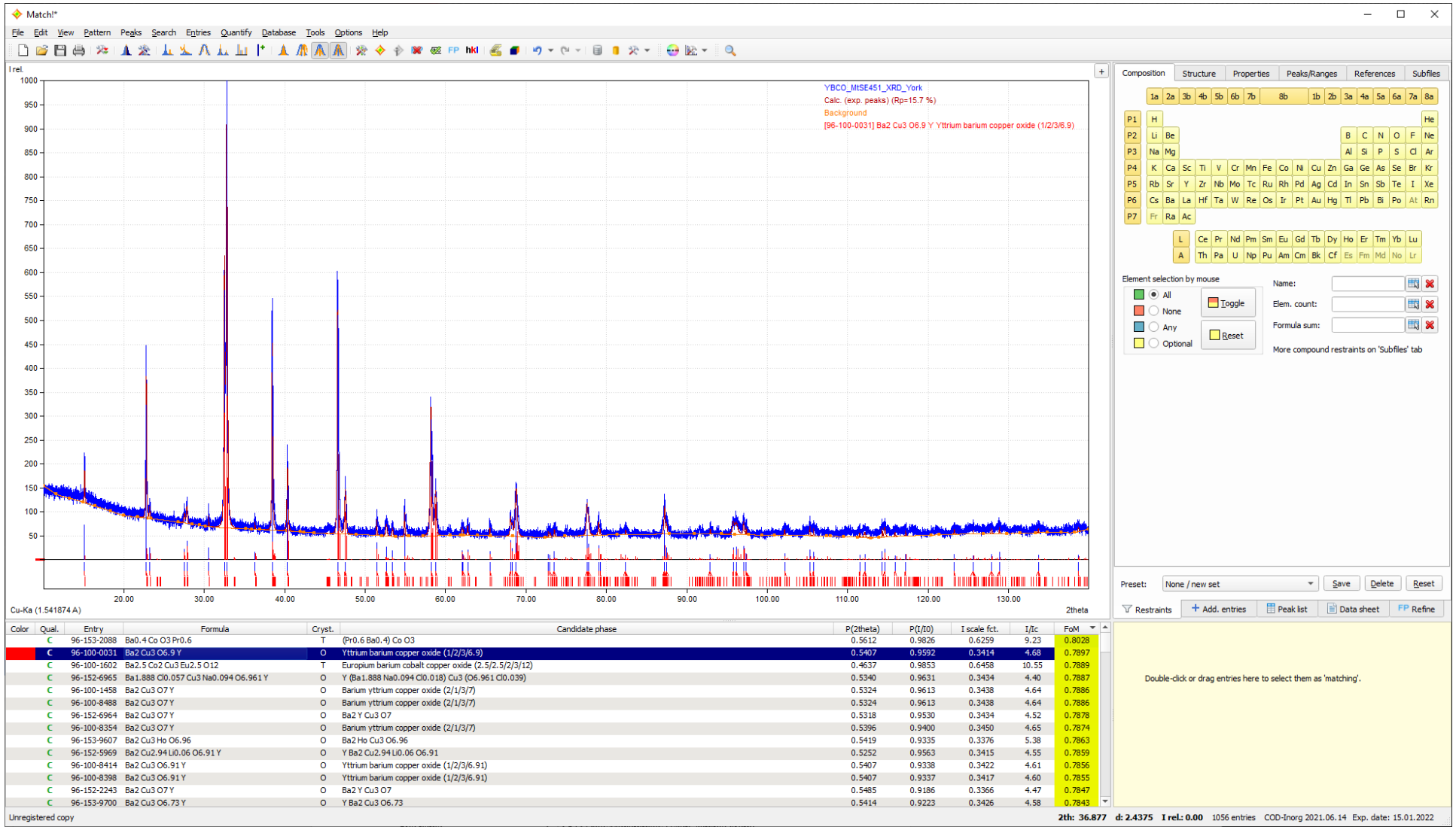
1.54187666667

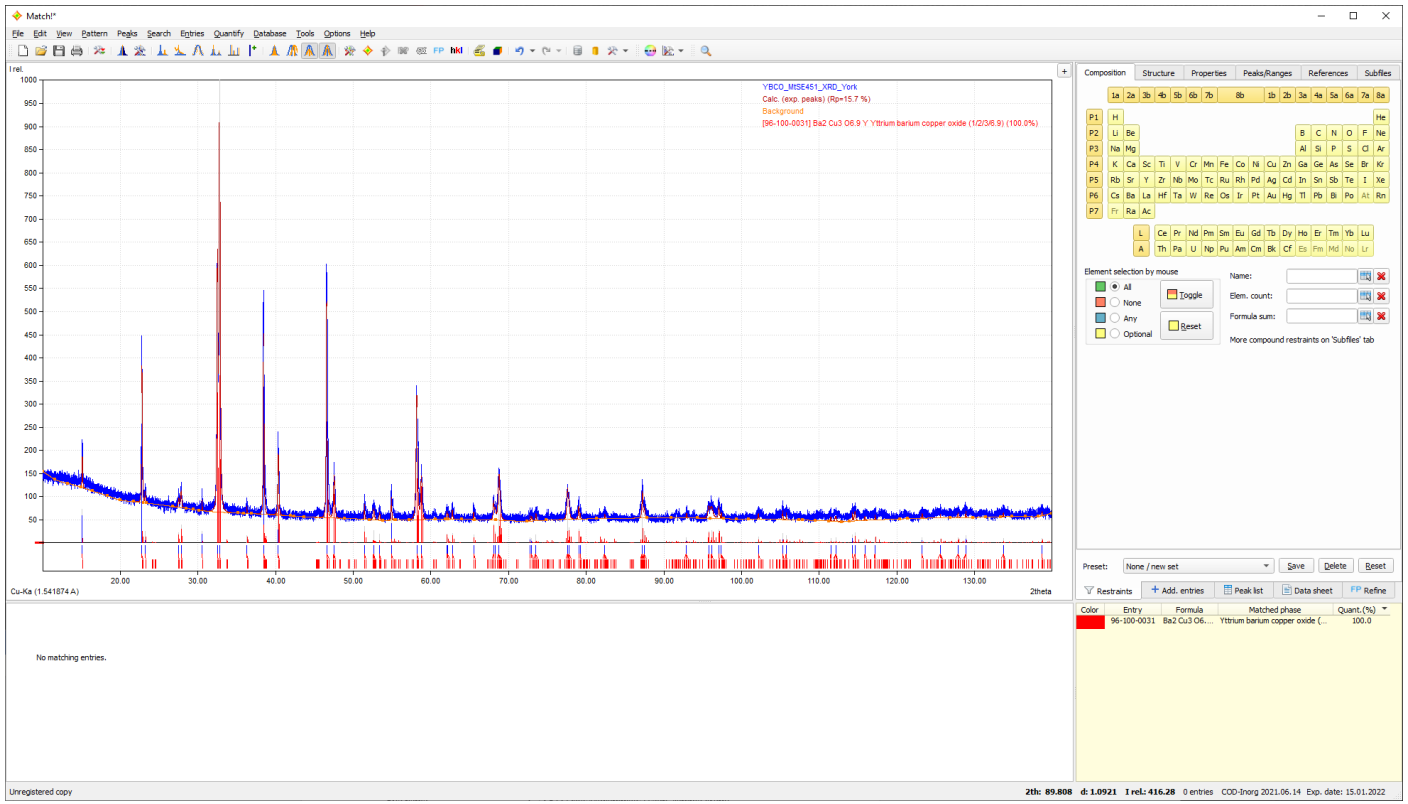
| | | | | | | |
|---|---|---|---|---|---|---|
| Rad \| Deg | x! | ( | ) | % | AC |
| Inv | sin | ln | 7 | 8 | 9 | ÷ |
| π | cos | log | 4 | 5 | 6 | × |
| e | tan | √ | 1 | 2 | 3 | − |
| Ans | EXP | $x^y$ | 0 | . | = | + |

More info

http://www.rsc.org › b904220b › b904220b PDF


Set Experimental Details
Please select the radiation type and wavelength applied in the diffraction experiment 'YBCO_MtSE451_XRD_York.xy'
Type of radiation
X-rays
Neutron
Wavelength
1.5418740 A (Cu-Ka)
Abscissa (value range: 10.00-140.00)
theta [°]
2theta [°]
d [Angstrom]
Help
OK


Match!*
File Edit View Pattern Peaks Search Entries Quantify Database Tools Options Help
I rel.
YBCO_MtSE451_XRD_York
Calc. (exp. peaks) (Rp=15.7 %)
Background
[96-100-0031] Ba2 Cu3 O6.9 Y Yttrium barium copper oxide (1/2/3/6.9)
Cu-Ka (1.541874 A)
2theta
Composition Structure Properties Peaks/Ranges References Subfiles
Element selection by mouse
All None Any Optional
Toggle Reset
Name:
Elem. count:
Formula sum:
More compound restraints on 'Subfiles' tab
Preset: None / new set Save Delete Reset
Restraints Add. entries Peak list Data sheet FP Refine
Double-click or drag entries here to select them as 'matching'.
Color Qual. Entry Formula Cryst. Candidate phase P(2theta) P(I/I0) I scale fct. I/Ic FoM
C 96-153-2088 Ba0.4 Co O3 Pr0.6 T (Pr0.6 Ba0.4) Co O3 0.5612 0.9826 0.6259 9.23 0.8028
C 96-100-0031 Ba2 Cu3 O6.9 Y O Yttrium barium copper oxide (1/2/3/6.9) 0.5407 0.9592 0.3414 4.68 0.7897
C 96-100-1602 Ba2.5 Co2 Cu3 Eu2.5 O12 T Europium barium cobalt copper oxide (2.5/2.5/2/3/12) 0.4637 0.9853 0.6458 10.55 0.7889
C 96-152-6965 Ba1.888 Cl0.057 Cu3 Na0.094 O6.961 Y O Y (Ba1.888 Na0.094 Cl0.018) Cu3 (O6.961 Cl0.039) 0.5340 0.9631 0.3434 4.40 0.7887
C 96-100-1458 Ba2 Cu3 O7 Y O Barium yttrium copper oxide (2/1/3/7) 0.5324 0.9613 0.3438 4.64 0.7886
C 96-100-8488 Ba2 Cu3 O7 Y O Barium yttrium copper oxide (2/1/3/7) 0.5324 0.9613 0.3438 4.64 0.7886
C 96-152-6964 Ba2 Cu3 O7 Y O Ba2 Y Cu3 O7 0.5318 0.9530 0.3434 4.52 0.7878
C 96-100-8354 Ba2 Cu3 O7 Y O Barium yttrium copper oxide (2/1/3/7) 0.5396 0.9400 0.3450 4.65 0.7874
C 96-153-9607 Ba2 Cu3 Ho O6.96 O Ba2 Ho Cu3 O6.96 0.5419 0.9335 0.3376 5.38 0.7863
C 96-152-5969 Ba2 Cu2.94 Li0.06 O6.91 Y O Y Ba2 Cu2.94 Li0.06 O6.91 0.5252 0.9563 0.3415 4.55 0.7859
C 96-100-8414 Ba2 Cu3 O6.91 Y O Yttrium barium copper oxide (1/2/3/6.91) 0.5407 0.9338 0.3422 4.61 0.7856
C 96-100-8398 Ba2 Cu3 O6.91 Y O Yttrium barium copper oxide (1/2/3/6.91) 0.5407 0.9337 0.3417 4.60 0.7855
C 96-152-2243 Ba2 Cu3 O7 Y O Ba2 Y Cu3 O7 0.5485 0.9186 0.3366 4.47 0.7847
C 96-153-9700 Ba2 Cu3 O6.73 Y O Y Ba2 Cu3 O6.73 0.5414 0.9223 0.3426 4.58 0.7843
Unregistered copy
2th: 36.877 d: 2.4375 I rel.: 0.00 1056 entries COD-Inorg 2021.06.14 Exp. date: 15.01.2022


Match!*
File Edit View Pattern Peaks Search Entries Quantify Database Tools Options Help
I rel.
YBCO_MISE451_XRD_York
Calc. (exp. peaks) (Rp=15.7 %)
Background
[96-100-0031] Ba2 Cu3 O6.9 Y Yttrium barium copper oxide (1/2/3/6.9) (100.0%)
Cu-Ka (1.541874 A)
2theta
No matching entries.
Composition
Structure
Properties
Peaks/Ranges
References
Subfiles
Element selection by mouse
All
None
Any
Optional
Toggle
Reset
Name:
Elem. count:
Formula sum:
More compound restraints on 'Subfiles' tab
Preset:
None / new set
Save
Delete
Reset
Restraints
Add. entries
Peak list
Data sheet
Refine
Color
Entry
Formula
Matched phase
Quant.(%)
96-100-0031
Ba2 Cu3 O6....
Yttrium barium copper oxide (...
100.0
Unregistered copy
2th: 89.808 d: 1.0921 I rel: 416.28 0 entries COD-Inorg 2021.06.14 Exp. date: 15.01.2022

FP

--Refine Scale factor and Run
--Refine shift on 2theta and Run
--Refine Specimen Displacement and Run
--Refine Unit Cell Parameters and Run
--First Background Parameter
-- Refine Profile Shape and Run
-- Reine W and run
-- Refine U and run
-- Refine V and run

Advanced
Peak Positions → Unit cell parameters
Peak Intensities → Intensity scaling of all phases

Atomic Coordinates in All phases

Overall Isotropic displacements parameters

Pref1, Preferred Orientation Factor 1

Pref2, Preferred Orientation Factor 2

Expert

Zero

Back1 1 -→ 10

show
Fpcalc.hkl

Fcalc.pcr

fpcalc.hkl

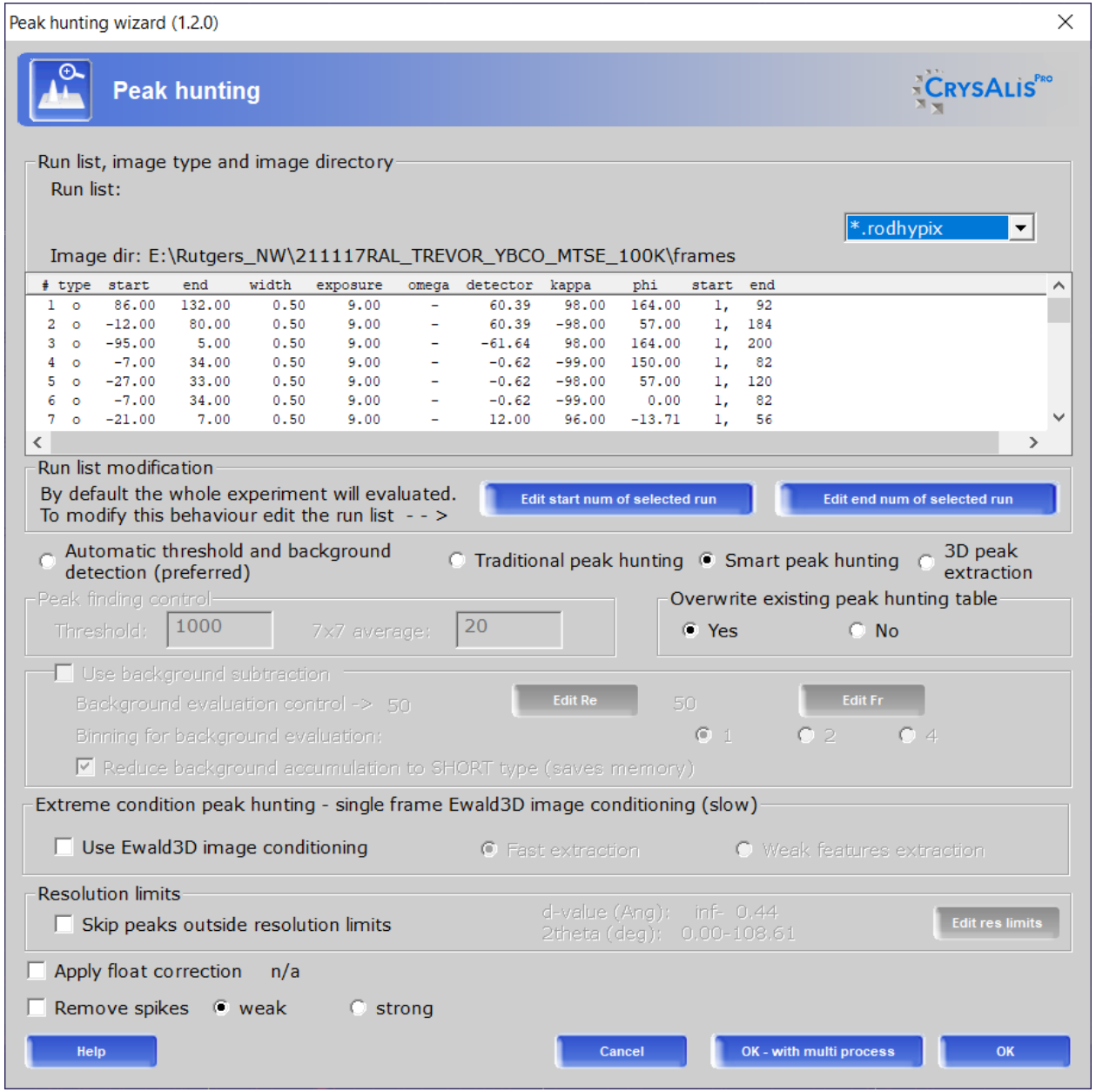
Pattern# 1 Phase No.: 1 Yttrium barium 483 reflections, N&T: 0 0.00 (The # of eff. reflections may be lower)

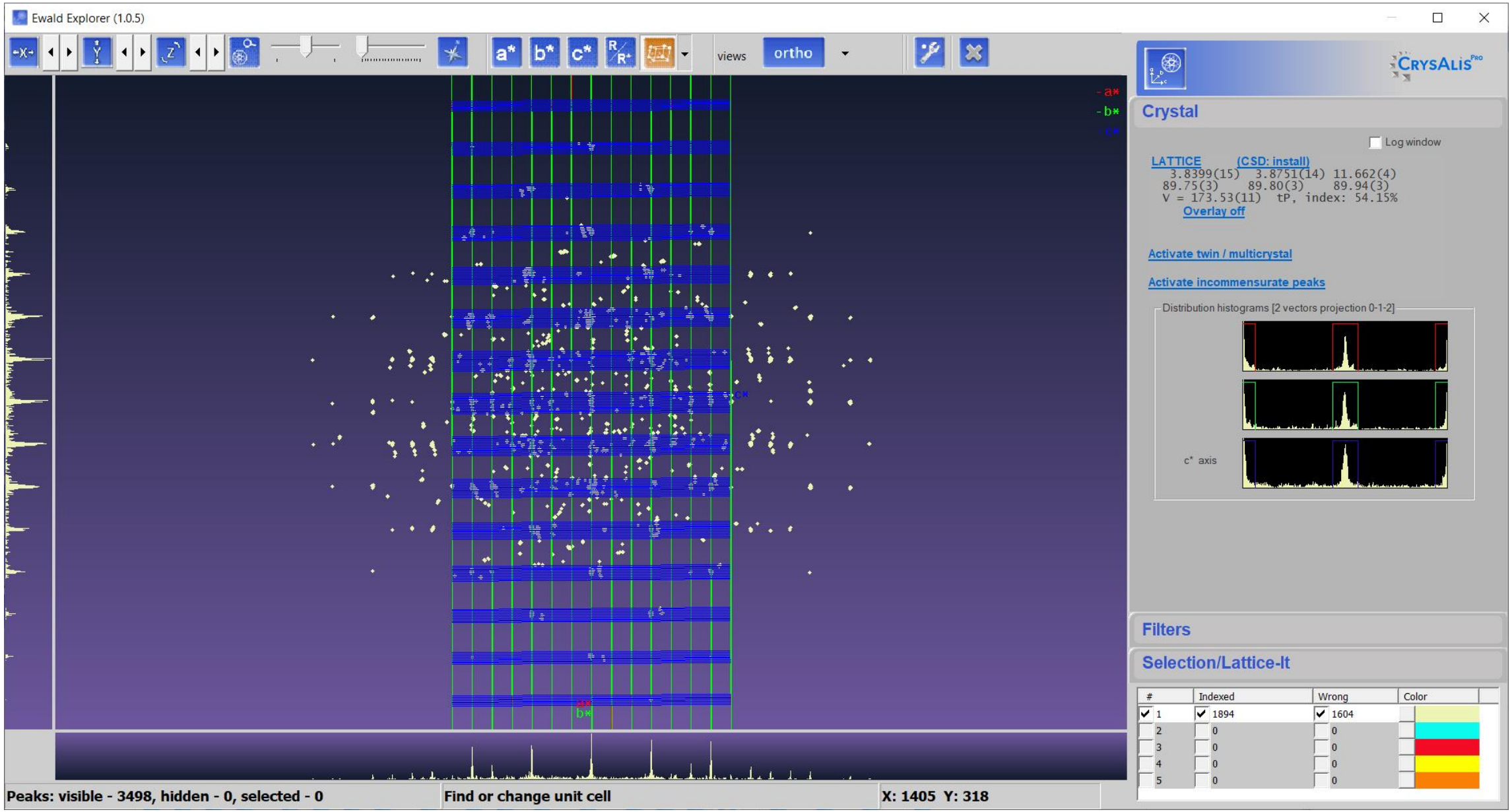
! SPGR: -P 2 2; CELL: 3.82050 3.88631 11.68000 90.00000 90.00000 90.00000

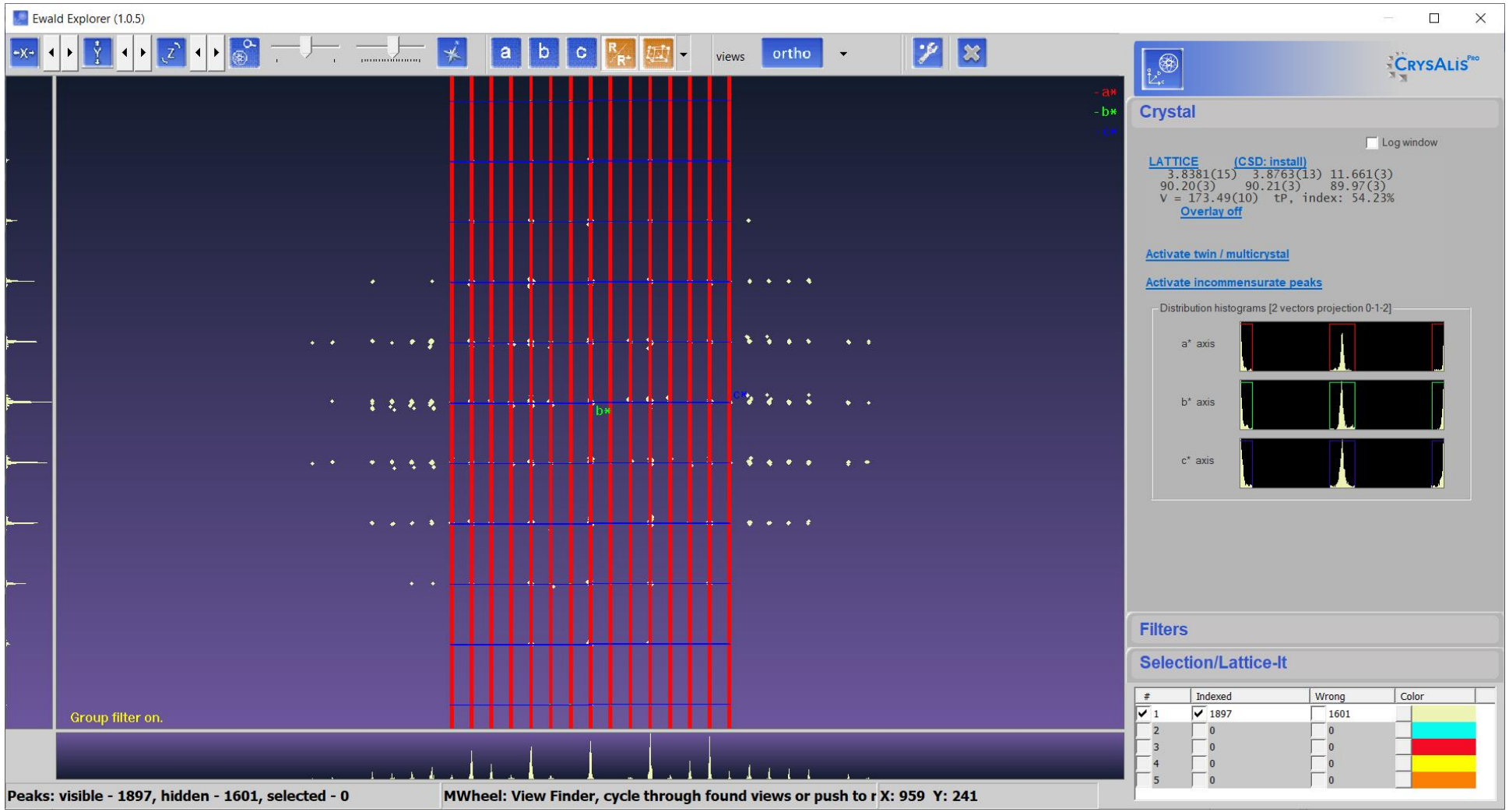
| Code | h | k | l | Mult | D(A) | 2T | HW | Iobs | Icalc | io-ic |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 2 | 2 | 5.840000 | 15.159 | 0.164836 | 66.0 | 11.5 | 54.6 |
| 2 | 0 | 0 | 2 | 2 | 5.840000 | 15.197 | 0.164835 | 33.6 | 5.7 | 27.9 |
| 1 | 0 | 0 | 3 | 2 | 3.893334 | 22.823 | 0.164857 | 65.7 | 26.7 | 39.0 |
| 1 | 0 | 1 | 0 | 2 | 3.886310 | 22.864 | 0.164858 | 73.4 | 32.2 | 41.2 |
| 2 | 0 | 0 | 3 | 2 | 3.893334 | 22.880 | 0.164858 | 28.7 | 13.3 | 15.5 |
| 2 | 0 | 1 | 0 | 2 | 3.886310 | 22.922 | 0.164859 | 29.4 | 16.0 | 13.4 |
| 1 | 1 | 0 | 0 | 2 | 3.820500 | 23.264 | 0.164867 | 14.2 | 18.7 | -4.5 |
| 2 | 1 | 0 | 0 | 2 | 3.820500 | 23.322 | 0.164868 | 6.0 | 9.3 | -3.2 |
| 1 | 0 | 1 | 1 | 4 | 3.687542 | 24.115 | 0.164889 | 0.0 | 2.3 | -2.3 |
| 2 | 0 | 1 | 1 | 4 | 3.687542 | 24.176 | 0.164891 | 0.0 | 1.1 | -1.1 |
| 1 | 1 | 0 | 1 | 4 | 3.631180 | 24.495 | 0.164900 | 0.0 | 0.7 | -0.7 |
| 2 | 1 | 0 | 1 | 4 | 3.631180 | 24.557 | 0.164902 | 0.0 | 0.3 | -0.3 |
| 1 | 0 | 1 | 2 | 4 | 3.235400 | 27.547 | 0.165015 | 2.1 | 16.1 | -14.1 |
| 2 | 0 | 1 | 2 | 4 | 3.235400 | 27.617 | 0.165018 | 2.8 | 8.0 | -5.2 |
| 1 | 1 | 0 | 2 | 4 | 3.197131 | 27.883 | 0.165031 | 10.3 | 28.1 | -17.8 |
| 2 | 1 | 0 | 2 | 4 | 3.197131 | 27.954 | 0.165034 | 4.1 | 14.0 | -9.9 |
| 1 | 0 | 0 | 4 | 2 | 2.920000 | 30.591 | 0.165179 | 10.6 | 2.7 | 7.8 |
| 2 | 0 | 0 | 4 | 2 | 2.920000 | 30.669 | 0.165184 | 4.7 | 1.4 | 3.4 |
| 1 | 0 | 1 | 3 | 4 | 2.750516 | 32.527 | 0.165310 | 258.9 | 285.9 | -27.1 |
| 2 | 0 | 1 | 3 | 4 | 2.750516 | 32.610 | 0.165316 | 140.0 | 142.2 | -2.1 |
| 1 | 1 | 0 | 3 | 4 | 2.726887 | 32.817 | 0.165331 | 255.9 | 319.3 | -63.4 |
| 1 | 1 | 1 | 0 | 4 | 2.724471 | 32.847 | 0.165334 | 243.5 | 307.5 | -64.1 |
| 2 | 1 | 0 | 3 | 4 | 2.726887 | 32.901 | 0.165338 | 123.7 | 158.8 | -35.1 |
| 2 | 1 | 1 | 0 | 4 | 2.724471 | 32.931 | 0.165340 | 119.3 | 152.9 | -33.6 |
| 1 | 1 | 1 | 1 | 8 | 2.653245 | 33.755 | 0.165404 | 7.1 | 6.4 | 0.7 |
| 2 | 1 | 1 | 1 | 8 | 2.653245 | 33.841 | 0.165411 | 3.2 | 3.2 | 0.0 |
| 1 | 1 | 1 | 2 | 8 | 2.469009 | 36.358 | 0.165632 | 7.3 | 14.0 | -6.7 |
| 2 | 1 | 1 | 2 | 8 | 2.469009 | 36.452 | 0.165641 | 2.4 | 7.0 | -4.5 |
| 1 | 0 | 0 | 5 | 2 | 2.336000 | 38.507 | 0.165852 | 126.1 | 34.8 | 91.3 |
| 1 | 0 | 1 | 4 | 4 | 2.334480 | 38.533 | 0.165855 | 67.7 | 18.8 | 48.9 |
| 2 | 0 | 0 | 5 | 2 | 2.336000 | 38.607 | 0.165863 | 54.0 | 17.3 | 36.8 |
| 2 | 0 | 1 | 4 | 4 | 2.334480 | 38.633 | 0.165866 | 26.9 | 9.3 | 17.5 |

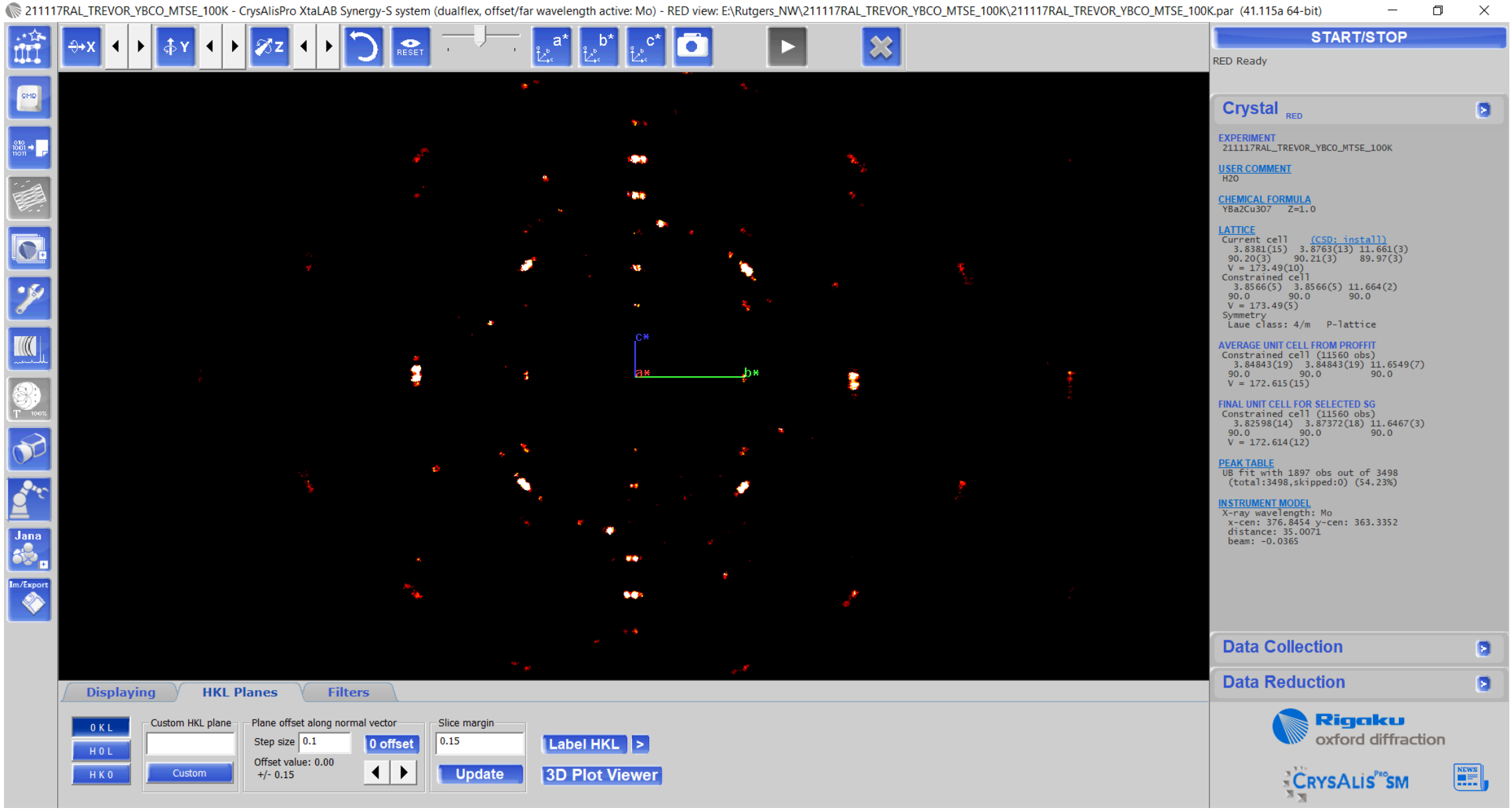
Close

# Single Crystal Analysis and YBCO

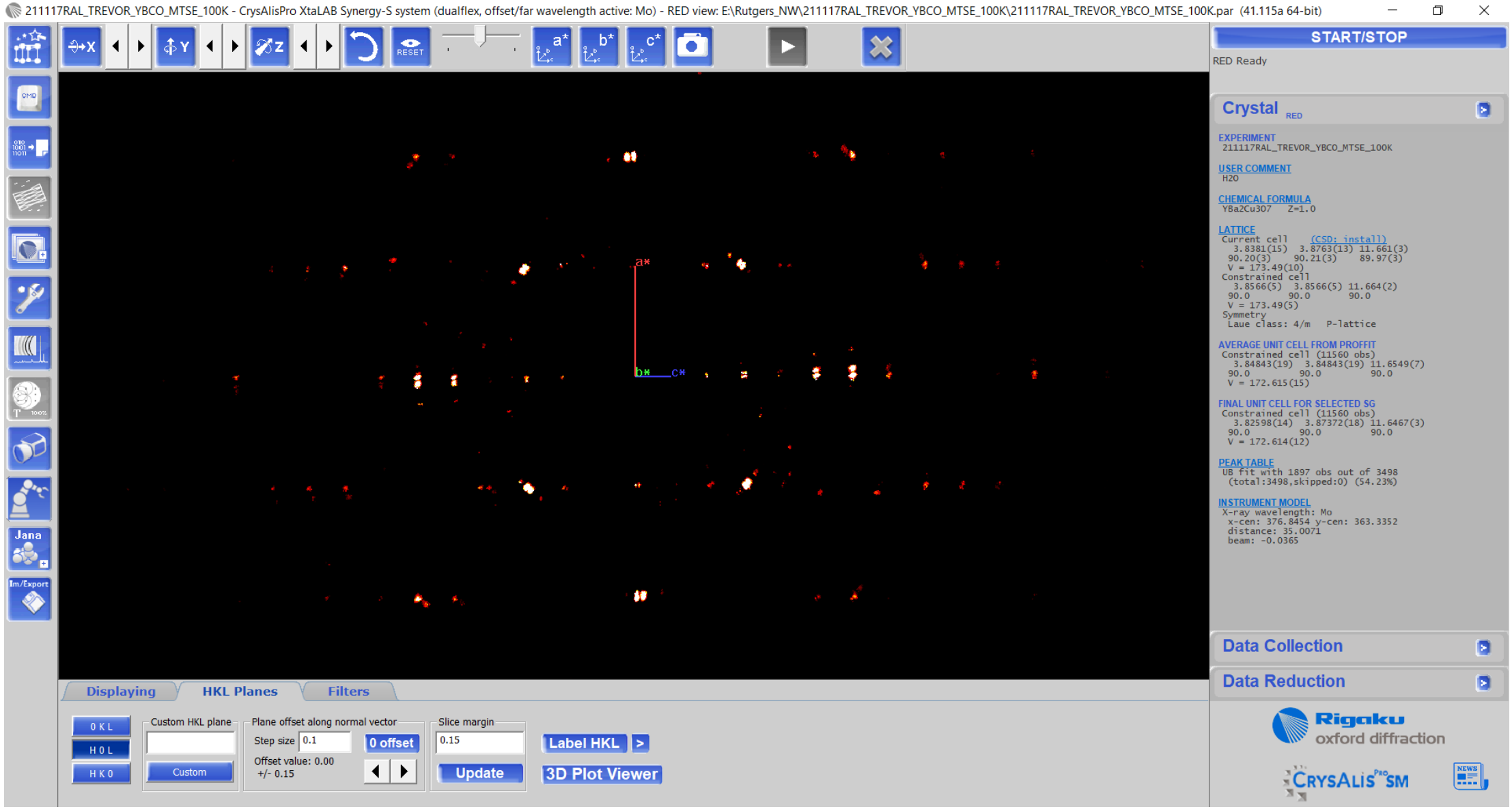

Peak hunting wizard (1.2.0)
Peak hunting
CrysAlis Pro
Run list, image type and image directory
Run list:
*.rodhypix
Image dir: E:\Rutgers_NW\211117RAL_TREVOR_YBCO_MTSE_100K\frames
# type start end width exposure omega detector kappa phi start end
1 o 86.00 132.00 0.50 9.00 - 60.39 98.00 164.00 1, 92
2 o -12.00 80.00 0.50 9.00 - 60.39 -98.00 57.00 1, 184
3 o -95.00 5.00 0.50 9.00 - -61.64 98.00 164.00 1, 200
4 o -7.00 34.00 0.50 9.00 - -0.62 -99.00 150.00 1, 82
5 o -27.00 33.00 0.50 9.00 - -0.62 -98.00 57.00 1, 120
6 o -7.00 34.00 0.50 9.00 - -0.62 -99.00 0.00 1, 82
7 o -21.00 7.00 0.50 9.00 - 12.00 96.00 -13.71 1, 56
Run list modification
By default the whole experiment will evaluated.
To modify this behaviour edit the run list - - >
Edit start num of selected run
Edit end num of selected run
Automatic threshold and background detection (preferred)
Traditional peak hunting
Smart peak hunting
3D peak extraction
Peak finding control
Threshold: 1000
7x7 average: 20
Overwrite existing peak hunting table
Yes
No
Use background subtraction
Background evaluation control -> 50
Edit Re
50
Edit Fr
Binning for background evaluation:
1
2
4
Reduce background accumulation to SHORT type (saves memory)
Extreme condition peak hunting - single frame Ewald3D image conditioning (slow)
Use Ewald3D image conditioning
Fast extraction
Weak features extraction
Resolution limits
Skip peaks outside resolution limits
d-value (Ang): inf- 0.44
2theta (deg): 0.00-108.61
Edit res limits
Apply float correction n/a
Remove spikes
weak
strong
Help
Cancel
OK - with multi process
OK


Ewald Explorer (1.0.5)
views
ortho
-a*
-b*
-c*
CrysAlis Pro
Crystal
Log window
LATTICE (CSD: install)
3.8399(15) 3.8751(14) 11.662(4)
89.75(3) 89.80(3) 89.94(3)
V = 173.53(11) tP, index: 54.15%
Overlay off
Activate twin / multicrystal
Activate incommensurate peaks
Distribution histograms [2 vectors projection 0-1-2]
c* axis
Filters
Selection/Lattice-It
# Indexed Wrong Color
1 1894 1604
2 0 0
3 0 0
4 0 0
5 0 0
Peaks: visible - 3498, hidden - 0, selected - 0
Find or change unit cell
X: 1405 Y: 318

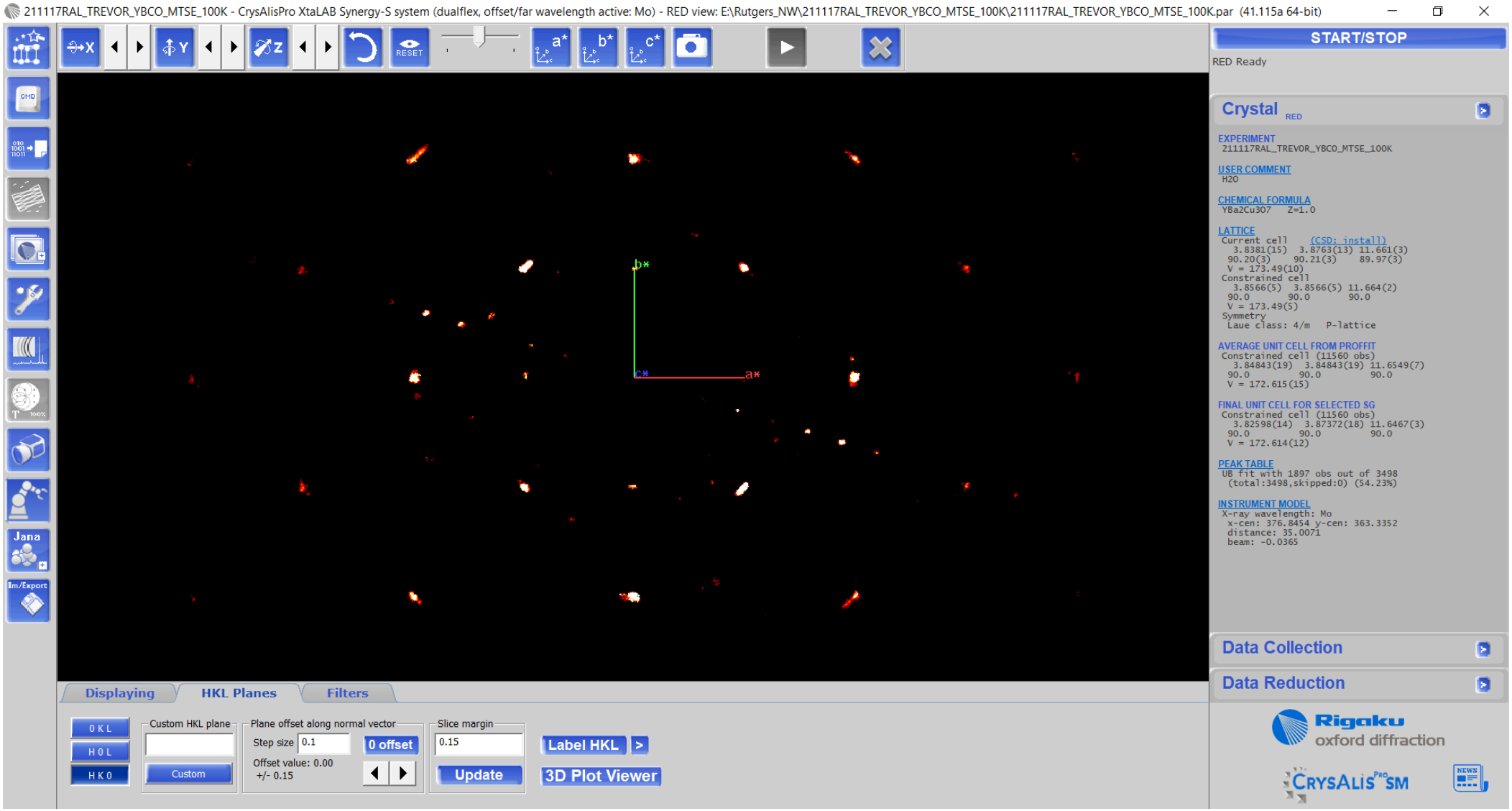

Ewald Explorer (1.0.5)
views
ortho
- a*
- b*
- c*
Group filter on.
Peaks: visible - 1897, hidden - 1601, selected - 0
MWheel: View Finder, cycle through found views or push to r
X: 959 Y: 241
CrysAlis Pro
Crystal
Log window
LATTICE (CSD: install)
3.8381(15) 3.8763(13) 11.661(3)
90.20(3) 90.21(3) 89.97(3)
V = 173.49(10) tP, index: 54.23%
Overlay off
Activate twin / multicrystal
Activate incommensurate peaks
Distribution histograms [2 vectors projection 0-1-2]
a* axis
b* axis
c* axis
Filters
Selection/Lattice-It
# Indexed Wrong Color
1 1897 1601
2 0 0
3 0 0
4 0 0
5 0 0


211117RAL_TREVOR_YBCO_MTSE_100K - CrysAlisPro XtaLAB Synergy-S system (dualflex, offset/far wavelength active: Mo) - RED view: E:\Rutgers_NW\211117RAL_TREVOR_YBCO_MTSE_100K\211117RAL_TREVOR_YBCO_MTSE_100K.par (41.115a 64-bit)
START/STOP
RED Ready
Crystal RED
EXPERIMENT
211117RAL_TREVOR_YBCO_MTSE_100K
USER COMMENT
H2O
CHEMICAL FORMULA
YBa2Cu3O7 Z=1.0
LATTICE
Current cell (CSD: install)
3.8381(15) 3.8763(13) 11.661(3)
90.20(3) 90.21(3) 89.97(3)
V = 173.49(10)
Constrained cell
3.8566(5) 3.8566(5) 11.664(2)
90.0 90.0 90.0
V = 173.49(5)
Symmetry
Laue class: 4/m P-lattice
AVERAGE UNIT CELL FROM PROFFIT
Constrained cell (11560 obs)
3.84843(19) 3.84843(19) 11.6549(7)
90.0 90.0 90.0
V = 172.615(15)
FINAL UNIT CELL FOR SELECTED SG
Constrained cell (11560 obs)
3.82598(14) 3.87372(18) 11.6467(3)
90.0 90.0 90.0
V = 172.614(12)
PEAK TABLE
UB fit with 1897 obs out of 3498
(total:3498,skipped:0) (54.23%)
INSTRUMENT MODEL
X-ray wavelength: Mo
x-cen: 376.8454 y-cen: 363.3352
distance: 35.0071
beam: -0.0365
Data Collection
Data Reduction
Rigaku
oxford diffraction
CrysAlis Pro SM
Displaying
HKL Planes
Filters
0 K L
H 0 L
H K 0
Custom HKL plane
Custom
Plane offset along normal vector
Step size 0.1
0 offset
Offset value: 0.00
+/- 0.15
Slice margin
0.15
Update
Label HKL
3D Plot Viewer

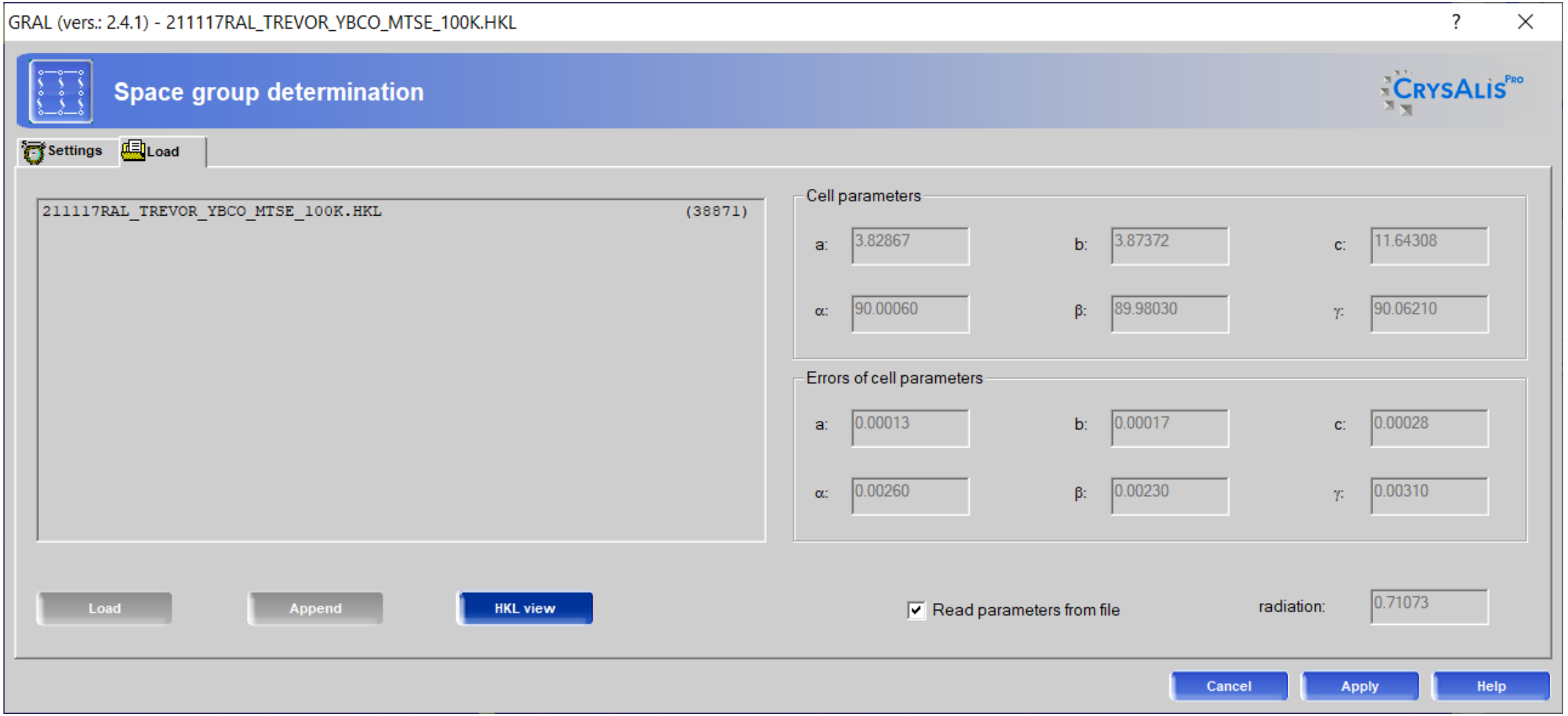
(0KL) Twinned

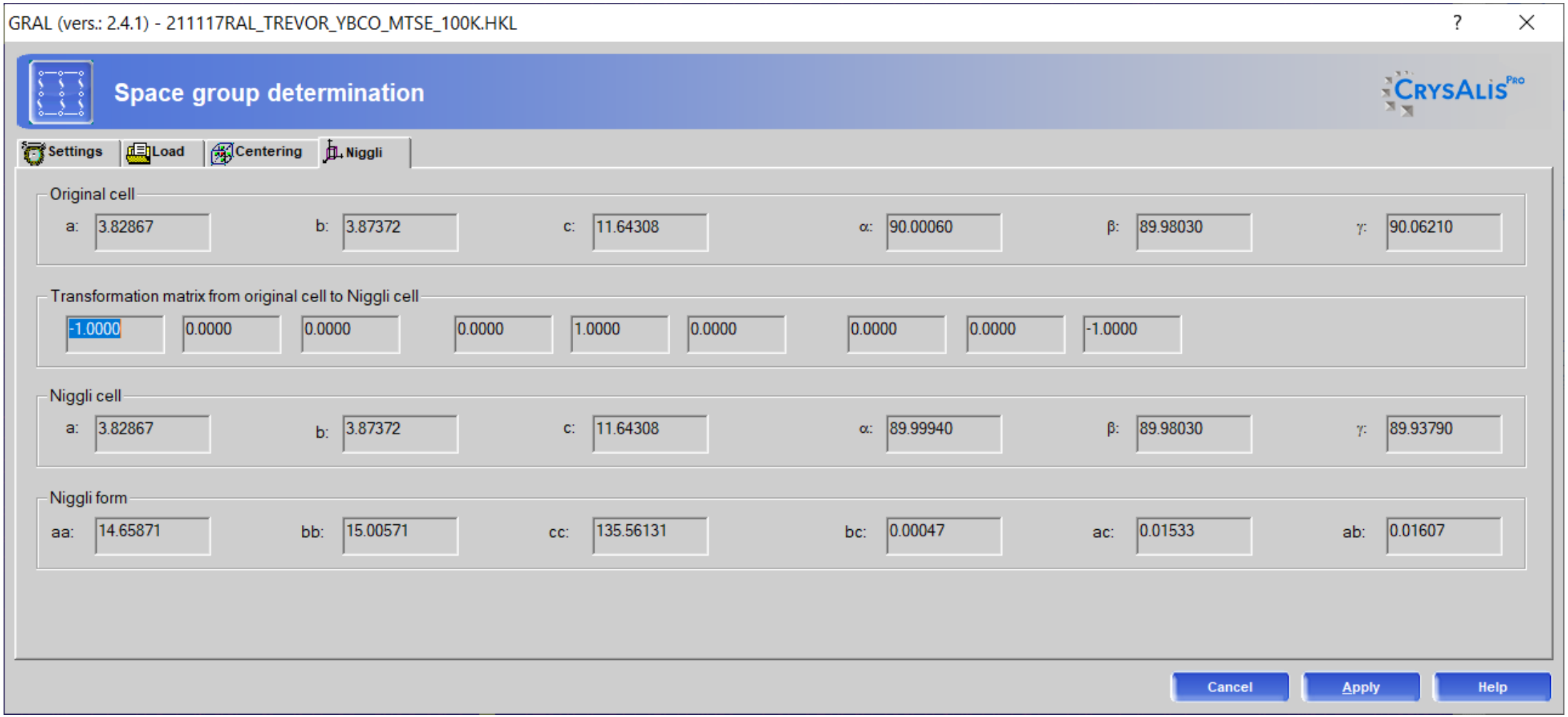

211117RAL_TREVOR_YBCO_MTSE_100K - CrysAlisPro XtaLAB Synergy-S system (dualflex, offset/far wavelength active: Mo) - RED view: E:\Rutgers_NW\211117RAL_TREVOR_YBCO_MTSE_100K\211117RAL_TREVOR_YBCO_MTSE_100K.par (41.115a 64-bit)
START/STOP
RED Ready
Crystal RED
EXPERIMENT
211117RAL_TREVOR_YBCO_MTSE_100K
USER COMMENT
H2O
CHEMICAL FORMULA
YBa2Cu3O7 Z=1.0
LATTICE
Current cell (CSD: install)
3.8381(15) 3.8763(13) 11.661(3)
90.20(3) 90.21(3) 89.97(3)
V = 173.49(10)
Constrained cell
3.8566(5) 3.8566(5) 11.664(2)
90.0 90.0 90.0
V = 173.49(5)
Symmetry
Laue class: 4/m P-lattice
AVERAGE UNIT CELL FROM PROFFIT
Constrained cell (11560 obs)
3.84843(19) 3.84843(19) 11.6549(7)
90.0 90.0 90.0
V = 172.615(15)
FINAL UNIT CELL FOR SELECTED SG
Constrained cell (11560 obs)
3.82598(14) 3.87372(18) 11.6467(3)
90.0 90.0 90.0
V = 172.614(12)
PEAK TABLE
UB fit with 1897 obs out of 3498
(total:3498,skipped:0) (54.23%)
INSTRUMENT MODEL
X-ray wavelength: Mo
x-cen: 376.8454 y-cen: 363.3352
distance: 35.0071
beam: -0.0365
Data Collection
Data Reduction
Rigaku
oxford diffraction
CrysAlis Pro SM
RESET
a*
b*
c*
Displaying
HKL Planes
Filters
0 K L
H 0 L
H K 0
Custom HKL plane
Custom
Plane offset along normal vector
Step size 0.1
0 offset
Offset value: 0.00
+/- 0.15
Slice margin
0.15
Update
Label HKL
3D Plot Viewer

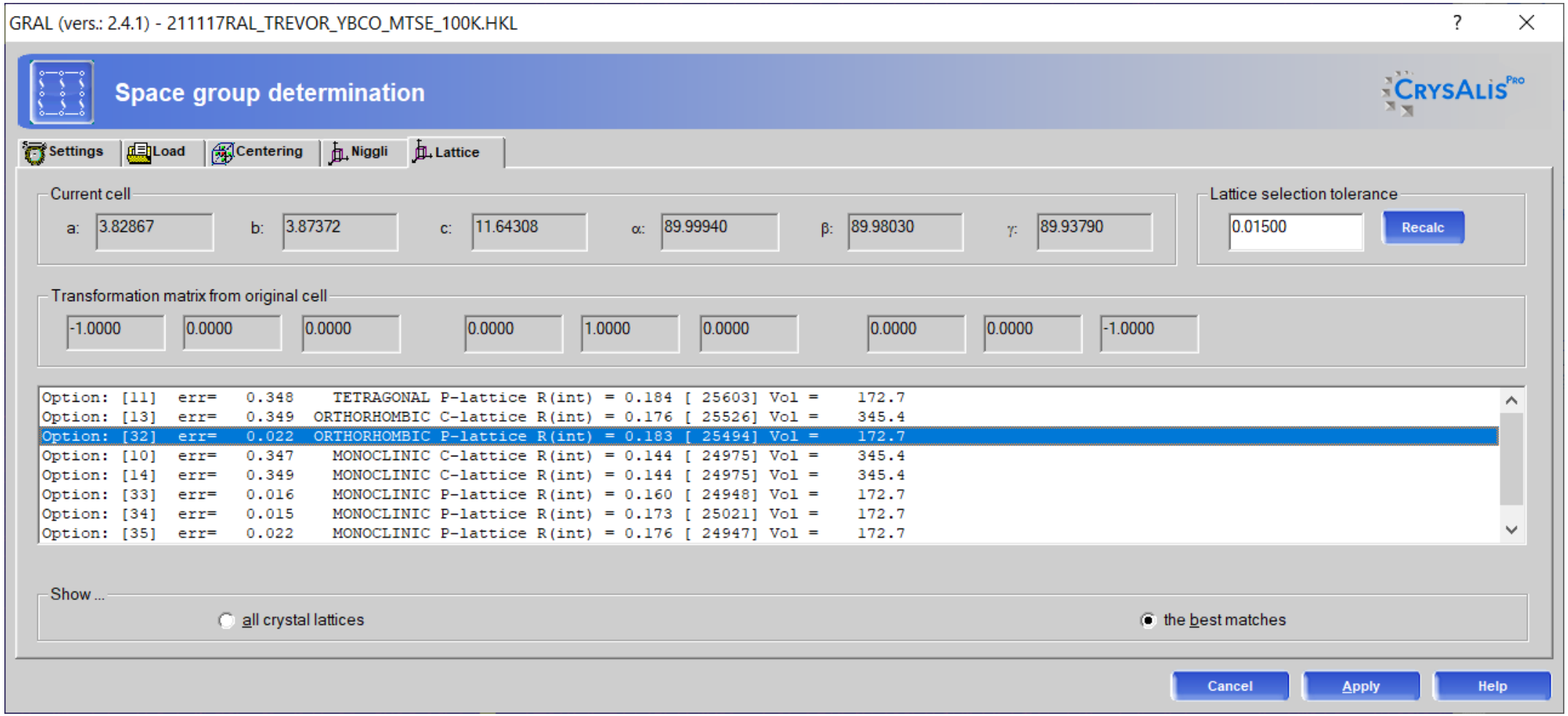
(H0L) Twinned


211117RAL_TREVOR_YBCO_MTSE_100K - CrysAlisPro XtaLAB Synergy-S system (dualflex, offset/far wavelength active: Mo) - RED view: E:\Rutgers_NW\211117RAL_TREVOR_YBCO_MTSE_100K\211117RAL_TREVOR_YBCO_MTSE_100K.par (41.115a 64-bit)
START/STOP
RED Ready
Crystal RED
EXPERIMENT
211117RAL_TREVOR_YBCO_MTSE_100K
USER COMMENT
H2O
CHEMICAL FORMULA
YBa2Cu3O7 Z=1.0
LATTICE
Current cell (CSD: install)
3.8381(15) 3.8763(13) 11.661(3)
90.20(3) 90.21(3) 89.97(3)
V = 173.49(10)
Constrained cell
3.8566(5) 3.8566(5) 11.664(2)
90.0 90.0 90.0
V = 173.49(5)
Symmetry
Laue class: 4/m P-lattice
AVERAGE UNIT CELL FROM PROFFIT
Constrained cell (11560 obs)
3.84843(19) 3.84843(19) 11.6549(7)
90.0 90.0 90.0
V = 172.615(15)
FINAL UNIT CELL FOR SELECTED SG
Constrained cell (11560 obs)
3.82598(14) 3.87372(18) 11.6467(3)
90.0 90.0 90.0
V = 172.614(12)
PEAK TABLE
UB fit with 1897 obs out of 3498
(total:3498,skipped:0) (54.23%)
INSTRUMENT MODEL
X-ray wavelength: Mo
x-cen: 376.8454 y-cen: 363.3352
distance: 35.0071
beam: -0.0365
Data Collection
Data Reduction
Rigaku
oxford diffraction
CrysAlisPro SM
Displaying
HKL Planes
Filters
0 K L
H 0 L
H K 0
Custom HKL plane
Custom
Plane offset along normal vector
Step size 0.1
0 offset
Offset value: 0.00
+/- 0.15
Slice margin
0.15
Update
Label HKL
3D Plot Viewer

(HK0) Twinned


GRAL (vers.: 2.4.1) - 211117RAL_TREVOR_YBCO_MTSE_100K.HKL
Space group determination
CrysAlis Pro
Settings
Load
211117RAL_TREVOR_YBCO_MTSE_100K.HKL (38871)
Cell parameters
a: 3.82867
b: 3.87372
c: 11.64308
α: 90.00060
β: 89.98030
γ: 90.06210
Errors of cell parameters
a: 0.00013
b: 0.00017
c: 0.00028
α: 0.00260
β: 0.00230
γ: 0.00310
Load
Append
HKL view
Read parameters from file
radiation: 0.71073
Cancel
Apply
Help


GRAL (vers.: 2.4.1) - 211117RAL_TREVOR_YBCO_MTSE_100K.HKL
Space group determination
CrysAlis Pro
Settings
Load
Centering
Niggli
Original cell
a: 3.82867
b: 3.87372
c: 11.64308
α: 90.00060
β: 89.98030
γ: 90.06210
Transformation matrix from original cell to Niggli cell
-1.0000 0.0000 0.0000
0.0000 1.0000 0.0000
0.0000 0.0000 -1.0000
Niggli cell
a: 3.82867
b: 3.87372
c: 11.64308
α: 89.99940
β: 89.98030
γ: 89.93790
Niggli form
aa: 14.65871
bb: 15.00571
cc: 135.56131
bc: 0.00047
ac: 0.01533
ab: 0.01607
Cancel
Apply
Help


GRAL (vers.: 2.4.1) - 211117RAL_TREVOR_YBCO_MTSE_100K.HKL
Space group determination
CrysAlis Pro
Settings
Load
Centering
Niggli
Lattice
Current cell
a: 3.82867
b: 3.87372
c: 11.64308
α: 89.99940
β: 89.98030
γ: 89.93790
Lattice selection tolerance
0.01500
Recalc
Transformation matrix from original cell
-1.0000 0.0000 0.0000
0.0000 1.0000 0.0000
0.0000 0.0000 -1.0000
Option: [11] err= 0.348 TETRAGONAL P-lattice R(int) = 0.184 [ 25603] Vol = 172.7
Option: [13] err= 0.349 ORTHORHOMBIC C-lattice R(int) = 0.176 [ 25526] Vol = 345.4
Option: [32] err= 0.022 ORTHORHOMBIC P-lattice R(int) = 0.183 [ 25494] Vol = 172.7
Option: [10] err= 0.347 MONOCLINIC C-lattice R(int) = 0.144 [ 24975] Vol = 345.4
Option: [14] err= 0.349 MONOCLINIC C-lattice R(int) = 0.144 [ 24975] Vol = 345.4
Option: [33] err= 0.016 MONOCLINIC P-lattice R(int) = 0.160 [ 24948] Vol = 172.7
Option: [34] err= 0.015 MONOCLINIC P-lattice R(int) = 0.173 [ 25021] Vol = 172.7
Option: [35] err= 0.022 MONOCLINIC P-lattice R(int) = 0.176 [ 24947] Vol = 172.7
Show ...
all crystal lattices
the best matches
Cancel
Apply
Help

GRAL (vers.: 2.4.1) - 211117RAL_TREVOR_YBCO_MTSE_100K.HKL

## Space group determination

CrysAlis Pro

Settings | Load | Centering | Niggli | Lattice | Centering | <E2-1> | Space Group

Systematic absence exceptions:

| | 21-- | b-- | c-- | n-- | -21- | -a- | -c- | -n- | --21 | --a | --b | --n |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| N | 44 | 1295 | 1312 | 1277 | 26 | 1621 | 1646 | 1603 | 132 | 432 | 420 | 406 |
| N I>3s | 19 | 842 | 865 | 975 | 23 | 922 | 974 | 1080 | 103 | 338 | 353 | 247 |
| <I> | 3.2 | 16.6 | 17.2 | 15.7 | 6.8 | 13.2 | 14.0 | 13.1 | 25.5 | 34.6 | 35.9 | 4.0 |
| <I/s> | 2.8 | 4.0 | 4.0 | 4.6 | 5.5 | 3.5 | 3.6 | 4.1 | 4.9 | 4.8 | 5.1 | 3.6 |

Active filter: (•) None ( ) Non-centro ( ) Chiral

| # | Space Group | No. | C/A | En. | O.A. | Pie. | Pyr. | CCDC | ICSD | R(int) | N(eq) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | P222 (abc) | 16 | A | Y | Y | Y | N | 20 | 8 | 0.181 | 25054 |
| 2 | Pmm2 (abc) | 25 | A | N | ? | Y | Y | 10 | 26 | 0.178 | 24821 |
| 3 | Pmm2 (-cba) | 25 | A | N | ? | Y | Y | 10 | 26 | 0.181 | 24908 |
| 4 | Pmm2 (a-cb) | 25 | A | N | ? | Y | Y | 10 | 26 | 0.176 | 24909 |
| 5 | Pmmm (abc) | 47 | C | N | N | N | N | 9 | 681 | 0.183 | 25494 |

Show ...

( ) all space groups ( ) all solutions on a branch (like in IT pp 42-47, 55-67) (•) most likely space groups ( ) advanced space group selection

Cancel | Apply | Help

GRAL (vers.: 2.4.1) - 211117RAL_TREVOR_YBCO_MTSE_100K.HKL

# Space group determination

CrysAlis Pro

Settings | Load | Centering | Niggli | Lattice | Centering | <E2-1> | Space Group | Ins-File

Z: 1

Import formula

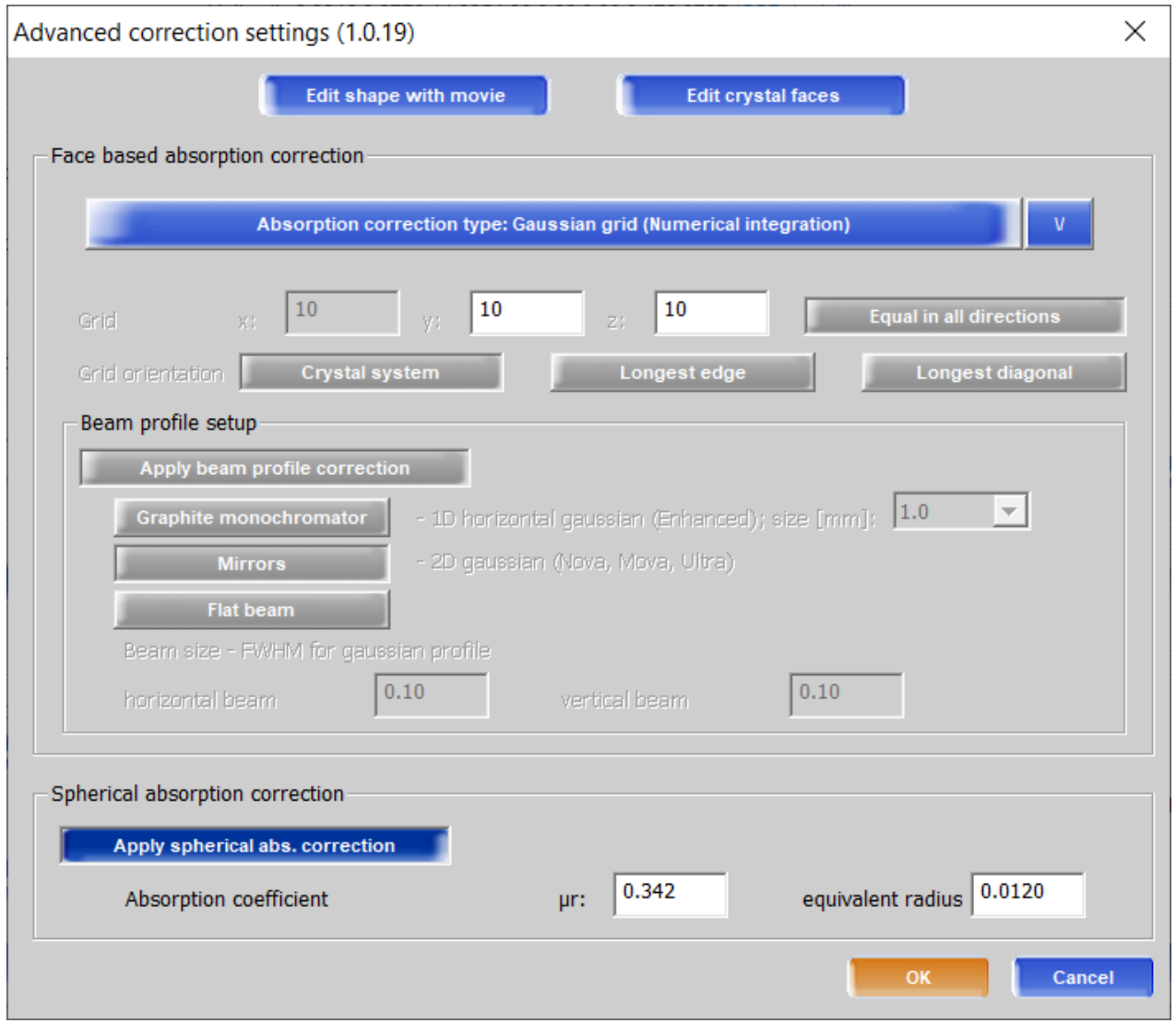
Chemical formula: YBa2Cu3O7

```
TITL 211117RAL_TREVOR_YBCO_MTSE_100K in Pmmm
REM Pmmm (#47 in standard setting)
CELL 0.71073   3.828670   3.873720  11.643080  89.9994  89.9803  89.9379
ZERR    1.00   0.000130   0.000170   0.000280   0.0026   0.0023   0.0031
LATT  1
SYMM -x,-y, z
SYMM -x, y,-z
SYMM  x,-y,-z
SFAC O Cu Y Ba
UNIT 7.00 3.00 1.00 2.00
REM  CrysAlisPro recorded range (K): Min=99.9; max=100.1; aver:100.0
TEMP -173
TREF
HKLF 4
END
```

```
Formula wt: 666.21
Mu(mm-1): 28.59
Density: 6.406
F(000): 294.00
At.vol: 13.28
Non-H : 13.28
4 element(s):
  O=7.00(16.81%)
  Cu=3.00(28.61%)
  Y=1.00(13.35%)
  Ba=2.00(41.23%)
```

NOTE: Unconstrained cell visible above will be afterwards replaced by a refined constrained one

Cancel | Finish | Help


Advanced correction settings (1.0.19)
Edit shape with movie
Edit crystal faces
Face based absorption correction
Absorption correction type: Gaussian grid (Numerical integration)
V
Grid
x:
10
y:
10
z:
10
Equal in all directions
Grid orientation
Crystal system
Longest edge
Longest diagonal
Beam profile setup
Apply beam profile correction
Graphite monochromator
- 1D horizontal gaussian (Enhanced); size [mm]:
1.0
Mirrors
- 2D gaussian (Nova, Mova, Ultra)
Flat beam
Beam size - FWHM for gaussian profile
horizontal beam
0.10
vertical beam
0.10
Spherical absorption correction
Apply spherical abs. correction
Absorption coefficient
μr:
0.342
equivalent radius
0.0120
OK
Cancel

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```
Select option [S]:


[A] Triclinic,  [M] Monoclinic,  [O] Orthorhombic,  [T] Tetragonal,
[H] Trigonal/Hexagonal,  [C] Cubic  or  [E] EXIT

Select option [T]: O


Lattice exceptions: P      A      B      C      I      F      Obv    Rev    All

N (total) =         0  19406  19388  19544  19358  29169  25882  25898  38853
N (int>3sigma) =    0   9101   9066   8855   9985  13511  12022  12006  18030
Mean intensity =  0.0  149.9  150.9  144.0  121.2  148.3  152.7  152.4  151.8
Mean int/sigma =  0.0    3.3    3.3    3.3    3.6    3.3    3.3    3.3    3.3

Lattice type [P, A, B, C, I, F, O(obv.), R(rev. rhomb. on hex. axes)]

Select option [P]:


Mean |E*E-1| = 0.906 [expected .968 centrosym and .736 non-centrosym]


Systematic absence exceptions:

        b--   c--   n--  21--   -c-   -a-   -n-  -21-   --a   --b   --n  --21

N      1614  1615  1617    44  2198  2171  2209    26   531   523   520   156
N I>3s  936   930  1036    21  1066  1050  1182    23   387   397   254   104
<I>   234.3 243.5 216.5  51.1 186.6 177.6 170.5 109.9 470.7 482.3  53.1 383.2
<I/s>   4.2   4.2   4.6   3.5   3.6   3.6   3.9   5.9   5.1   5.3   3.4   5.0


Identical indices and Friedel opposites combined before calculating R(sym)

Option  Space Group  No.  Type  Axes  CSD  R(sym) N(eq)  Syst. Abs.   CFOM

[A] P222           # 16  chiral   1    14  0.105   2937  0.0 /  3.3  12.57
[B] Pmm2           # 25  non-cen  1     9  0.105   2937  0.0 /  3.3  15.91
[C] Pmm2           # 25  non-cen  5     9  0.105   2937  0.0 /  3.3  15.91
[D] Pmm2           # 25  non-cen  3     9  0.105   2937  0.0 /  3.3  15.91
[E] Pmmm           # 47  centro   1     7  0.105   2937  0.0 /  3.3  15.91

Select option [A]: E
```

PgUp/PgDn scrolls text;  only graphics window may be resized

| Resolution | #Data | #Theory | %Complete | Redundancy | Mean I | Mean I/s | Rmerge | Rsigma |
|---|---|---|---|---|---|---|---|---|
| Inf - 1.99 | 20 | 21 | 95.2 | 11.86 | 1129.00 | 24.14 | 0.1437 | 0.0408 |
| 1.99 - 1.28 | 49 | 49 | 100.0 | 35.92 | 841.33 | 38.28 | 0.1155 | 0.0278 |
| 1.28 - 1.02 | 60 | 60 | 100.0 | 46.48 | 446.42 | 40.36 | 0.1297 | 0.0199 |
| 1.02 - 0.88 | 63 | 63 | 100.0 | 46.02 | 240.43 | 34.01 | 0.1169 | 0.0242 |
| 0.88 - 0.77 | 69 | 69 | 100.0 | 43.90 | 247.08 | 33.55 | 0.1491 | 0.0229 |
| 0.77 - 0.72 | 64 | 64 | 100.0 | 36.12 | 135.44 | 21.30 | 0.1489 | 0.0322 |
| 0.72 - 0.68 | 60 | 60 | 100.0 | 37.53 | 138.70 | 22.66 | 0.1632 | 0.0326 |
| 0.68 - 0.64 | 65 | 65 | 100.0 | 36.35 | 119.16 | 21.44 | 0.1915 | 0.0385 |
| 0.64 - 0.61 | 61 | 61 | 100.0 | 33.97 | 72.69 | 15.25 | 0.2137 | 0.0509 |
| 0.61 - 0.58 | 82 | 82 | 100.0 | 31.84 | 79.20 | 14.05 | 0.2240 | 0.0525 |
| 0.58 - 0.56 | 53 | 53 | 100.0 | 33.32 | 69.16 | 14.66 | 0.2342 | 0.0554 |
| 0.56 - 0.54 | 75 | 75 | 100.0 | 29.15 | 57.69 | 11.44 | 0.2836 | 0.0767 |
| 0.54 - 0.52 | 90 | 90 | 100.0 | 27.50 | 53.89 | 10.68 | 0.2966 | 0.0797 |
| 0.52 - 0.51 | 40 | 40 | 100.0 | 28.83 | 53.52 | 11.16 | 0.2881 | 0.0754 |
| 0.51 - 0.50 | 44 | 44 | 100.0 | 27.05 | 29.44 | 6.89 | 0.3907 | 0.1312 |
| 0.50 - 0.48 | 98 | 98 | 100.0 | 25.17 | 35.23 | 7.83 | 0.3744 | 0.1173 |
| 0.48 - 0.47 | 74 | 74 | 100.0 | 22.41 | 29.12 | 6.54 | 0.3768 | 0.1462 |
| 0.47 - 0.46 | 71 | 71 | 100.0 | 20.97 | 32.33 | 6.57 | 0.4063 | 0.1355 |
| 0.46 - 0.45 | 67 | 67 | 100.0 | 18.99 | 25.91 | 5.98 | 0.4118 | 0.1627 |
| 0.45 - 0.44 | 81 | 97 | 83.5 | 8.88 | 22.14 | 3.88 | 0.4099 | 0.2774 |
| 0.54 - 0.44 | 565 | 581 | 97.2 | 21.63 | 34.90 | 7.33 | 0.3506 | 0.1283 |
| Inf - 0.44 | 1286 | 1303 | 98.7 | 29.82 | 144.76 | 16.50 | 0.1625 | 0.0421 |

Merged [A], lowest resolution = 5.83 Angstroms

Graphical output: 1=<I/s>, 2=Rmerge, 3=Rsigma, <Enter>=none:

```
Current formula is:
YBa2Cu3O7


Tentative Z (number of formula units/cell) =   1.0  giving rho = 6.406,
non-H atomic volume =  13.3  and following cell contents and analysis:

O       7.00    16.81 %             Cu      3.00    28.62 %
Y       1.00    13.35 %             Ba      2.00    41.23 %

[Z] change Z,  [F] new FORMULA,   [R] change RADIATION,
[E] EXIT to main menu  or  [Q] QUIT program

Select option [E]:
```

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Contents
Current events
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What links here
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# Yttrium barium copper oxide

From Wikipedia, the free encyclopedia

**Yttrium barium copper oxide** (**YBCO**) is a family of crystalline chemical compounds, famous for displaying high-temperature superconductivity. It includes the first material ever discovered to become superconducting above the boiling point of liquid nitrogen (77 K) at about 92 K. Many YBCO compounds have the general formula $YBa_2Cu_3O_{7-x}$ (also known as Y123), although materials with other Y:Ba:Cu ratios exist, such as $YBa_2Cu_4O_y$ (Y124) or $Y_2Ba_4Cu_7O_y$ (Y247). At present, there is no singularly recognised theory for high-temperature superconductivity.

It is part of the more general group of rare-earth barium copper oxides (ReBCO) in which, instead of yttrium, other rare earths are present.

Contents [hide]



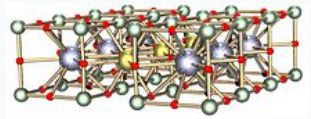
## History [ edit ]

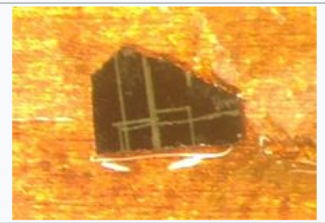
In April 1986, Georg Bednorz and Karl Müller, working at IBM in Zurich, discovered that certain semiconducting oxides became superconducting at relatively high temperature, in particular, a lanthanum barium copper oxide becomes superconducting at 35 K. This oxide was an oxygen-deficient perovskite-related material that proved promising and stimulated the search for related compounds with higher superconducting transition temperatures. In 1987, Bednorz and Müller were jointly awarded the Nobel Prize in Physics for this work.

Following Bednorz and Müller's disovery, a team at the University of Alabama in Huntsville and University of Houston discovered that YBCO has a superconducting transition critical temperature ($T_c$) of 93 K.[3] The first samples were $Y_{1.2}Ba_{0.8}CuO_4$, but this was an average composition for two phases, a black and a green one. Workers at the Carnegie Institution of Washington found that the black phase (which turned out to be the superconductor) had the composition $YBa_2Cu_3O_{7-\delta}$.[4]

YBCO was the first material found to become superconducting above 77 K, the boiling point of liquid

**Yttrium barium copper oxide**





| Names | |
|---|---|
| IUPAC name | barium copper yttrium oxide |
| Other names | YBCO, Y123, yttrium barium cuprate |
| **Identifiers** | |
| CAS Number | 107539-20-8 ✓ |
| ChemSpider | 17339938 |
| ECHA InfoCard | 100.121.379 |
| EC Number | 619-720-7 |
| PubChem CID | 21871996 |
| CompTox Dashboard (EPA) | DTXSID90148081 |
| **Properties** | |
| Chemical formula | $YBa_2Cu_3O_7$ |
| Molar mass | 666.19 g/mol |
| Appearance | Black solid |
| Density | 6.3 g/cm$^3$[1][2] |
| Melting point | >1000 °C |
| Solubility in water | Insoluble |
| **Structure** | |
| Crystal structure | Based on the perovskite structure. |

Languages
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YBCO was the first material found to become superconducting above 77 K, the boiling point of liquid nitrogen, whereas the majority of other superconductors require more expensive cryogens. Nonetheless, YBCO and its many related materials have yet to displace superconductors requiring liquid helium for cooling.

## Synthesis [edit]

Relatively pure YBCO was first synthesized by heating a mixture of the metal carbonates at temperatures between 1000 and 1300 K.[5][6]

$$4\ BaCO_3 + Y_2(CO_3)_3 + 6\ CuCO_3 + (1/2{-}x)\ O_2 \rightarrow 2\ YBa_2Cu_3O_{7-x} + 13\ CO_2$$

Modern syntheses of YBCO use the corresponding oxides and nitrates.[6]

The superconducting properties of $YBa_2Cu_3O_{7-x}$ are sensitive to the value of $x$, its oxygen content. Only those materials with $0 \le x \le 0.65$ are superconducting below $T_c$, and when $x \sim 0.07$, the material superconducts at the highest temperature of 95 K,[6] or in highest magnetic fields: 120 T for **B** perpendicular and 250 T for **B** parallel to the $CuO_2$ planes.[7]

In addition to being sensitive to the stoichiometry of oxygen, the properties of YBCO are influenced by the crystallization methods used. Care must be taken to sinter YBCO. YBCO is a crystalline material, and the best superconductive properties are obtained when crystal grain boundaries are aligned by careful control of annealing and quenching temperature rates.

Numerous other methods to synthesize YBCO have developed since its discovery by Wu and his co-workers, such as chemical vapor deposition (CVD),[5][6] sol-gel,[8] and aerosol[9] methods. These alternative methods, however, still require careful sintering to produce a quality product.

However, new possibilities have been opened since the discovery that trifluoroacetic acid (TFA), a source of fluorine, prevents the formation of the undesired barium carbonate ($BaCO_3$). Routes such as CSD (chemical solution deposition) have opened a wide range of possibilities, particularly in the preparation of long YBCO tapes.[10] This route lowers the temperature necessary to get the correct phase to around 700 °C. This, and the lack of dependence on vacuum, makes this method a very promising way to get scalable YBCO tapes.

| | |
|---|---|
| PubChem CID | 21871996 |
| CompTox Dashboard (EPA) | DTXSID90148081 |
| **Properties** | |
| Chemical formula | $YBa_2Cu_3O_7$ |
| Molar mass | 666.19 g/mol |
| Appearance | Black solid |
| Density | 6.3 g/cm$^3$[1][2] |
| Melting point | >1000 °C |
| Solubility in water | Insoluble |
| **Structure** | |
| Crystal structure | Based on the perovskite structure. |
| Coordination geometry | Orthorhombic |
| **Hazards** | |
| GHS pictograms |  |
| GHS Signal word | **Warning** |
| GHS hazard statements | H302, H315, H319, H335 |
| GHS precautionary statements | P261, P264, P270, P271, P280, P301+312, P302+352, P304+340, P305+351+338, P312, P321, P330, P332+313, P337+313, P362, P403+233, P405, P501 |
| **Related compounds** | |
| Related high-$T_c$ superconductors | Cuprate superconductors |
| Related compounds | Yttrium(III) oxide<br>Barium oxide<br>Copper(II) oxide |

Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa).

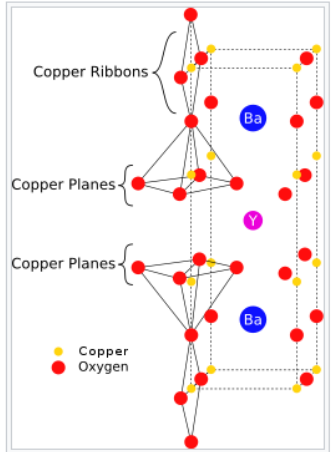
✓ verify (what is ✓✗ ?)

Infobox references

However, new possibilities have been opened since the discovery that trifluoroacetic acid (TFA), a source of fluorine, prevents the formation of the undesired barium carbonate ($BaCO_3$). Routes such as CSD (chemical solution deposition) have opened a wide range of possibilities, particularly in the preparation of long YBCO tapes.[10] This route lowers the temperature necessary to get the correct phase to around 700 °C. This, and the lack of dependence on vacuum, makes this method a very promising way to get scalable YBCO tapes.

## Structure [ edit ]

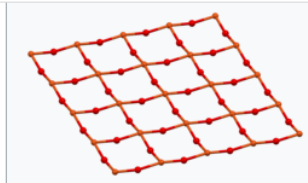
YBCO crystallizes in a defect perovskite structure consisting of layers. The boundary of each layer is defined by planes of square planar $CuO_4$ units sharing 4 vertices. The planes can sometimes be slightly puckered.[5] Perpendicular to these $CuO_4$ planes are $CuO_2$ ribbons sharing 2 vertices. The yttrium atoms are found between the $CuO_4$ planes, while the barium atoms are found between the $CuO_2$ ribbons and the $CuO_4$ planes. This structural feature is illustrated in the figure to the right.



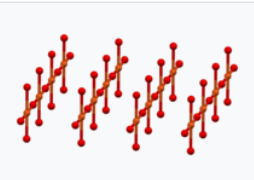

Part of the lattice structure of yttrium barium copper oxide

**Coordination geometry of metal centres in YBCO**[11][6]

| cubic $\{YO_8\}$ | $\{BaO_{10}\}$ | square planar $\{CuO_4\}$ | square pyramidal $\{CuO_5\}$ | $YBa_2Cu_3O_{7-\delta}$ unit cell |
|---|---|---|---|---|



puckered Cu plane



Cu ribbons

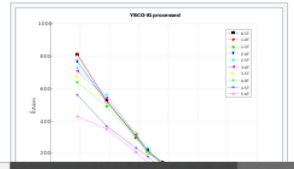
Although $YBa_2Cu_3O_7$ is a well-defined chemical compound with a specific structure and stoichiometry, materials with fewer than seven oxygen atoms per formula unit are non-stoichiometric compounds. The structure of these materials depends on the oxygen content. This non-stoichiometry is denoted by the x in the chemical formula $YBa_2Cu_3O_{7-x}$. When $x = 1$, the O(1) sites in the Cu(1) layer are vacant and the structure is tetragonal. The tetragonal form of YBCO is insulating and does not superconduct. Increasing the oxygen content slightly causes more of the O(1) sites to become occupied. For $x < 0.65$, Cu-O chains along the *b* axis of the crystal are formed. Elongation of the *b* axis changes the structure to orthorhombic, with lattice parameters of $a = 3.82$, $b = 3.89$, and $c = 11.68$ Å.[citation needed] Optimum superconducting properties occur when $x \sim 0.07$, i.e., almost all of the O(1) sites are occupied, with few vacancies.

Like many type-II superconductors, YBCO can exhibit flux pinning: lines of magnetic flux may be pinned in place in a crystal, with a force required to move a piece from a particular magnetic field configuration. A piece of YBCO placed above a magnetic track can thus levitate at a fixed height.[5]

In experiments where other elements are substituted on the Cu and Ba[why?] sites, evidence has shown that conduction occurs in the Cu(2)O planes while the Cu(1)O(1) chains act as charge reservoirs, which provide carriers to the CuO planes. However, this model fails to address superconductivity in the homologue Pr123 (praseodymium instead of yttrium).[12] This (conduction in the copper planes) confines conductivity to the *a*-*b* planes and a large anisotropy in transport properties is observed. Along the *c* axis, normal conductivity is 10 times smaller than in the *a*-*b* plane. For other cuprates in the same general class, the anisotropy is even greater and inter-plane transport is highly restricted.

Furthermore, the superconducting length scales show similar anisotropy, in both penetration depth ($\lambda_{ab} \approx 150$ nm, $\lambda_c \approx 800$ nm) and coherence length, ($\xi_{ab} \approx 2$ nm, $\xi_c \approx 0.4$ nm). Although the coherence length in the *a*-*b* plane is 5 times greater than that along the *c* axis it is quite small compared to classic superconductors such as niobium (where $\xi \approx 40$ nm). This modest coherence length means that the superconducting state is more susceptible to local disruptions from interfaces or defects on the order of a single unit cell, such as the boundary between twinned crystal domains. This sensitivity to small defects complicates fabricating devices with YBCO, and the material is also sensitive to degradation from humidity.

## Proposed applications [ edit ]

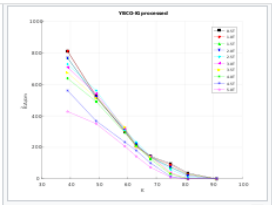


Many possible applications of this and related high temperature superconducting materials have been discussed. For example, superconducting materials are finding use as magnets in magnetic resonance imaging, magnetic levitation, and Josephson junctions. (The most used material for power cables and magnets is BSCCO.)[citation needed]

YBCO has yet to be used in many applications involving superconductors for two primary reasons:

- First, although single crystals of YBCO have a very high critical current density, polycrystals have a very low

Yttrium barium copper oxide - W | (16) (PDF) Relationship between | en.wikipedia.org/wiki/Yttrium_barium_copper_oxide



Critical current (KA/cm$^2$) vs absolute temperature (K), at different intensity of magnetic field (T) in YBCO prepared by infiltration-growth.[13]

Many possible applications of this and related high temperature superconducting materials have been discussed. For example, superconducting materials are finding use as magnets in magnetic resonance imaging, magnetic levitation, and Josephson junctions. (The most used material for power cables and magnets is BSCCO.)[citation needed]

YBCO has yet to be used in many applications involving superconductors for two primary reasons:

- First, although single crystals of YBCO have a very high critical current density, polycrystals have a very low critical current density: only a small current can be passed while maintaining superconductivity. This problem is due to crystal grain boundaries in the material. When the grain boundary angle is greater than about 5°, the supercurrent cannot cross the boundary. The grain boundary problem can be controlled to some extent by preparing thin films via CVD or by texturing the material to align the grain boundaries.[citation needed]
- A second problem limiting the use of this material in technological applications is associated with processing of the material. Oxide materials such as this are brittle, and forming them into superconducting wires by any conventional process does not produce a useful superconductor. (Unlike BSCCO, the powder-in-tube process does not give good results with YBCO.)[citation needed]

YBCO superconductor at TTU

The most promising method developed to utilize this material involves deposition of YBCO on flexible metal tapes coated with buffering metal oxides. This is known as *coated conductor*. Texture (crystal plane alignment) can be introduced into the metal tape (the RABiTS process) or a textured ceramic buffer layer can be deposited, with the aid of an ion beam, on an untextured alloy substrate (the IBAD process). Subsequent oxide layers prevent diffusion of the metal from the tape into the superconductor while transferring the template for texturing the superconducting layer. Novel variants on CVD, PVD, and solution deposition techniques are used to produce long lengths of the final YBCO layer at high rates. Companies pursuing these processes include American Superconductor, Superpower (a division of Furukawa Electric), Sumitomo, Fujikura, Nexans Superconductors, Commonwealth Fusion Systems, and European Advanced Superconductors. A much larger number of research institutes have also produced YBCO tape by these methods.[citation needed]

The superconducting tape may be the key to a tokamak fusion reactor design that can achieve breakeven energy production.[14] YBCO is often categorized as a rare-earth barium copper oxide (REBCO).[15]

## Surface modification [ edit ]

Surface modification of materials has often led to new and improved properties. Corrosion inhibition, polymer adhesion and nucleation, preparation of organic superconductor/insulator/high-$T_c$ superconductor trilayer structures, and the fabrication of metal/insulator/superconductor tunnel junctions have been developed using surface-modified YBCO.[16]

These molecular layered materials are synthesized using cyclic voltammetry. Thus far, YBCO layered with alkylamines, arylamines, and thiols have been produced with varying stability of the molecular layer. It has been proposed that amines act as Lewis bases and bind to Lewis acidic Cu surface sites in $YBa_2Cu_3O_7$ to form stable coordination bonds.

## Hobbyist use [ edit ]

Shortly after it was discovered, physicist and science author Paul Grant published in the U.K. Journal *New Scientist* a straightforward guide for

been produced with varying stability of the molecular layer. It has been proposed that amines act as Lewis bases and bind to Lewis acidic Cu surface sites in $YBa_2Cu_3O_7$ to form stable coordination bonds.

## Hobbyist use [ edit ]

Shortly after it was discovered, physicist and science author Paul Grant published in the U.K. Journal *New Scientist* a straightforward guide for synthesizing YBCO superconductors using widely-available equipment.[17] Thanks in part to this article and similar publications at the time, YBCO has become a popular high-temperature superconductor for use by hobbyists and in education, as the magnetic levitation effect can be easily demonstrated using liquid nitrogen as coolant.

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17. ^ Grant, Paul (30 July 1987). "Do-it-yourself Superconductors". *New Scientist*. Reed Business Information. **115** (1571): 36. Retrieved 12 January 2019.

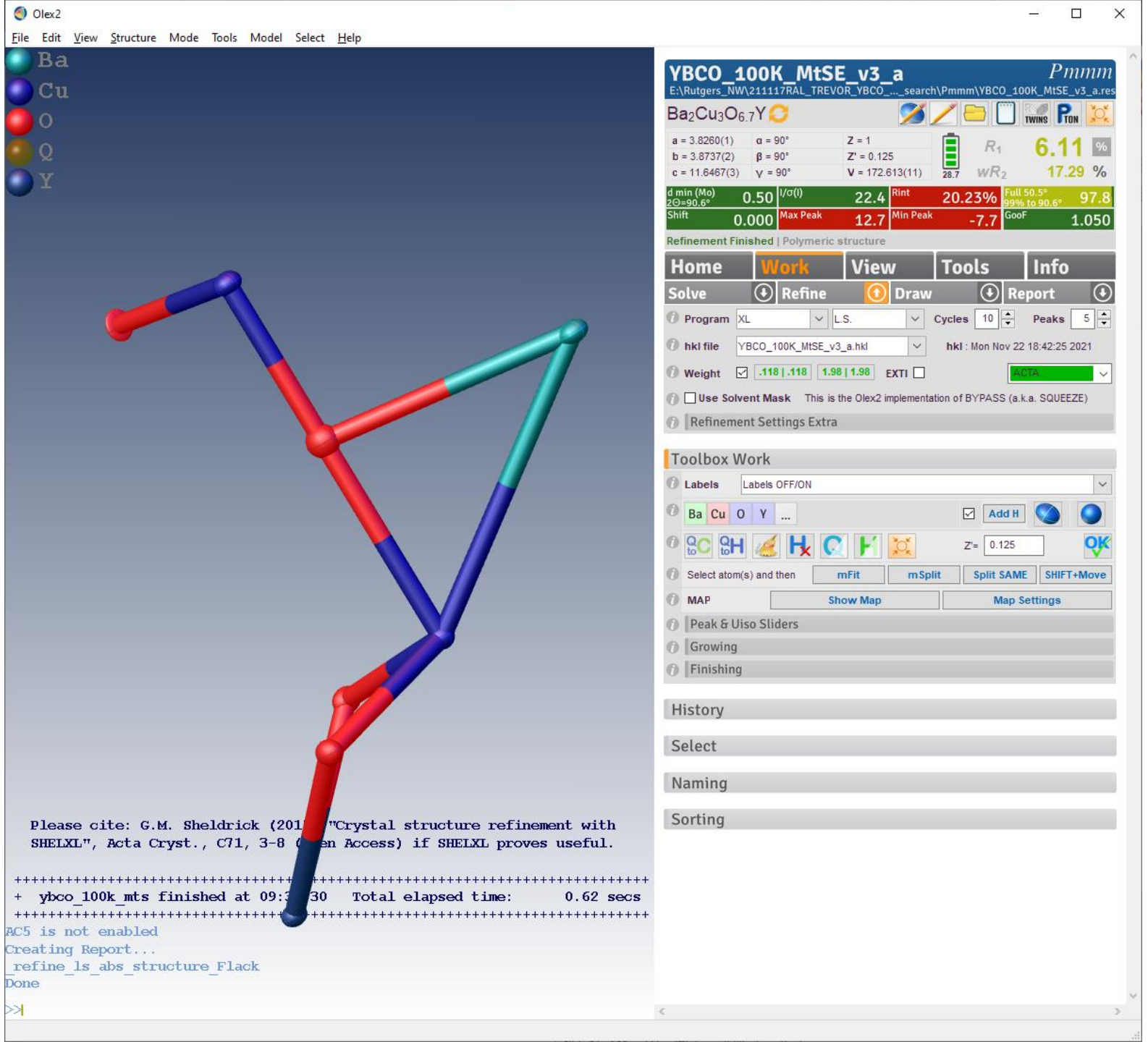
## External links [edit]

- Diagram of YBCO structure
- New World Record For Superconducting Magnet 26.8T April 2007
- External MSDS Data Sheet (safety classifications) for YBCO.
- Superconductivity in everyday life : Interactive exhibition – little if any specific to YBCO.

Wikimedia Commons has media related to ***Yttrium barium copper oxide***.

| | | |
|---|---|---|
| V·T·E | **Yttrium compounds** | [show] |
| V·T·E | **Barium compounds** | [show] |
| V·T·E | **Copper compounds** | [show] |
| V·T·E | **Oxides** | [show] |

Categories: Yttrium compounds | Barium compounds | Copper compounds | High-temperature superconductors | Mixed valence compounds | Transition metal oxides | Non-stoichiometric compounds | Ceramic materials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Please cite: G.M. Sheldrick (201 "Crystal structure refinement with
SHELXL", Acta Cryst., C71, 3-8 en Access) if SHELXL proves useful.
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Ba2Cu3O6.7Y
a = 3.8260(1) α = 90° Z = 1
b = 3.8737(2) β = 90° Z' = 0.125
c = 11.6467(3) γ = 90° V = 172.613(11)
28.7
R1 6.11 %
wR2 17.29 %
d min (Mo) 2Θ=90.6° 0.50
I/σ(I) 22.4
Rint 20.23%
Full 50.5° 99% to 90.6° 97.8
Shift 0.000
Max Peak 12.7
Min Peak -7.7
GooF 1.050
Refinement Finished | Polymeric structure
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Solve Refine Draw Report
Program XL L.S. Cycles 10 Peaks 5
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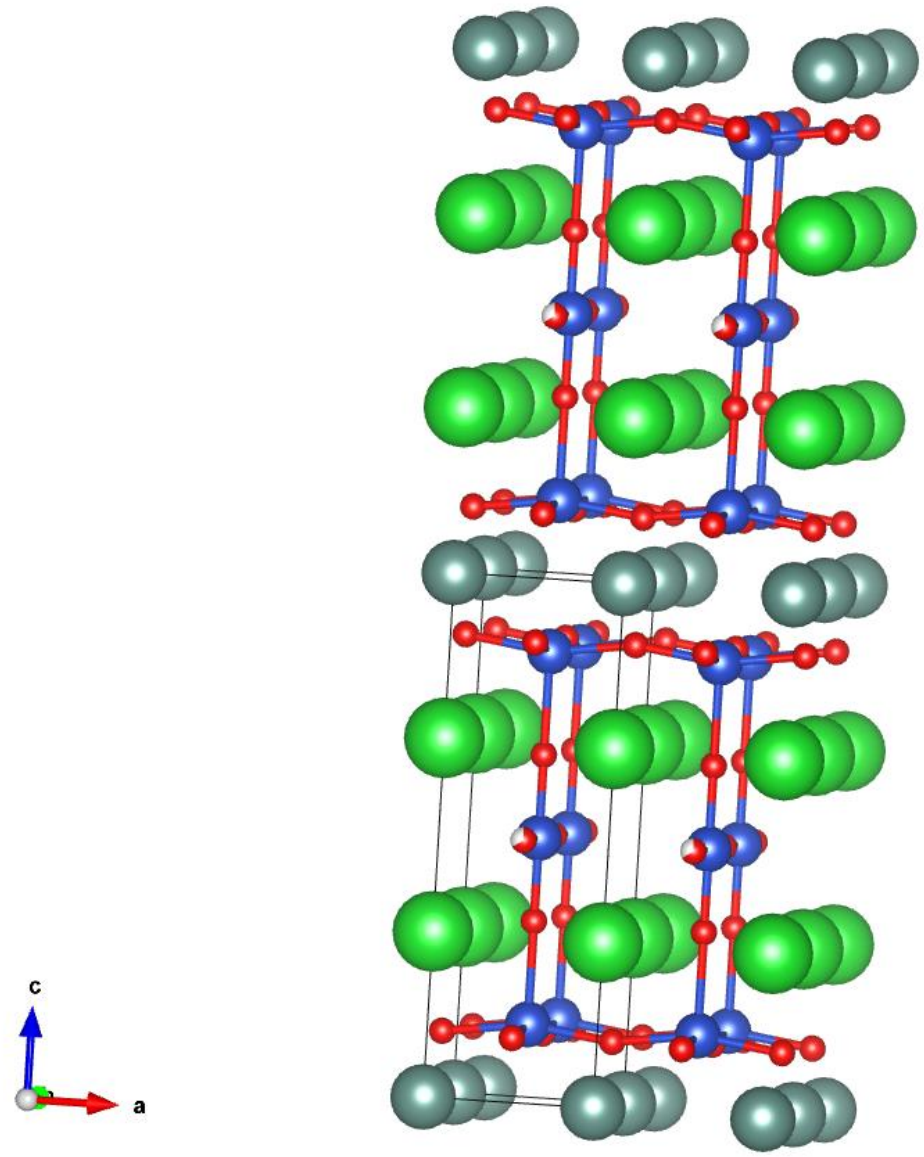

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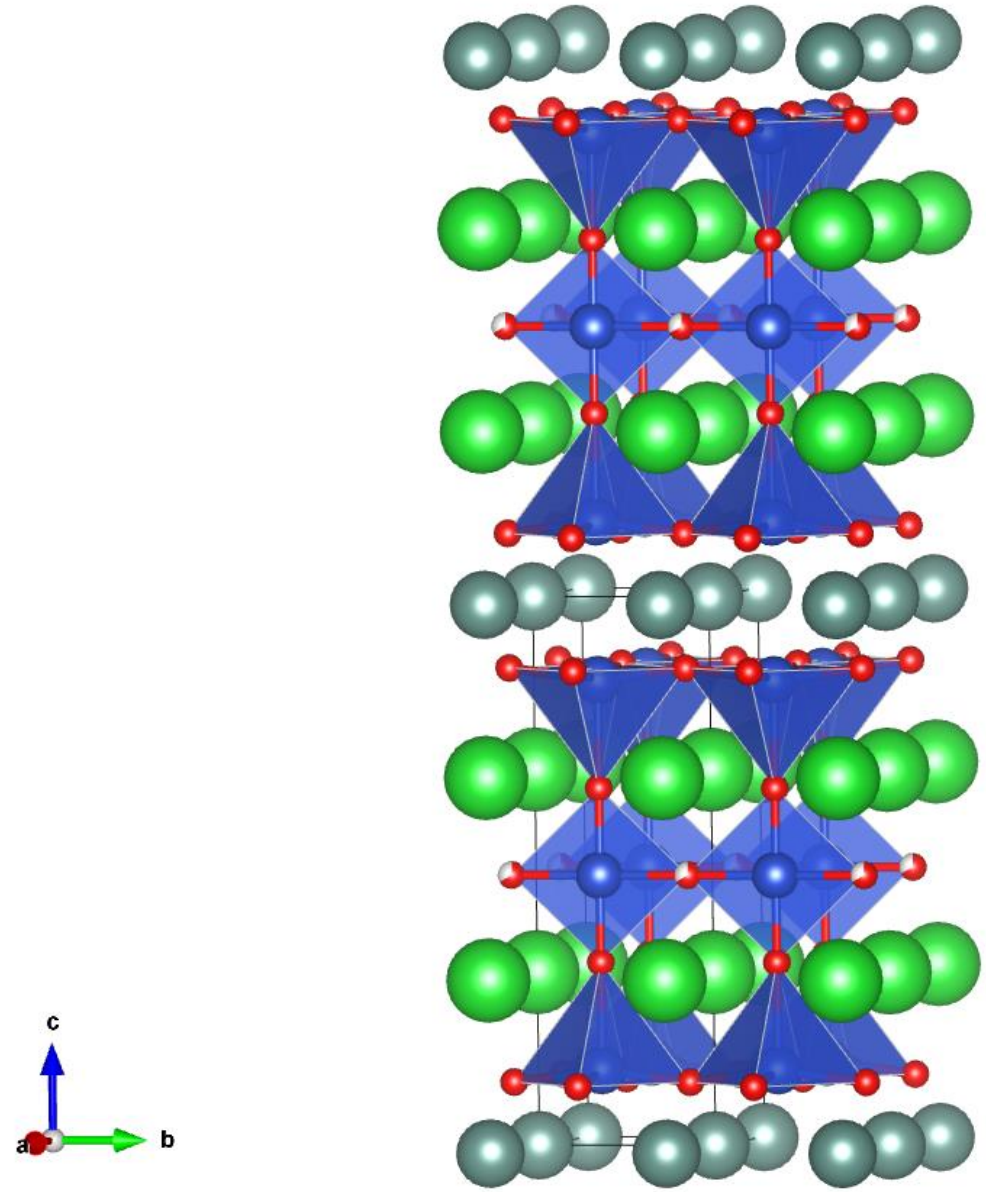


# YBCO_100K_MtSE_v3_a

**Table 1 Crystal data and structure refinement for YBCO_100K_MtSE_v3_a.**

| | |
|---|---|
| Identification code | YBCO_100K_MtSE_v3_a |
| Empirical formula | $Ba_2Cu_3O_{6.67}Y$ |
| Formula weight | 660.93 |
| Temperature/K | 293(2) |
| Crystal system | orthorhombic |
| Space group | Pmmm |
| a/Å | 3.82600(10) |
| b/Å | 3.8737(2) |
| c/Å | 11.6467(3) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 172.613(11) |
| Z | 1 |
| $\rho_{calc}$g/cm$^3$ | 6.358 |
| μ/mm$^{-1}$ | 28.594 |
| F(000) | 291.0 |
| Crystal size/mm$^3$ | ? × ? × ? |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 6.998 to 90.564 |
| Index ranges | -7 ≤ h ≤ 7, -7 ≤ k ≤ 7, -23 ≤ l ≤ 23 |
| Reflections collected | 30938 |
| Independent reflections | 889 [$R_{int}$ = 0.2023, $R_{sigma}$ = 0.0446] |
| Data/restraints/parameters | 889/0/31 |
| Goodness-of-fit on F$^2$ | 1.050 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0611, w$R_2$ = 0.1592 |
| Final R indexes [all data] | $R_1$ = 0.0741, w$R_2$ = 0.1729 |
| Largest diff. peak/hole / e Å$^{-3}$ | 12.66/-7.70 |

**Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for YBCO_100K_MtSE_v3_a. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| Ba01 | 10000 | 10000 | 6845.3(4) | 9.30(16) |
| Y02 | 0 | 0 | 10000 | 7.0(2) |
| Cu03 | 5000 | 5000 | 5000 | 8.7(3) |
| Cu04 | 5000 | 5000 | 8556.3(10) | 7.30(19) |
| O05 | 5000 | 0 | 5000 | 8(3) |
| O06 | 5000 | 5000 | 6586(7) | 13.1(12) |
| O07 | 0 | 5000 | 8784(6) | 8.3(9) |
| O08 | 5000 | 0 | 8773(6) | 8.3(9) |

**Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for YBCO_100K_MtSE_v3_a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Ba01 | 11.8(2) | 10.5(2) | 5.6(2) | 0 | 0 | 0 |
| Y02 | 7.8(4) | 7.6(4) | 5.4(4) | 0 | 0 | 0 |
| Cu03 | 10.4(6) | 9.8(6) | 6.0(5) | 0 | 0 | 0 |
| Cu04 | 7.5(4) | 7.7(4) | 6.8(4) | 0 | 0 | 0 |
| O05 | 11(5) | 1(4) | 12(5) | 0 | 0 | 0 |
| O06 | 11(2) | 15(3) | 13(3) | 0 | 0 | 0 |
| O07 | 6.5(19) | 11(2) | 8(2) | 0 | 0 | 0 |
| O08 | 11(2) | 6(2) | 8(2) | 0 | 0 | 0 |

**Table 4 Bond Lengths for YBCO_100K_MtSE_v3_a.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Ba01 | Cu04[1] | 3.3737(7) | Y02 | O07 | 2.400(4) |
| Ba01 | Cu04[2] | 3.3737(7) | Y02 | O07[5] | 2.400(4) |
| Ba01 | O05[2] | 2.8772(4) | Y02 | O07[8] | 2.400(4) |
| Ba01 | O05[1] | 2.8772(4) | Y02 | O08 | 2.388(5) |
| Ba01 | O06[3] | 2.7390(9) | Y02 | O08[9] | 2.388(4) |
| Ba01 | O06[2] | 2.7390(10) | Y02 | O08[5] | 2.388(4) |
| Ba01 | O06[1] | 2.7390(9) | Y02 | O08[10] | 2.388(4) |
| Ba01 | O06 | 2.7390(10) | Cu03 | O05 | 1.93685(10) |
| Ba01 | O07[2] | 2.974(6) | Cu03 | O05[1] | 1.93685(10) |
| Ba01 | O07[3] | 2.974(6) | Cu03 | O06[11] | 1.847(8) |
| Ba01 | O08[1] | 2.950(6) | Cu03 | O06 | 1.847(8) |
| Ba01 | O08[2] | 2.950(6) | Cu04 | O06 | 2.295(8) |
| Y02 | Cu04[4] | 3.1997(6) | Cu04 | O07[3] | 1.9312(11) |
| Y02 | Cu04[5] | 3.1997(6) | Cu04 | O07 | 1.9312(10) |
| Y02 | Cu04 | 3.1997(6) | Cu04 | O08[1] | 1.9532(10) |
| Y02 | Cu04[6] | 3.1997(6) | Cu04 | O08 | 1.9532(10) |
| Y02 | O07[7] | 2.400(4) | | | |

[1]+X,1+Y,+Z; [2]1+X,1+Y,+Z; [3]1+X,+Y,+Z; [4]-1+X,-1+Y,+Z; [5]-X,-Y,2-Z; [6]1-X,1-Y,2-Z; [7]+X,-1+Y,+Z; [8]-X,1-Y,2-Z; [9]1-X,-Y,2-Z; [10]-1+X,+Y,+Z; [11]1-X,1-Y,1-Z

**Table 7 Atomic Occupancy for YBCO_100K_MtSE_v3_a.**

| Atom | *Occupancy* | Atom | *Occupancy* | Atom | *Occupancy* |
|---|---|---|---|---|---|
| O05 | 0.67(6) | | | | |

**Experimental**

Single crystals of $Ba_2Cu_3O_{6.67}Y$ [YBCO_100K_MtSE_v3_a] were []. A suitable crystal was selected and [] on a diffractometer. The crystal was kept at 293(2) K during data collection. Using Olex2 [1], the structure was solved with olex2.solve [2] structure solution program using Charge Flipping and refined with the XL [3] refinement package using Least Squares minimisation.


1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H. (2015). Acta Cryst. A71, 59-75.
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.


**Crystal structure determination of [YBCO_100K_MtSE_v3_a]**

**Crystal Data** for $Ba_2Cu_3O_{6.67}Y$ ($M$ =660.93 g/mol): orthorhombic, space group Pmmm (no. 47), $a$ = 3.82600(10) Å, $b$ = 3.8737(2) Å, $c$ = 11.6467(3) Å, $V$ = 172.613(11) Å$^3$, $Z$ = 1, $T$ = 293(2) K, μ(MoKα) = 28.594 mm$^{-1}$, *Dcalc* 6.358 g/cm$^3$, 30938 reflections measured (6.998° ≤ 2Θ ≤ 90.564°), 889 unique ($R_{int}$ = 0.2023, $R_{sigma}$ = 0.0446) which were used in all calculations. The final $R_1$ was 0.0611 (I > 2σ(I)) and $wR_2$ was 0.1729 (all data).

**Refinement model description**

Number of restraints - 0, number of constraints - unknown.

Details:

N/A

# Crystal structure of the $YBa_2Cu_3O_7$ superconductor by single-crystal X-ray diffraction

**G. Calestani & C. Rizzoli***

Istituto di Strutturistica Chimica, Università di Parma and *Centro di Studio per la Strutturistica Diffrattometrica del CNR Viale delle Scienze, 43100 Parma, Italy

**Just after Wu *et al.*[1] reported superconductivity above 90 K in barium, yttrium and copper ternary oxides, the formula ($YBa_2Cu_3O_{7-x}$) and the structural arrangement (oxygen-deficient tripled-perovskite-type structure) of the superconducting phase was proposed by different groups. As theoretical proposals depend crucially on the details of the atomic arrangement reducing the dimensionality of the system, a number of structural determinations were carried out by X-ray, neutron and electron diffraction. Although these studies established the structure of the metal**

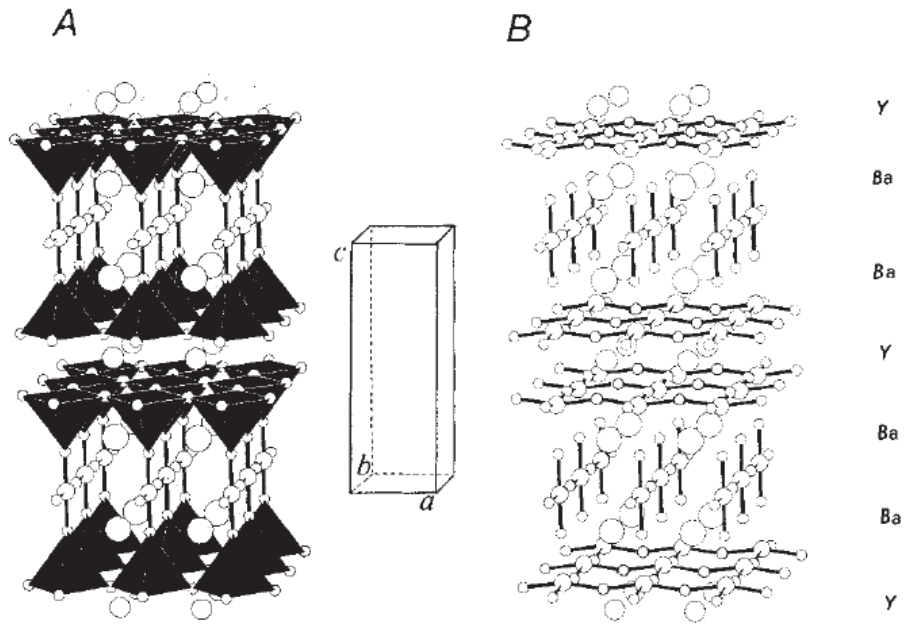
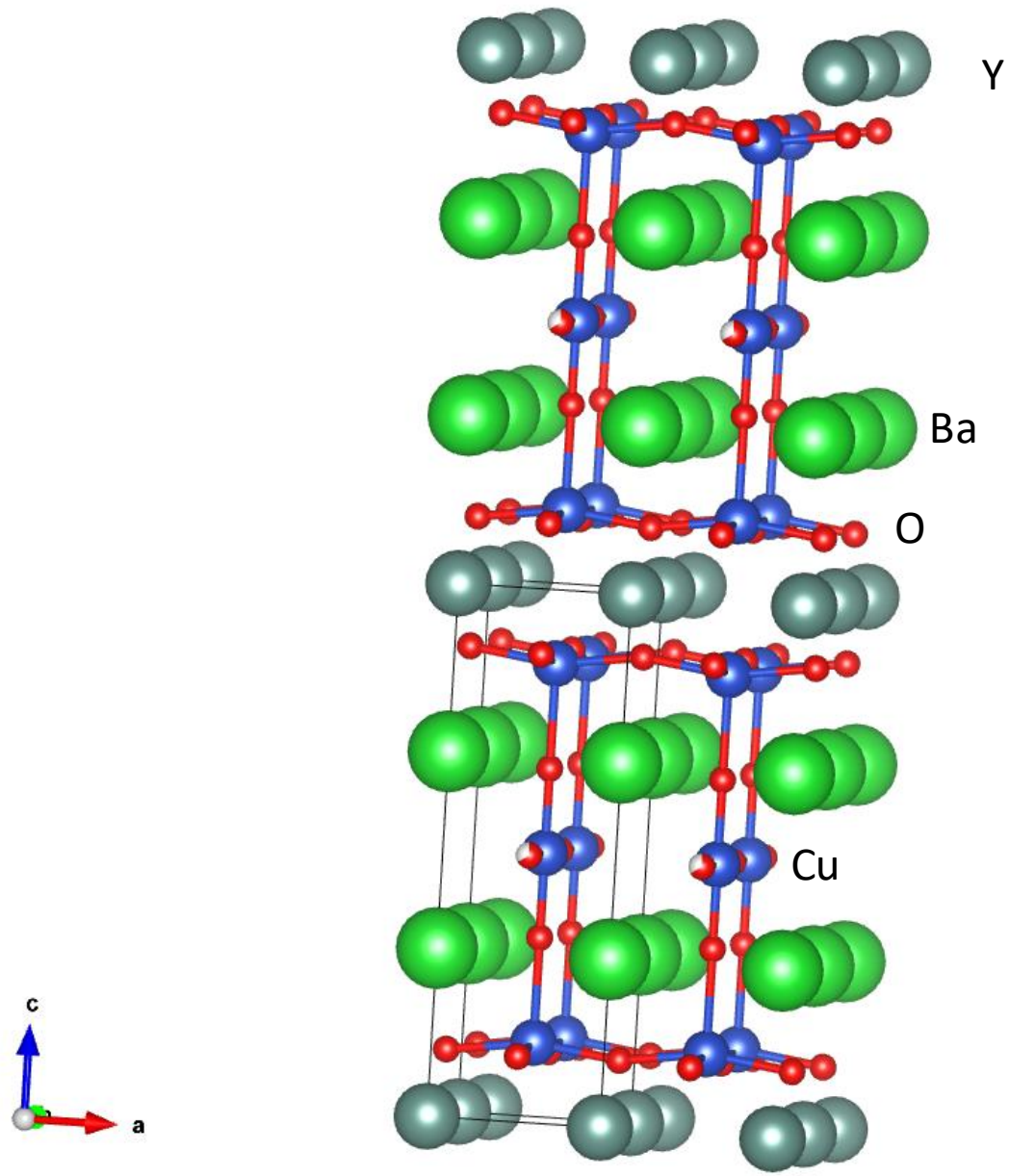



**Fig. 1** Crystal structure representation of $YBa_2Cu_3O_7$ showing the copper coordinations (*A*) and the puckered sheets of square planar-like groups (*B*).


Y
Ba
O
Cu
c
a

# Crystal structure of the $YBa_2Cu_3O_7$ superconductor by single-crystal X-ray diffraction

G. Calestani & C. Rizzoli*

**Table 1** Fractional atomic coordinates and thermal parameters ($\times 10^4$ Å$^2$) for $YBa_2Cu_3O_7$

| Atom | $a/a$ | $y/b$ | $z/c$ | $U_{11}$ | $U_{22}$ | $U_{33}$ |
|---|---|---|---|---|---|---|
| Y | 0.5000 | 0.5000 | 0.5000 | 123 (26) | 162 (29) | 1 (30) |
| Ba | 0.5000 | 0.5000 | 0.1850 (2) | 68 (10) | 45 (9) | 87 (14) |
| Cu (1) | 0.0000 | 0.0000 | 0.0000 | 144 (36) | 237 (44) | 32 (33) |
| Cu(2) | 0.0000 | 0.0000 | 0.3565 (5) | 55 (21) | 57 (20) | 90 (32) |
| O (1) | 0.0000 | 0.5000 | 0.0000 | 587 (360) | 68 (196) | 35 (158) |
| O (2) | 0.0000 | 0.0000 | 0.1566 (23) | 1 (98) | 226 (130) | 59 (89) |
| O (3) | 0.5000 | 0.0000 | 0.3776 (21) | 23 (106) | 112 (125) | 168 (121) |
| O (4) | 0.0000 | 0.5000 | 0.3765 (21) | 22 (113) | 256 (172) | 131 (122) |

Thermal parameters are in the form: $\exp(-2\pi^2 U_{11} h^2 a^{*2} + \cdots + U_{12} hka^* b^*)$.
$U_{12} = U_{23} = U_{13} = 0$ by symmetry requirements.

This experiment

**Table 4 Bond Lengths for YBCO_100K_MtSE_v3_a.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Ba01 | $Cu04^{1}$ | 3.3737(7) | Y02 | O07 | 2.400(4) |
| Ba01 | $Cu04^{2}$ | 3.3737(7) | Y02 | $O07^{5}$ | 2.400(4) |
| Ba01 | $O05^{2}$ | 2.8772(4) | Y02 | $O07^{8}$ | 2.400(4) |
| Ba01 | $O05^{1}$ | 2.8772(4) | Y02 | O08 | 2.388(5) |
| Ba01 | $O06^{3}$ | 2.7390(9) | Y02 | $O08^{9}$ | 2.388(4) |
| Ba01 | $O06^{2}$ | 2.7390(10) | Y02 | $O08^{5}$ | 2.388(4) |
| Ba01 | $O06^{1}$ | 2.7390(9) | Y02 | $O08^{10}$ | 2.388(4) |
| Ba01 | O06 | 2.7390(10) | Cu03 | O05 | 1.93685(10) |
| Ba01 | $O07^{2}$ | 2.974(6) | Cu03 | $O05^{1}$ | 1.93685(10) |
| Ba01 | $O07^{3}$ | 2.974(6) | Cu03 | $O06^{11}$ | 1.847(8) |
| Ba01 | $O08^{1}$ | 2.950(6) | Cu03 | O06 | 1.847(8) |
| Ba01 | $O08^{2}$ | 2.950(6) | Cu04 | O06 | 2.295(8) |
| Y02 | $Cu04^{4}$ | 3.1997(6) | Cu04 | $O07^{3}$ | 1.9312(11) |
| Y02 | $Cu04^{5}$ | 3.1997(6) | Cu04 | O07 | 1.9312(10) |
| Y02 | Cu04 | 3.1997(6) | Cu04 | $O08^{1}$ | 1.9532(10) |
| Y02 | $Cu04^{6}$ | 3.1997(6) | Cu04 | O08 | 1.9532(10) |
| Y02 | $O07^{7}$ | 2.400(4) | | | |

$^{1}$+X,1+Y,+Z; $^{2}$1+X,1+Y,+Z; $^{3}$1+X,+Y,+Z; $^{4}$-1+X,-1+Y,+Z; $^{5}$-X,-Y,2-Z; $^{6}$1-X,1-Y,2-Z; $^{7}$+X,-1+Y,+Z; $^{8}$-X,1-Y,2-Z; $^{9}$1-X,-Y,2-Z; $^{10}$-1+X,+Y,+Z; $^{11}$1-X,1-Y,1-Z

# Crystal structure of the $YBa_2Cu_3O_7$ superconductor by single-crystal X-ray diffraction

G. Calestani & C. Rizzoli*

**Table 2** Selected bond distances (Å) and angles (°) for $YBa_2Cu_3O_7$

| | | | |
|---|---|---|---|
| Y-O (3) | 4 × 2.418 (15) | Cu (1)-O (1) | 2 × 1.947 (5) |
| Y-O (4) | 4 × 2.399 (15) | Cu (1)-O (2) | 2 × 1.834 (27) |
| | | Cu (2)-O (2) | 2.341 (28) |
| Ba-O (1) | 2 × 2.891 (2) | Cu (2)-O (3) | 2 × 1.929 (3) |
| Ba-O (2) | 4 × 2.750 (3) | Cu (2)-O (4) | 2 × 1.961 (3) |
| Ba-O (3) | 2 × 2.980 (19) | | |
| Ba-O (4) | 2 × 2.948 (19) | | |

| | |
|---|---|
| O (1)-Cu (1)-O (2) | 90.0 (5) |
| O (2)-Cu (1)-O (2) | 180.0 (7) |
| O (1)-Cu (1)-O (1) | 180.0 (0) |
| O (4)-Cu (2)-O (4) | 166.3 (1) |
| O (3)-Cu (2)-O (3) | 165.3 (7) |
| O (3)-Cu (2)-O (4) | 89.1 (0) |
| O (2)-Cu (2)-O (4) | 96.9 (6) |
| O (2)-Cu (2)-O (3) | 97.4 (6) |

The numbers in parentheses are estimated standard deviations.

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# STRUCTURAL ANOMALIES, OXYGEN ORDERING AND SUPERCONDUCTIVITY IN OXYGEN DEFICIENT $Ba_2YCu_3O_x$

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Revised manuscript received 15 December 1989

We report the characterization of series of oxygen deficient $Ba_2YCu_3O_x$ samples for $7 \geq x \geq 6$ prepared by Zr gettered annealing at 440°C. Measurements include complete crystal structure analysis at 5 K by powder neutron diffraction, electron microscopy study of the oxygen ordering, and magnetic measurements of the superconducting transitions, with particular attention to the transition widths. The results show for the first time that the 90 K and 60 K plateaus in $T_c$ as a function of oxygen stoichiometry are associated with plateaus in the effective valence of the plane coppers. We also correlate the disappearance of superconductivity for $x < 6.5$ with an abrupt transfer of negative charge into the $CuO_2$ planes. We propose that different ordering schemes of oxygen have different characteristic $T_c$'s between 90 and 60 K.

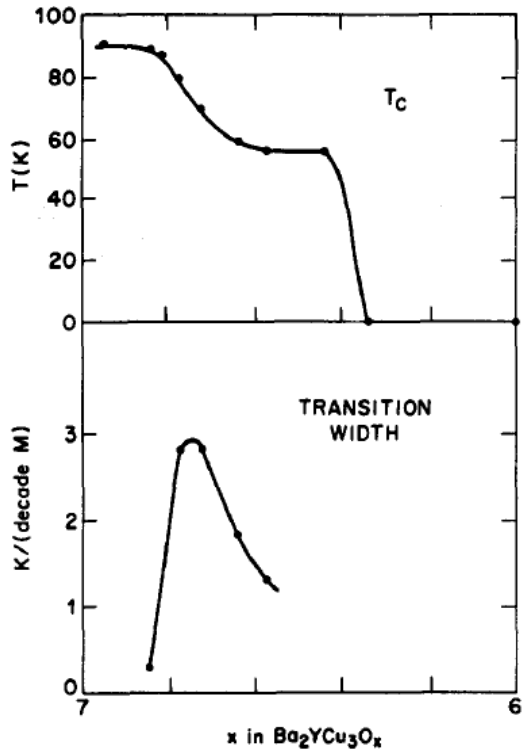


Fig. 1. Superconductive transition temperature $T_c$ for the ten samples of $Ba_2YCu_3O_x$ employed in this study. The width of the superconducting transitions in kelvins per decade of magnetization is also shown.

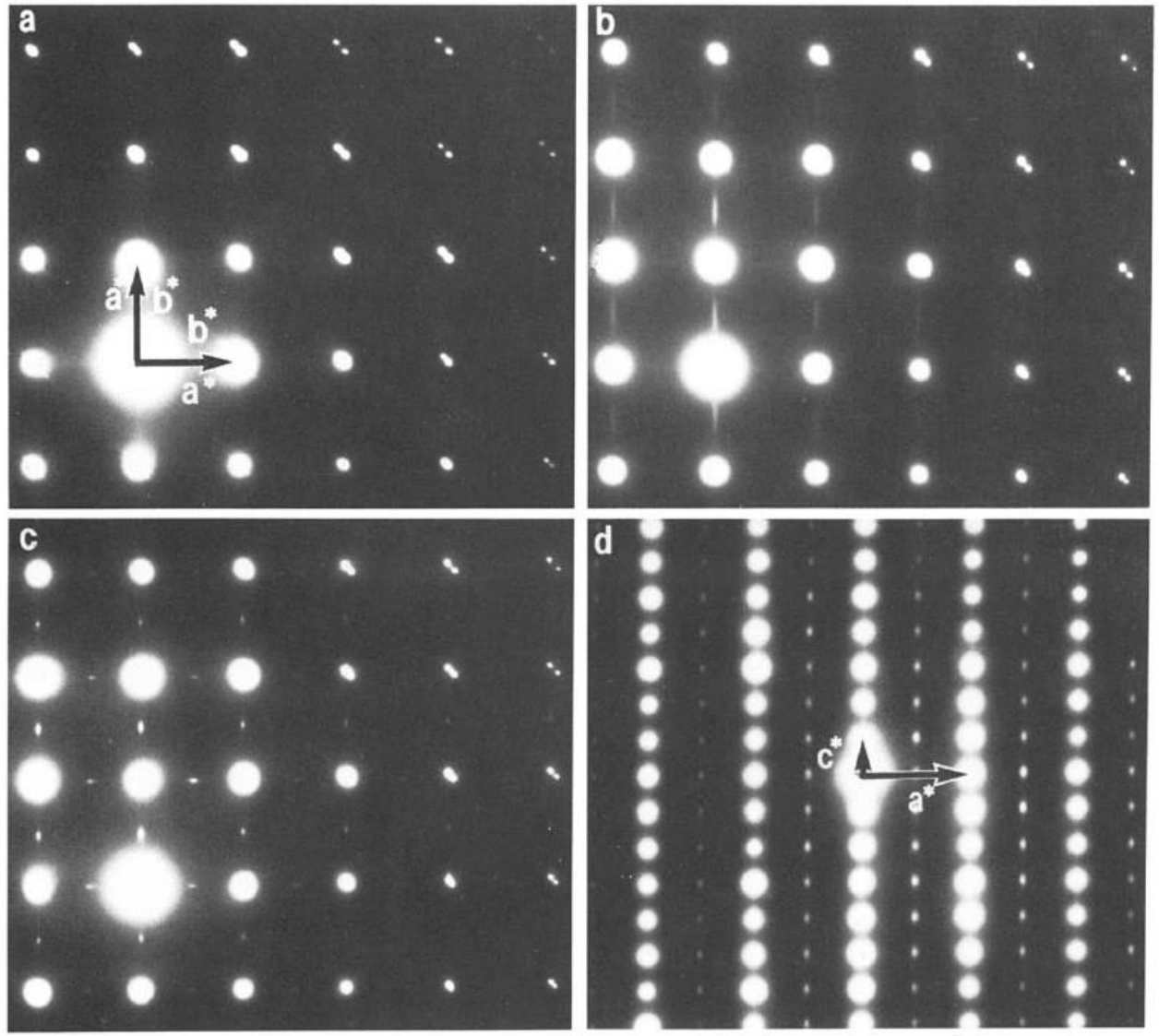


Fig. 2. Electron diffraction patterns from orthorhombic $Ba_2YCu_3O_x$ showing: (a) typical twinning with no diffuse scattering for $x > 6.8$, (b) short range superstructure for $x = 6.64$, (c) long range superstructure in the $x$–$y$ plane for $6.58 \geq x \geq 6.45$, (d) long range order also along the c-axis for $6.58 \geq x \geq 6.45$.

R.J. Cava et al. / A series of oxygen

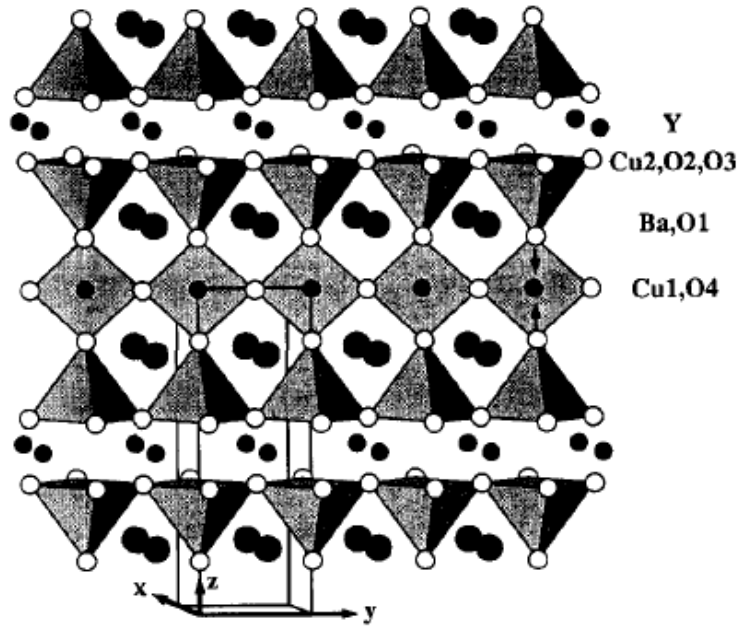


Fig. 3. The structure of $Ba_2YCu_3O_7$, showing the atom labels used in the present paper.

used for all atoms. No attempt was made to refine a double minimum site for the chain oxygen O(4), as done by Francois et al. [18], because the longer

Table II
Structural parameters at 5 K for $YBa_2Cu_3O_x$ with various oxygen stoichiometries. The relative cell dimensions $a$, $b$, $c$ are reliable within the quoted standard deviations, but these do not include the uncertainty in the effective neutron wavelength $\lambda = 1.5946(3)$ Å.

| $x=$ | | 6.95 | 6.84 | 6.81 | 6.78 | 6.73 | 6.64 | 6.58 | 6.45 | 6.35 | 6.00 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $a$ | | 3.8136(1) | 3.8153(1) | 3.8163(1) | 3.8170(1) | 3.8193(1) | 3.8224(1) | 3.8252(1) | 3.8293(1) | 3.8580(1) | 3.8544(1) |
| $b$ | | 3.8845(1) | 3.8848(1) | 3.8845(1) | 3.8836(1) | 3.8835(1) | 3.8811(1) | 3.8786(1) | 3.8750(1) | 3.8580(1) | 3.8544(1) |
| $c$ | | 11.6603(3) | 11.6692(3) | 11.6739(3) | 11.6768(3) | 11.6832(2) | 11.6912(3) | 11.6987(3) | 11.7101(4) | 11.7913(3) | 11.8175(4) |
| Ba | ($z$) | 0.1843(2) | 0.1856(2) | 0.1859(2) | 0.1862(2) | 0.1867(2) | 0.1873(3) | 0.1877(2) | 0.1878(3) | 0.1931(2) | 0.1944(3) |
| | ($B$) | 0.34(4) | 0.41(4) | 0.25(4) | 0.27(40) | 0.32(3) | 0.16(5) | 0.43(4) | 0.05(6) | 0.68(6) | 0.37(6) |
| Y | ($B$) | 0.67(4) | 0.41(4) | 0.44(4) | 0.18(4) | 0.37(3) | 0.18(5) | 0.63(4) | 0.14(6) | 0.48(5) | 0.15(5) |
| Cu(1) | ($B$) | 0.44(4) | 0.43(4) | 0.34(4) | 0.26(4) | 0.29(3) | 0.11(4) | 0.46(4) | 0.06(6) | 0.76(5) | 0.44(5) |
| Cu(2) | ($z$) | 0.3546(2) | 0.3552(1) | 0.3561(1) | 0.3559(1) | 0.3561(1) | 0.3571(2) | 0.3574(1) | 0.3573(2) | 0.3603(2) | 0.3602(2) |
| | ($B$) | 0.22(3) | 0.28(3) | 0.17(3) | 0.14(3) | 0.23(2) | 0.01(3) | 0.47(3) | 0.09(4) | 0.59(3) | 0.23(3) |
| O(1) | ($z$) | 0.1572(2) | 0.1579(2) | 0.1570(2) | 0.1565(2) | 0.1568(2) | 0.1564(2) | 0.1553(2) | 0.1541(3) | 0.1515(3) | 0.1511(3) |
| | ($B$) | 0.65(4) | 0.71(4) | 0.65(4) | 0.55(4) | 0.68(3) | 0.51(4) | 0.86(4) | 0.54(6) | 1.06(5) | 0.61(5) |
| O(2) | ($z$) | 0.3781(2) | 0.3785(2) | 0.3786(2) | 0.3787(2) | 0.3786(2) | 0.3786(2) | 0.3792(2) | 0.3781(3) | 0.3788(2) | 0.3791(2) |
| | ($B$) | 0.55(4) | 0.53(4) | 0.55(4) | 0.43(4) | 0.50(3) | 0.38(4) | 0.74(4) | 0.30(6) | 0.59(3) | 0.27(3) |
| O(3) | ($z$) | 0.3777(2) | 0.3777(2) | 0.3780(2) | 0.3779(2) | 0.3778(2) | 0.3786(3) | 0.3776(2) | 0.3768(4) | 0.3788 | 0.3791 |
| | ($B$) | 0.33(4) | 0.22(4) | 0.25(4) | 0.15(4) | 0.31(3) | 0.15(4) | 0.62(4) | 0.10(6) | 0.59 | 0.27 |
| O(4) | ($B$) | 0.97(8) | 0.72(8) | 0.56(8) | 0.49(8) | 0.61(7) | 0.65(11) | 0.86(10) | 0.10(18) | 3.14(50) | |
| | ($n$) | 0.475 | 0.420 | 0.405 | 0.390 | 0.375 | 0.320 | 0.290 | 0.225 | 0.175 | 0.000 |
| $R_I$ | | 6.57 | 8.14 | 7.32 | 5.61 | 4.46 | 7.54 | 7.28 | 10.95 | 8.06 | 8.57 |
| $R_P$ | | 10.42 | 9.32 | 10.61 | 9.85 | 8.03 | 10.92 | 9.50 | 15.51 | 12.63 | 12.93 |

R.J. Cava et al. / A series of oxygen deficient $Ba_2YCu_3O_x$ samples

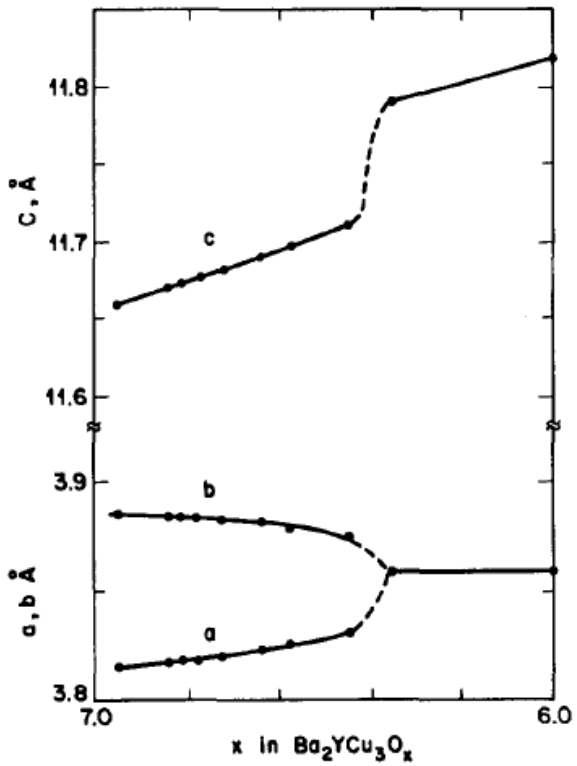


Fig. 5. Refined crystallographic cell parameters for $Ba_2YCu_3O_x$ prepared by Zr gettering at 440°C.

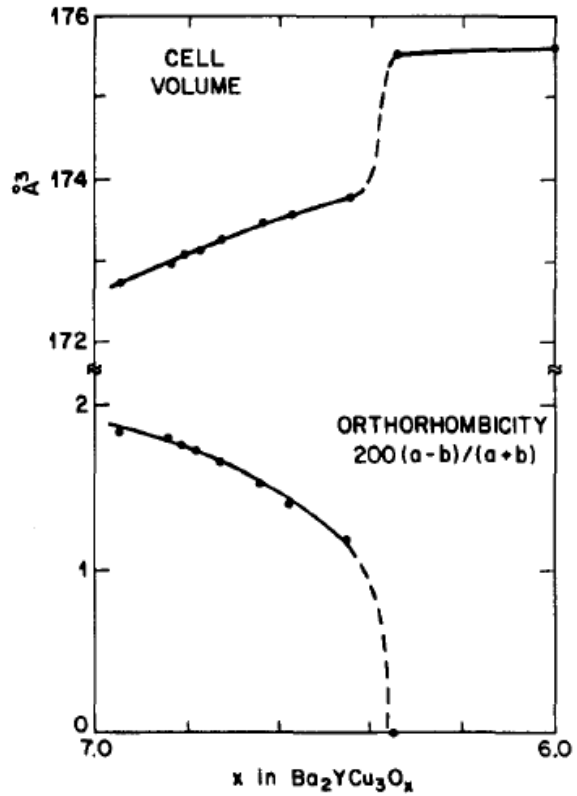


Fig. 6. Crystallographic cell volume and orthorhombicity f $Ba_2YCu_3O_x$ prepared by Zr gettering at 440°C.

More Recent Data

PHYSICAL REVIEW B VOLUME 41, NUMBER 4 1 FEBRUARY 1990

# Structural properties of oxygen-deficient $YBa_2Cu_3O_{7-\delta}$

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(Received 17 July 1989; revised manuscript received 25 September 1989)

The structural properties of oxygen-deficient $YBa_2Cu_3O_{7-\delta}$ have been determined by neutron powder diffraction for $0.07 < \delta < 0.91$. The samples were produced by quenching into liquid nitrogen from controlled oxygen partial pressures at 520 °C, and they exhibit a clearly defined "plateau" behavior of $T_c$ versus $\delta$. Superconductivity disappears at the orthorhombic-to-tetragonal transition that occurs near $\delta = 0.65$. Structural parameters, including the copper-oxygen bond lengths, vary smoothly with $\delta$ within each phase but exhibit different behavior in the superconducting and nonsuperconducting phases. These observations are consistent with a model in which superconducting behavior is controlled by charge transfer between the conducting two-dimensional $CuO_2$ planes and the $CuO_x$ chains, which act as reservoirs of charge.

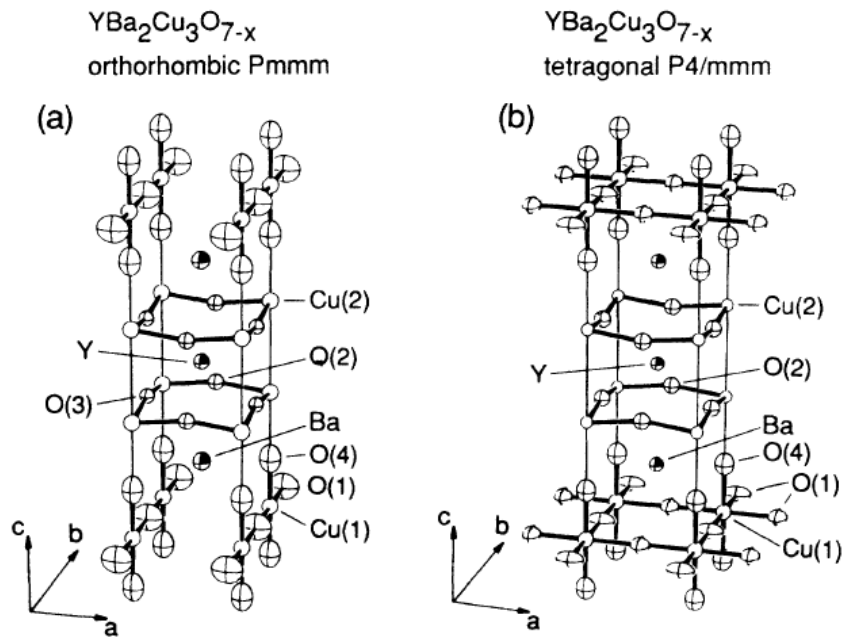



FIG. 1. (a) Orthorhombic and (b) tetragonal structures of $YBa_2Cu_3O_{7-\delta}$. In the tetragonal structure (b) the different atom symbol for the O(1) site is used to indicate that this site is not fully occupied.

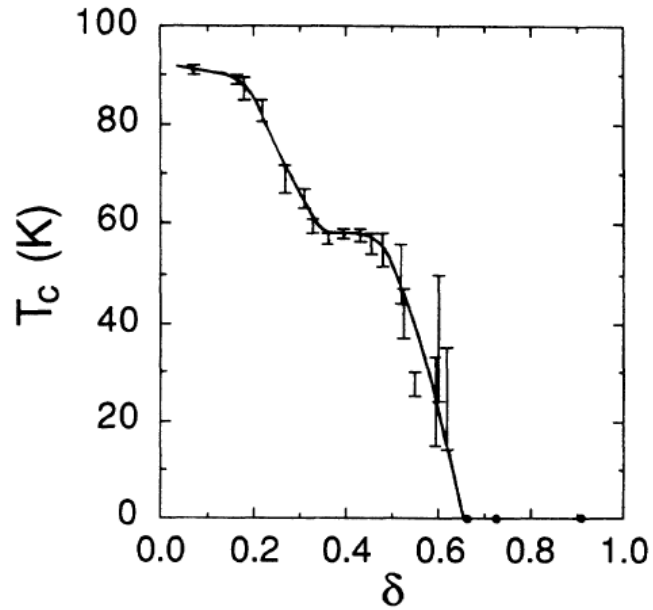
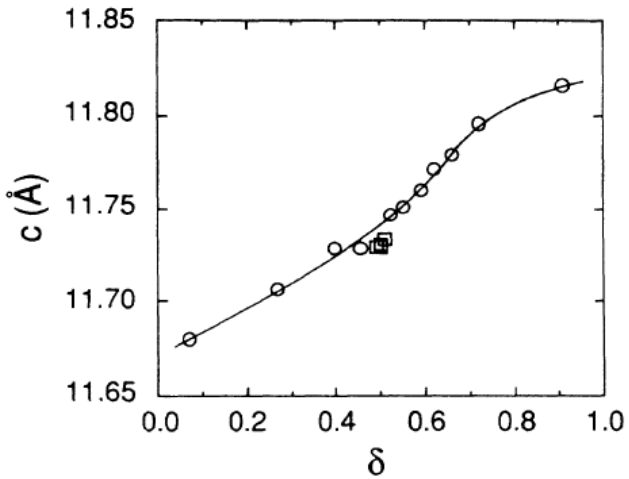
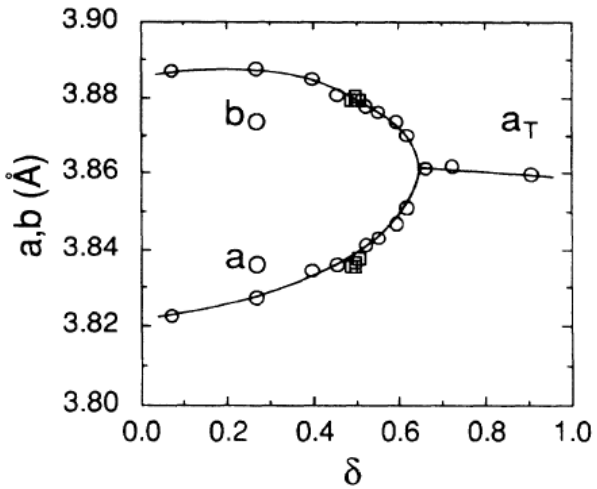
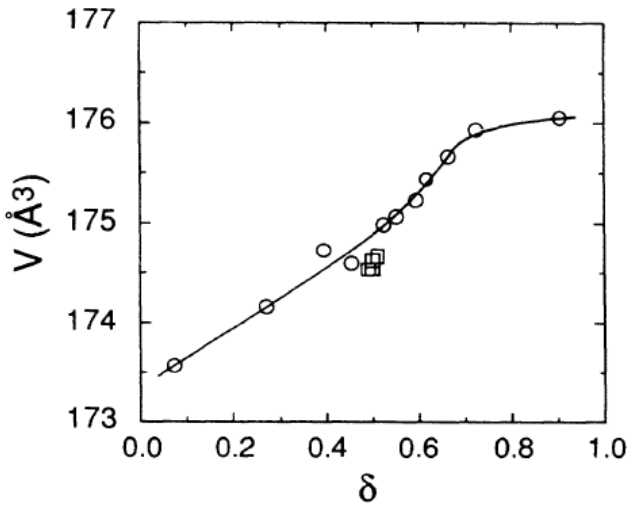



FIG. 3. Superconducting transition temperatures, $T_c$, for oxygen-deficient samples of $YBa_2Cu_3O_{7-\delta}$, produced by quenching into liquid nitrogen from various oxygen partial pressures at 520°C. The error bars for $T_c$ extend from the Meissner onset temperature to the temperature at which the Meissner signal is 50% of its maximum value. The oxygen compositions, $\delta$, are determined from weight-loss measurements referenced to a starting composition of $YBa_2Cu_3O_{6.93}$ (see text).


11.85
11.80
11.75
11.70
11.65
c (Å)
0.0
0.2
0.4
0.6
0.8
1.0
δ


3.90
3.88
3.86
3.84
3.82
3.80
a,b (Å)
b_O
a_T
a_O
0.0
0.2
0.4
0.6
0.8
1.0
δ


177
176
175
174
173
V (Å3)
0.0
0.2
0.4
0.6
0.8
1.0
δ

# YBCO_100K_MtSE_v3_a

**Table 1 Crystal data and structure refinement for YBCO_100K_MtSE_v3_a.**

| | |
|---|---|
| Identification code | YBCO_100K_MtSE_v3_a |
| Empirical formula | $Ba_2Cu_3O_{6.67}Y$ |
| Formula weight | 660.93 |
| Temperature/K | 293(2) |
| Crystal system | orthorhombic |
| Space group | Pmmm |
| a/Å | 3.82600(10) |
| b/Å | 3.8737(2) |
| c/Å | 11.6467(3) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 172.613(11) |
| Z | 1 |
| $\rho_{calc}$g/cm$^3$ | 6.358 |
| μ/mm$^{-1}$ | 28.594 |
| F(000) | 291.0 |
| Crystal size/mm$^3$ | ? × ? × ? |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 6.998 to 90.564 |
| Index ranges | -7 ≤ h ≤ 7, -7 ≤ k ≤ 7, -23 ≤ l ≤ 23 |
| Reflections collected | 30938 |
| Independent reflections | 889 [$R_{int}$ = 0.2023, $R_{sigma}$ = 0.0446] |
| Data/restraints/parameters | 889/0/31 |
| Goodness-of-fit on F$^2$ | 1.050 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0611, $wR_2$ = 0.1592 |
| Final R indexes [all data] | $R_1$ = 0.0741, $wR_2$ = 0.1729 |
| Largest diff. peak/hole / e Å$^{-3}$ | 12.66/-7.70 |



## STRUCTURAL PROPERTIES OF OXYGEN-DEFICIENT $YBa_2Cu_3O_{7-\delta}$

TABLE II. Structural parameters for oxygen-deficient samples of $YBa_2Cu_3O_{7-\delta}$, annealed in controlled oxygen atmospheres at 520°C and then quenched into liquid nitrogen. Rietveld refinements were done in the orthorhombic *Pmmm* or tetragonal *P4/mmm* space groups. Atom positions are Y($\frac{1}{2},\frac{1}{2},\frac{1}{2}$), Ba($\frac{1}{2},\frac{1}{2},z$), Cu(1)(0,0,0), Cu(2)(0,0,$z$), O(1)(0,$\frac{1}{2}$,0), O(2)($\frac{1}{2}$,0,$z$), O(3)(0,$\frac{1}{2}$,$z$), O(4)(0,0,$z$), and O(5)($\frac{1}{2}$,0,0). Numbers in parentheses are statistical standard deviations of the last significant digit.

| δ (weight loss) | | 0.07[a] | 0.27 | 0.40 | 0.45 |
|---|---|---|---|---|---|
| | a (Å) | 3.8227(1) | 3.8275(1) | 3.8349(1) | 3.8362(1) |
| | b (Å) | 3.8872(2) | 3.8875(1) | 3.8851(1) | 3.8808(1) |
| | c (Å) | 11.6802(2) | 11.7063(2) | 11.7279(2) | 11.7286(2) |
| | $V$ (Å$^3$) | 173.56 | 174.18 | 174.73 | 174.61 |
| Y: | $B$ (Å$^2$) | 0.28(3) | 0.33(3) | 0.24(4) | 0.36(3) |
| Ba: | $z$ | 0.1843(2) | 0.1871(2) | 0.1879(2) | 0.1892(2) |
| | $B$ (Å$^2$) | 0.44(3) | 0.48(3) | 0.40(4) | 0.44(4) |
| Cu(1): | $B$ (Å$^2$) | 0.41(3) | 0.53(3) | 0.61(4) | 0.63(4) |
| Cu(2): | $z$ | 0.3556(1) | 0.3569(1) | 0.3578(1) | 0.3579(1) |
| | $B$ (Å$^2$) | 0.20(2) | 0.24(2) | 0.18(3) | 0.21(2) |
| O(1): | $U^2_{11}$ (Å$^2$) | 0.022(3) | 0.031(3) | 0.033(5) | 0.036(5) |
| | $U^2_{22}$ (Å$^2$) | −0.001(2) | 0.006(2) | 0.012(3) | 0.002(3) |
| | $U^2_{33}$ (Å$^2$) | 0.019(2) | 0.013(3) | 0.016(4) | 0.023(5) |
| | $n$ | 0.90(1) | 0.74(1) | 0.69(2) | 0.56(1) |
| O(2): | $z$ | 0.3779(2) | 0.3788(2) | 0.3786(2) | 0.3787(2) |
| | $B$ (Å$^2$) | 0.51(4) | 0.46(4) | 0.45(5) | 0.47(4) |
| O(3): | $z$ | 0.3790(2) | 0.3780(2) | 0.3779(2) | 0.3784(2) |
| | $B$ (Å$^2$) | 0.35(3) | 0.28(3) | 0.07(4) | 0.34(4) |
| O(4): | $z$ | 0.1590(2) | 0.1572(2) | 0.1561(2) | 0.1559(2) |
| | $U^2_{11}$ (Å$^2$) | 0.009(1) | 0.015(1) | 0.016(2) | 0.011(1) |
| | $U^2_{22}$ (Å$^2$) | 0.007(1) | 0.18(1) | 0.018(2) | 0.015(1) |
| | $U^2_{33}$ (Å$^2$) | 0.010(1) | 0.003(1) | −0.005(1) | 0.009(1) |
| | $n$ | 2.06(2) | 2.03(2) | 1.94(2) | 2.00(2) |
| O(5): | $n$ | 0.03(1) | 0.03(1) | 0.04(1) | 0.04(1) |
| | Peak width | 8.1(1) | 7.3(1) | 7.5(1) | 7.3(1) |
| | $R_{wp}$ (%) | 5.96 | 5.69 | 6.74 | 5.98 |
| | $R_{expt}$ (%) | 3.33 | 3.64 | 3.77 | 3.65 |