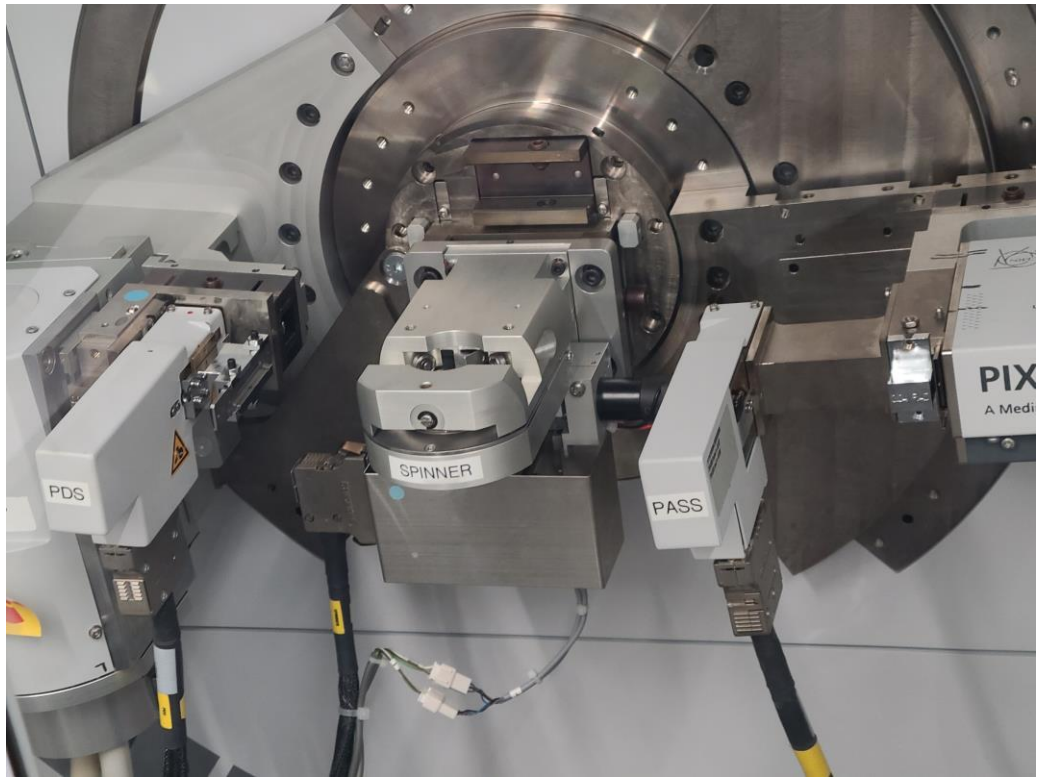
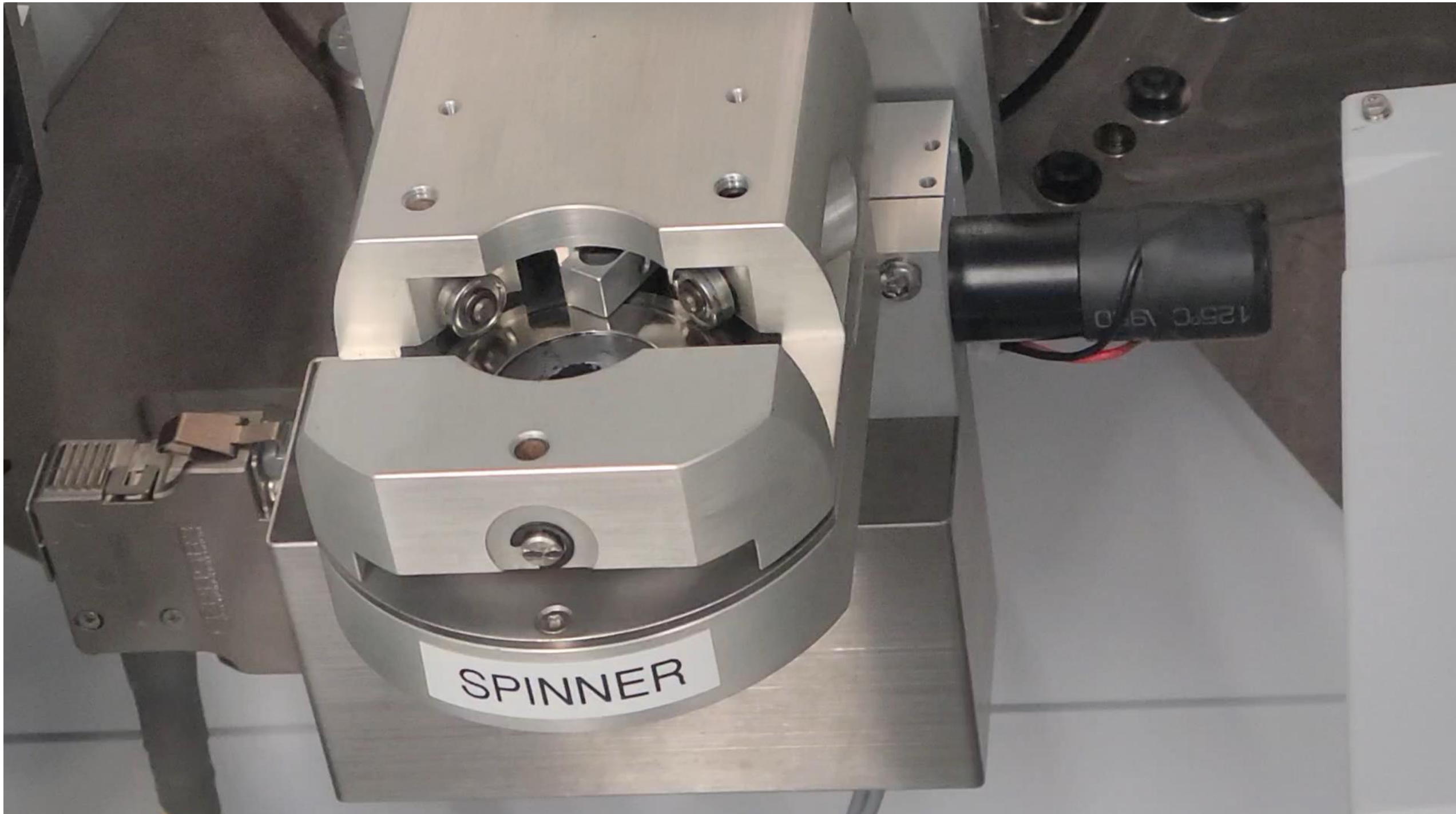
York Ctr XRD Experiment on YBCO

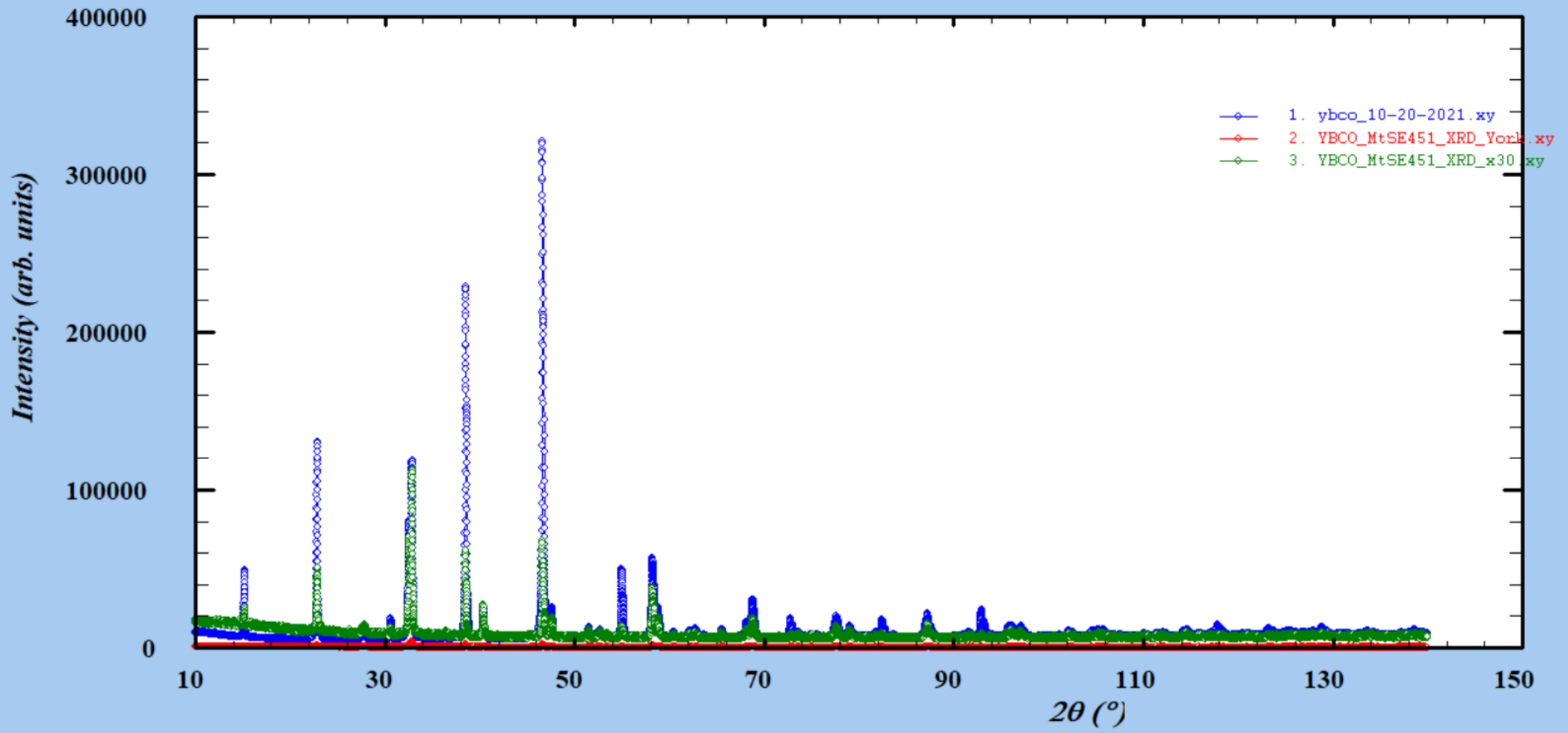

STANDBY 45/20
45 40
In case of Emergency situati
Press the Red Button on the XRD
and then leave this lab immediately.
Thanks,
Shim


PDS
SPINNER
PASS


SPINNER

WinPLOTR [CDIFX UMR6226 Rennes / ILL Grenoble]

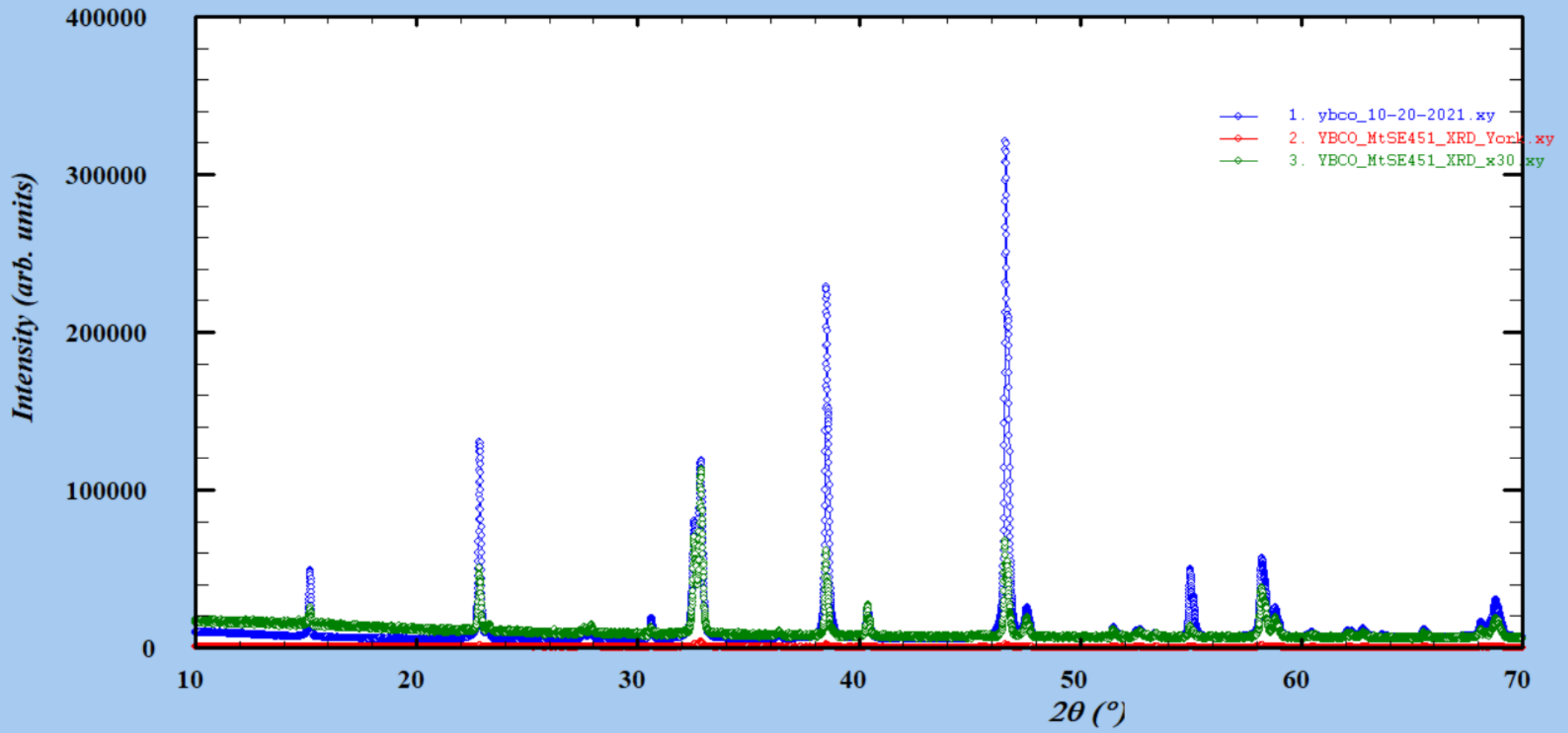
File Plot Options Points Selection X space Calculations Rietveld plot options Text External applications Tools Help



11-02-2021 | 14:37 | NUM | 2Th = 98.48959 (°) [d= 1.01689 A (wl = 1.54060 A)] | Y = 0.17459E+06

WinPLOTR [CDIFX UMR6226 Rennes / ILL Grenoble]

File Plot Options Points Selection X space Calculations Rietveld plot options Text External applications Tools Help



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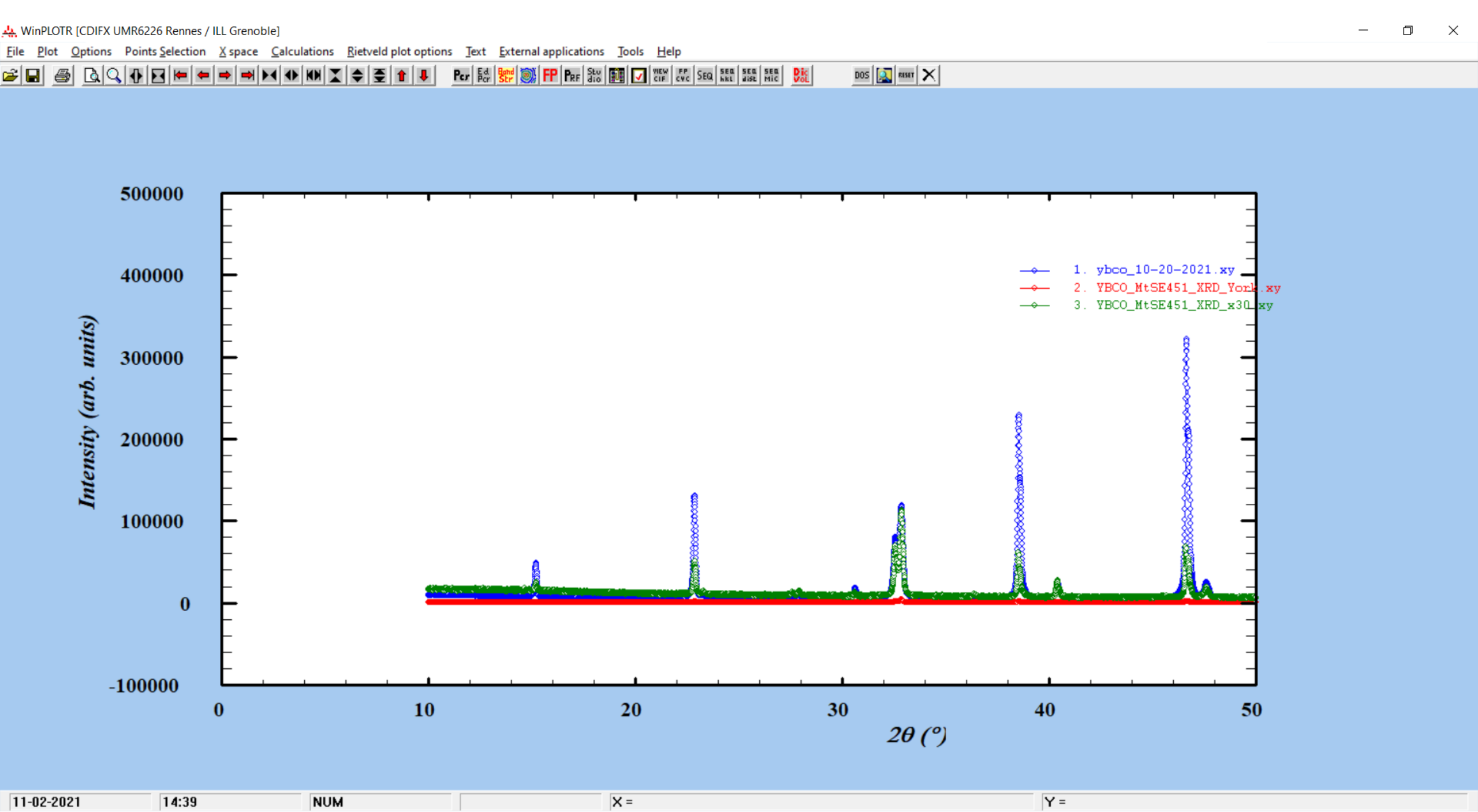
WinPLOTR [CDIFX UMR6226 Rennes / ILL Grenoble]
File Plot Options Points Selection X space Calculations Rietveld plot options Text External applications Tools Help
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200000
100000
0
-100000
Intensity (arb. units)
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10
20
30
40
50
2θ (°)
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2. YBCO_MtSE451_XRD_York.xy
3. YBCO_MtSE451_XRD_x30.xy
11-02-2021
14:39
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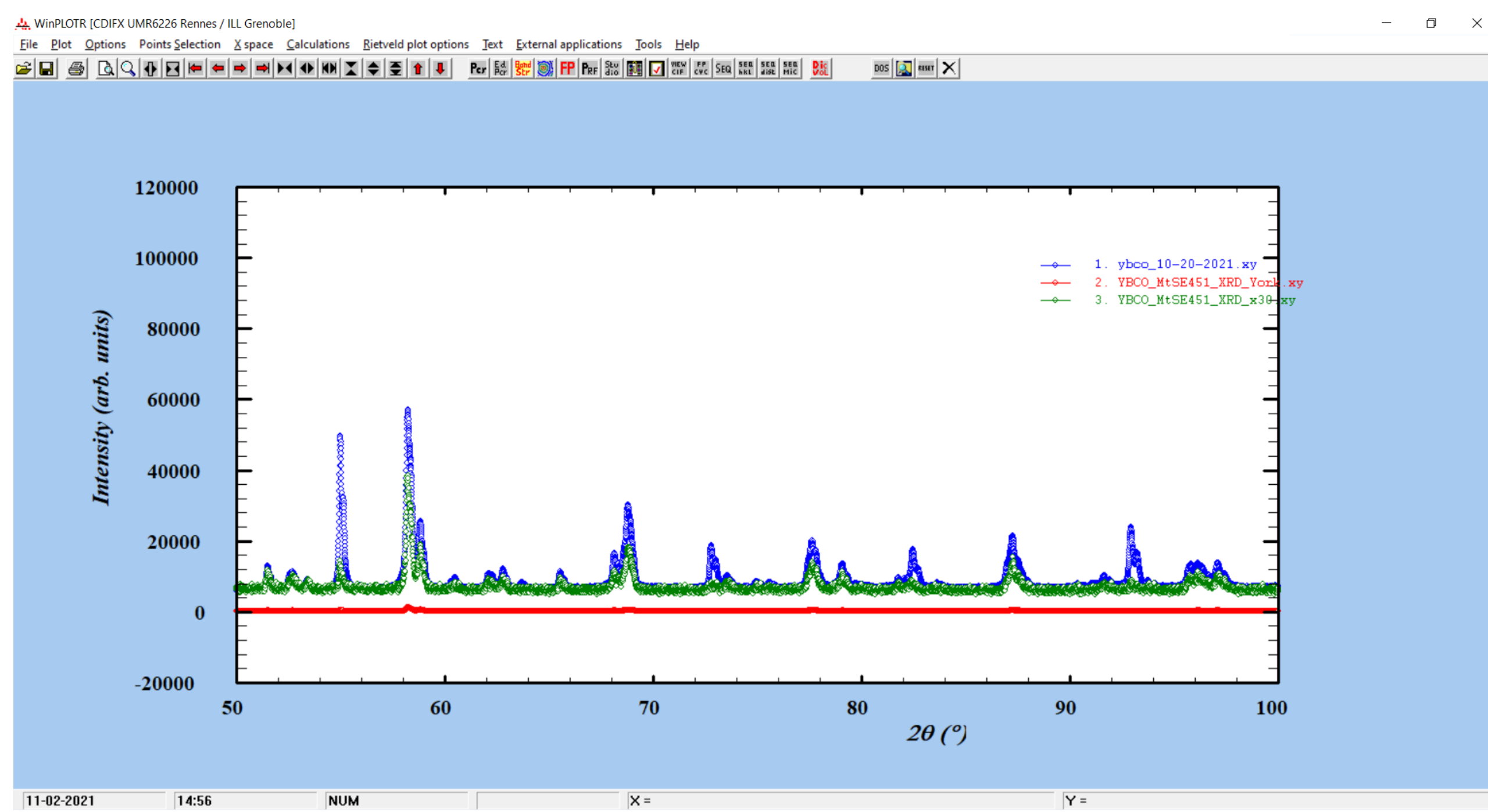
Y =


WinPLOTR [CDIFX UMR6226 Rennes / ILL Grenoble]
File Plot Options Points Selection X space Calculations Rietveld plot options Text External applications Tools Help
120000
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80000
60000
40000
20000
0
-20000
Intensity (arb. units)
50
60
70
80
90
100
2θ (°)
1. ybco_10-20-2021.xy
2. YBCO_MtSE451_XRD_York.xy
3. YBCO_MtSE451_XRD_x30.xy
11-02-2021
14:56
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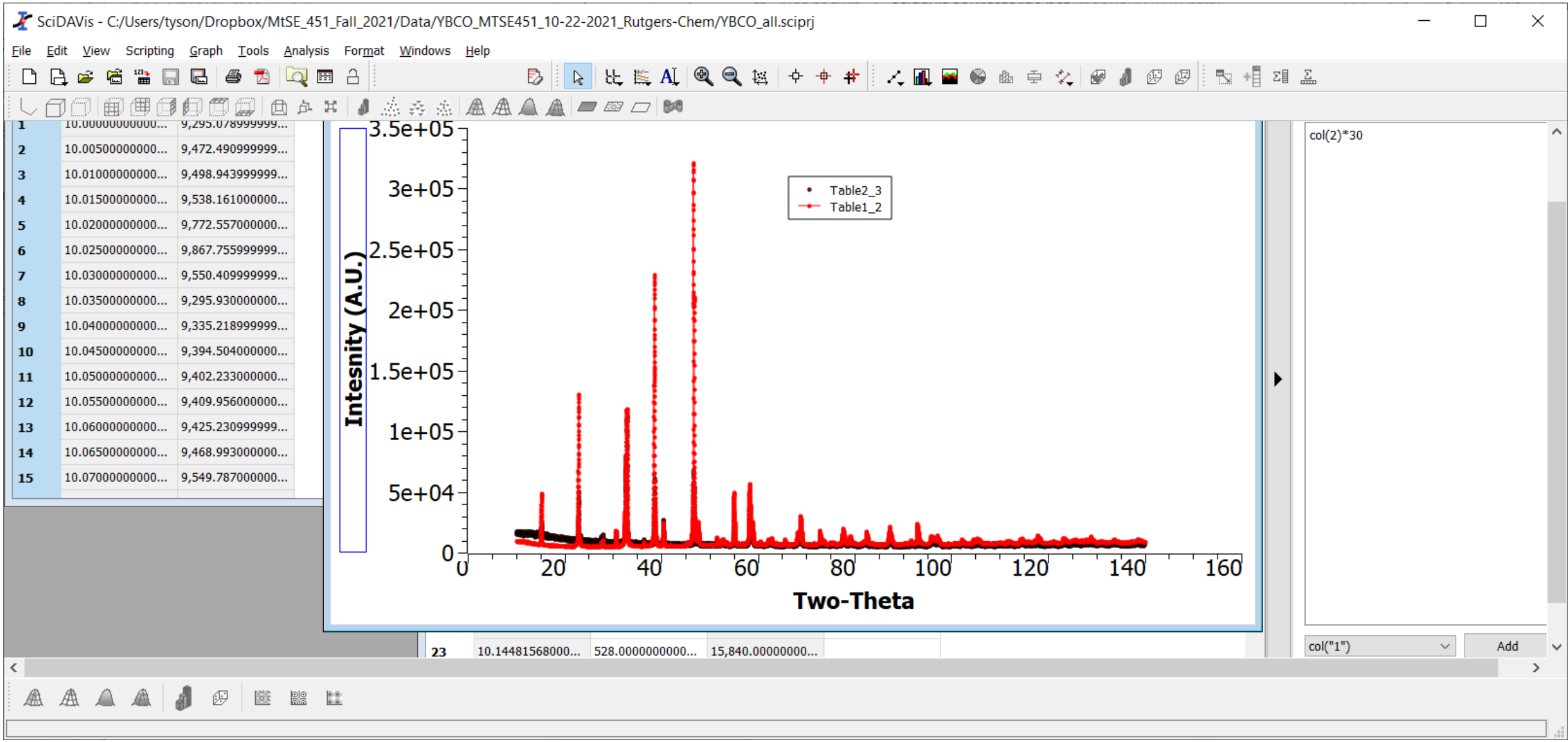
X =
Y =

Install SciDAVis
Plotting Program



$2d\sin\theta = \lambda$ Cu $K_\alpha \Rightarrow \lambda = 1.5406\text{Å}$

$$\frac{1}{d_{hkl}^2} = \left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right) + \left(\frac{l}{c}\right)^2$$

fix h k

$$\Delta\left(\frac{1}{d^2}\right) = \frac{l_1^2 - l_2^2}{c^2}$$

$1^2 - 0^2$ →	1
$2^2 - 0$	4
$3^2 - 0$	9
$4^2 - 0$	16

$2^2 - 1^2$ →	3
$3^2 - 1^2$	8

$3^2 - 2^2$	5
$4^2 - 2^2$	12
$5^2 - 2^2$	21

$4^2 - 3^2$	7
$5^2 - 4^2$	9

25

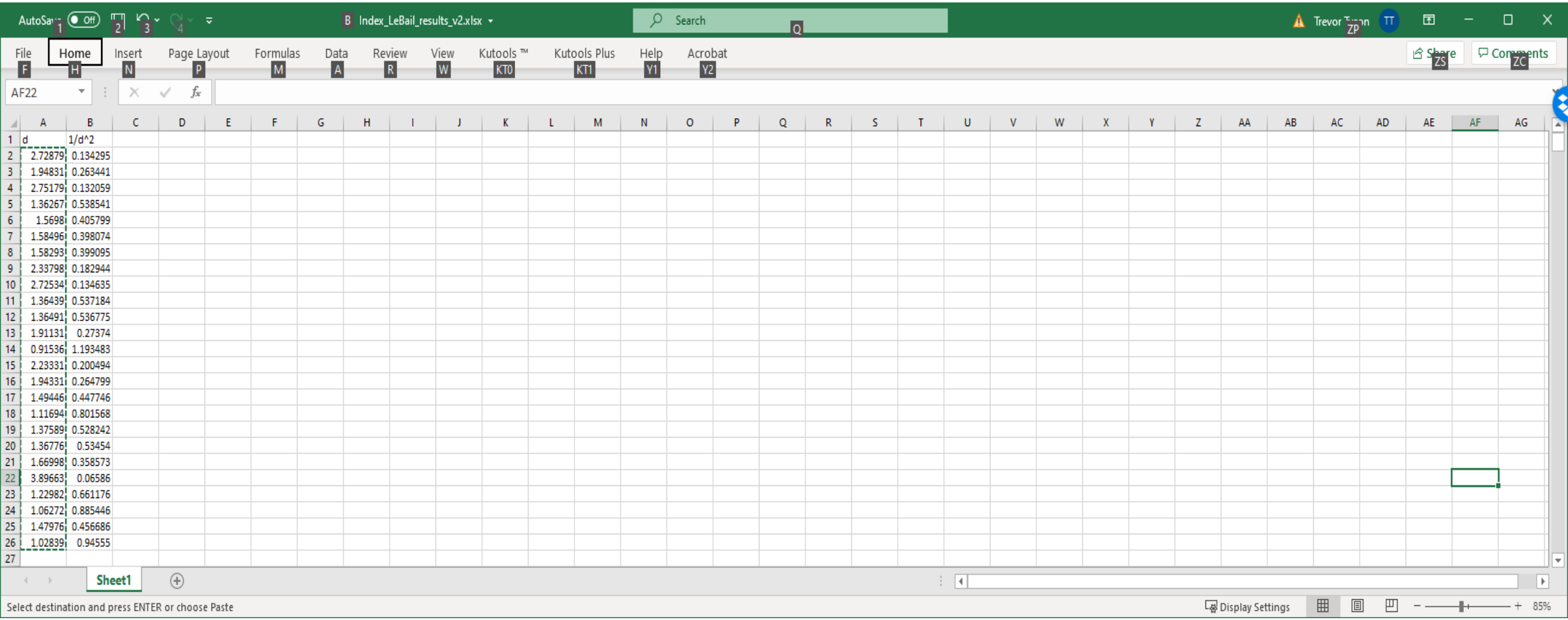
$\Delta\left(\frac{1}{d^2}\right) = (1, 3, 4, 5, 7, 8, 9 \ldots)/c^2$

$\Delta\left(\frac{1}{\square^{11}}\right) = (1, 3, 5, 78, 9 \ldots)/6^2$

$\Delta\left(\frac{4}{\square^{11}}\right) = (1\ 3,\ 5,\ 7, 89)/b^2$

$\Delta\left(\frac{1}{d^2}\right) = \frac{n}{a^2}$ find c

$a = \sqrt{\frac{n}{\Delta\left(\frac{1}{d^2}\right)}}$ $n = 1, 3, 4, 5, 7, 8$



	A	B
1	d	1/d^2
2	2.72879	0.134295
3	1.94831	0.263441
4	2.75179	0.132059
5	1.36267	0.538541
6	1.5698	0.405799
7	1.58496	0.398074
8	1.58293	0.399095
9	2.33798	0.182944
10	2.72534	0.134635
11	1.36439	0.537184
12	1.36491	0.536775
13	1.91131	0.27374
14	0.91536	1.193483
15	2.23331	0.200494
16	1.94331	0.264799
17	1.49446	0.447746
18	1.11694	0.801568
19	1.37589	0.528242
20	1.36776	0.53454
21	1.66998	0.358573
22	3.89663	0.06586
23	1.22982	0.661176
24	1.06272	0.885446
25	1.47976	0.456686
26	1.02839	0.94555
27		

AutoSave Off | Index_LeBail_results_v2.xlsx | Search | Trevor Tyson

File Home Insert Page Layout Formulas Data Review View Kutools ™ Kutools Plus Help Acrobat | Share | Comments

AF22

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG
22	3.89663	0.06586																															
23	1.22982	0.661176																															
24	1.06272	0.885446																															
25	1.47976	0.456686																															
26	1.02839	0.94555																															
27																																	
28																																	
29																																	
30																																	
31		0.06586	0.132059	0.134295	0.134635	0.182944	0.200494	0.263441	0.264799	0.27374	0.358573	0.398074	0.399095	0.405799	0.447746	0.456686	0.528242	0.53454	0.536775	0.537184	0.538541	0.661176	0.801568	0.885446	0.94555	1.193483							
32	0.06586	0	-0.0662	-0.06843	-0.06878	-0.11708	-0.13463	-0.19758	-0.19894	-0.20788	-0.29271	-0.33221	-0.33324	-0.33994	-0.38189	-0.39083	-0.46238	-0.46868	-0.47091	-0.47132	-0.47268	-0.59532	-0.73571	-0.81959	-0.87969	-1.12762							
33	0.132059	0.066199	0	-0.00224	-0.00258	-0.05088	-0.06843	-0.13138	-0.13274	-0.14168	-0.22651	-0.26601	-0.26704	-0.27374	-0.31569	-0.32463	-0.39618	-0.40248	-0.40472	-0.40512	-0.40648	-0.52912	-0.66951	-0.75339	-0.81349	-1.06142							
34	0.134295	0.068435	0.002236	0	-0.00034	-0.04865	-0.0662	-0.12915	-0.1305	-0.13944	-0.22428	-0.26378	-0.2648	-0.2715	-0.31345	-0.32239	-0.39395	-0.40025	-0.40248	-0.40289	-0.40425	-0.52688	-0.66727	-0.75115	-0.81125	-1.05919							
35	0.134635	0.068775	0.002576	0.00034	0	-0.04831	-0.06586	-0.12881	-0.13016	-0.1391	-0.22394	-0.26344	-0.26446	-0.27116	-0.31311	-0.32205	-0.39361	-0.3999	-0.40214	-0.40255	-0.40391	-0.52654	-0.66693	-0.75081	-0.81091	-1.05885							
36	0.182944	0.117084	0.050885	0.048649	0.048309	0	-0.01755	-0.0805	-0.08185	-0.0908	-0.17563	-0.21513	-0.21615	-0.22286	-0.2648	-0.27374	-0.3453	-0.3516	-0.35383	-0.35424	-0.3556	-0.47823	-0.61862	-0.7025	-0.76261	-1.01054							
37	0.200494	0.134634	0.068435	0.066199	0.065859	0.01755	0	-0.06295	-0.0643	-0.07325	-0.15808	-0.19758	-0.1986	-0.20531	-0.24725	-0.25619	-0.32775	-0.33405	-0.33628	-0.33669	-0.33805	-0.46068	-0.60107	-0.68495	-0.74506	-0.99299							
38	0.263441	0.197581	0.131382	0.129146	0.128806	0.080497	0.062947	0	-0.00136	-0.0103	-0.09513	-0.13463	-0.13565	-0.14236	-0.1843	-0.19324	-0.2648	-0.2711	-0.27333	-0.27374	-0.2751	-0.39773	-0.53813	-0.62201	-0.68211	-0.93004							
39	0.264799	0.198939	0.132739	0.130504	0.130163	0.081855	0.064304	0.001357	0	-0.00894	-0.09377	-0.13327	-0.1343	-0.141	-0.18295	-0.19189	-0.26344	-0.26974	-0.27198	-0.27239	-0.27374	-0.39638	-0.53677	-0.62065	-0.68075	-0.92868							
40	0.27374	0.20788	0.14168	0.139445	0.139104	0.090796	0.073245	0.010298	0.008941	0	-0.08483	-0.12433	-0.12536	-0.13206	-0.17401	-0.18295	-0.2545	-0.2608	-0.26303	-0.26344	-0.2648	-0.38744	-0.52783	-0.61171	-0.67181	-0.91974							
41	0.358573	0.292713	0.226513	0.224278	0.223938	0.175629	0.158079	0.095132	0.093774	0.084833	0	-0.0395	-0.04052	-0.04723	-0.08917	-0.09811	-0.16967	-0.17597	-0.1782	-0.17861	-0.17997	-0.3026	-0.44299	-0.52687	-0.58698	-0.83491							
42	0.398074	0.332214	0.266014	0.263779	0.263438	0.21513	0.197579	0.134632	0.133275	0.124334	0.039501	0	-0.00102	-0.00773	-0.04967	-0.05861	-0.13017	-0.13647	-0.1387	-0.13911	-0.14047	-0.2631	-0.40349	-0.48737	-0.54748	-0.79541							
43	0.399095	0.333235	0.267036	0.2648	0.26446	0.216151	0.198601	0.135654	0.134297	0.125356	0.040522	0.001022	0	-0.0067	-0.04865	-0.05759	-0.12915	-0.13544	-0.13768	-0.13809	-0.13945	-0.26208	-0.40247	-0.48635	-0.54645	-0.79439							
44	0.405799	0.339939	0.27374	0.271504	0.271164	0.222855	0.205305	0.142358	0.141001	0.13206	0.047226	0.007726	0.006704	0	-0.04195	-0.05089	-0.12244	-0.12874	-0.13098	-0.13138	-0.13274	-0.25538	-0.39577	-0.47965	-0.53975	-0.78768							
45	0.447746	0.381886	0.315686	0.313451	0.31311	0.264802	0.247251	0.184304	0.182947	0.174006	0.089173	0.049672	0.04865	0.041946	0	-0.00894	-0.0805	-0.08679	-0.08903	-0.08944	-0.0908	-0.21343	-0.35382	-0.4377	-0.4978	-0.74574							
46	0.456686	0.390826	0.324626	0.322391	0.322051	0.273742	0.256191	0.193244	0.191887	0.182946	0.098113	0.058612	0.05759	0.050886	0.00894	0	-0.07156	-0.07785	-0.08009	-0.0805	-0.08186	-0.20449	-0.34488	-0.42876	-0.48886	-0.7368							
47	0.528242	0.462382	0.396182	0.393947	0.393606	0.345297	0.327747	0.2648	0.263443	0.254502	0.169669	0.130168	0.129146	0.122442	0.080496	0.071556	0	-0.0063	-0.00853	-0.00894	-0.0103	-0.13293	-0.27333	-0.3572	-0.41731	-0.66524							
48	0.53454	0.46868	0.402481	0.400245	0.399905	0.351596	0.334046	0.271099	0.269741	0.2608	0.175967	0.136466	0.135445	0.128741	0.086794	0.077854	0.006298	0	-0.00223	-0.00264	-0.004	-0.12664	-0.26703	-0.35091	-0.41101	-0.65894							
49	0.536775	0.470915	0.404715	0.40248	0.402139	0.353831	0.33628	0.273333	0.271976	0.263035	0.178202	0.138701	0.137679	0.130975	0.089029	0.080089	0.008533	0.002235	0	-0.00041	-0.00177	-0.1244	-0.26479	-0.34867	-0.40877	-0.65671							
50	0.537184	0.471324	0.405124	0.402889	0.402549	0.35424	0.33669	0.273743	0.272385	0.263444	0.178611	0.13911	0.138089	0.131384	0.089438	0.080498	0.008942	0.002644	0.000409	0	-0.00136	-0.12399	-0.26438	-0.34826	-0.40837	-0.6563							
51	0.538541	0.472681	0.406481	0.404246	0.403906	0.355597	0.338047	0.275099	0.273742	0.264801	0.179968	0.140467	0.139446	0.132741	0.090795	0.081855	0.010299	0.004001	0.001766	0.001357	0	-0.12263	-0.26303	-0.34691	-0.40701	-0.65494							
52	0.661176	0.595316	0.529116	0.526881	0.526541	0.478232	0.460681	0.397734	0.396377	0.387436	0.302603	0.263102	0.26208	0.255376	0.21343	0.20449	0.132934	0.126636	0.124401	0.123992	0.122635	0	-0.14039	-0.22427	-0.28437	-0.53231							
53	0.801568	0.735708	0.669508	0.667273	0.666933	0.618624	0.601074	0.538127	0.536769	0.527828	0.442995	0.403494	0.402473	0.395769	0.353822	0.344882	0.273326	0.267028	0.264793	0.264384	0.263027	0.140392	0	-0.08388	-0.14398	-0.39191							
54	0.885446	0.819586	0.753387	0.751151	0.750811	0.702502	0.684952	0.622005	0.620648	0.611707	0.526874	0.487373	0.486351	0.479647	0.437701	0.428761	0.357205	0.350906	0.348672	0.348263	0.346906	0.224271	0.083879	0	-0.0601	-0.30804							
55	0.94555	0.87969	0.81349	0.811255	0.810914	0.762605	0.745055	0.682108	0.680751	0.67181	0.586977	0.547476	0.546454	0.53975	0.497804	0.488864	0.417308	0.41101	0.408775	0.408366	0.407009	0.284374	0.143982	0.060103	0	-0.24793							
56	1.193483	1.127623	1.061423	1.059188	1.058848	1.010539	0.992988	0.930041	0.928684	0.919743	0.83491	0.795409	0.794387	0.787683	0.745737	0.736797	0.665241	0.658943	0.656708	0.656299	0.654942	0.532307	0.391915	0.308036	0.247933	0							
57																																	
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Sheet1

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D	E	F	G	H	I	J	K	L	M	N
	0.040522									
	0.041946									
	0.047226									
	0.090796									
	0.093774									

6.133182	7.75793		
6.094074	7.708462		
5.991651	7.578905		

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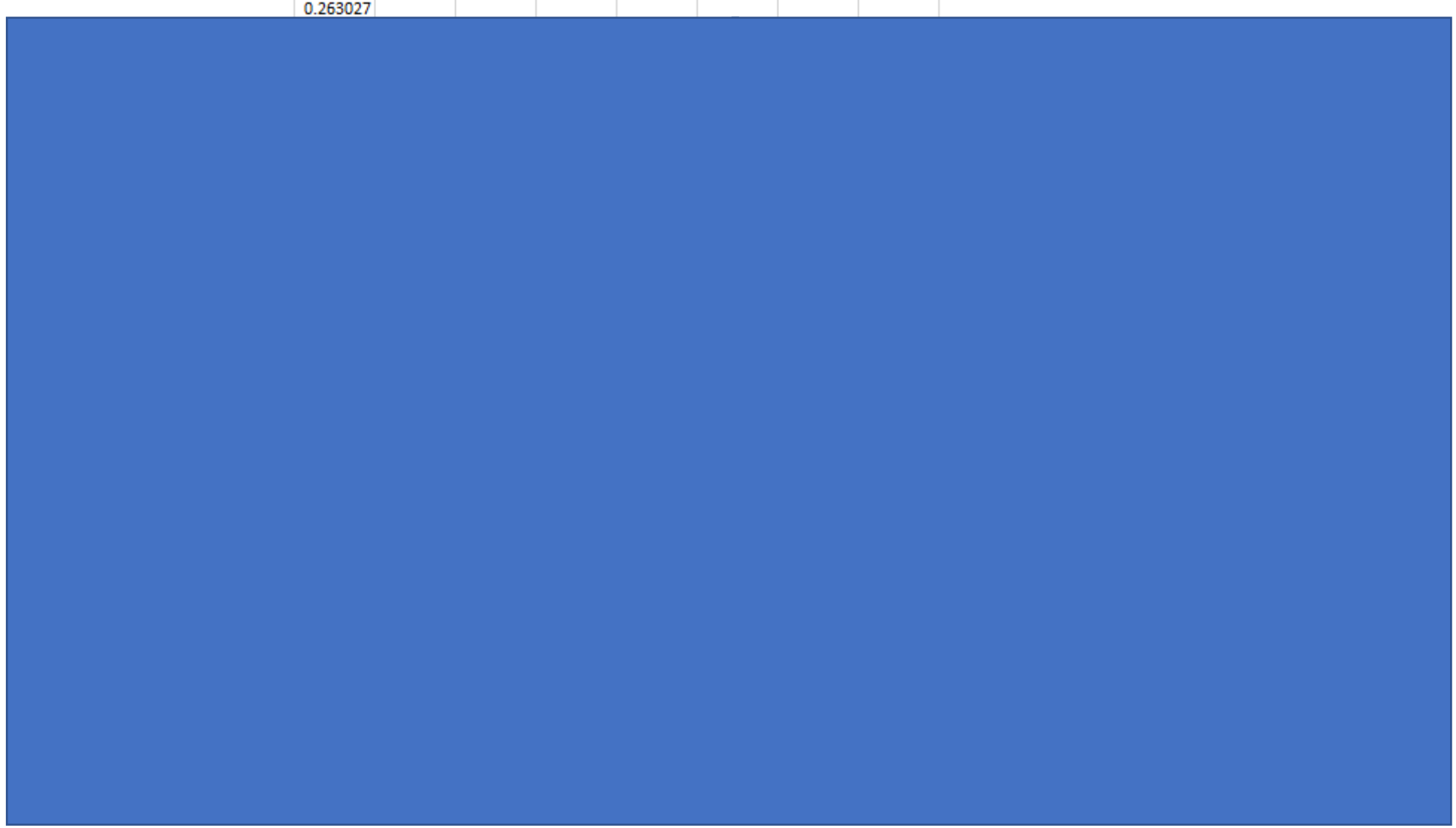


Whole powder pattern decomposition methods and applications: A retrospection

Armel Le Bail[a)]
Laboratoire des Oxydes et Fluorures, CNRS UMR 6010, Université du Maine, avenue O. Messiaen, 72085 Le Mans Cedex 9, France

(Received 30 June 2005; accepted 12 October 2005)

Methods extracting fast all the peak intensities from a complete powder diffraction pattern are reviewed. The genesis of the modern whole powder pattern decomposition methods (the so-called Pawley and Le Bail methods) is detailed and their importance and domains of application are decoded from the most cited papers citing them. It is concluded that these methods represented a decisive step toward the possibility to solve more easily, if not routinely, a structure solely from a powder sample. The review enlightens the contributions from the Louër's group during the rising years 1987–1993. © *2005 International Centre for Diffraction Data.* [DOI: 10.1154/1.2135315]

Key words: powder diffraction, whole powder pattern decomposition, intensity extraction, *ab initio* structure determination

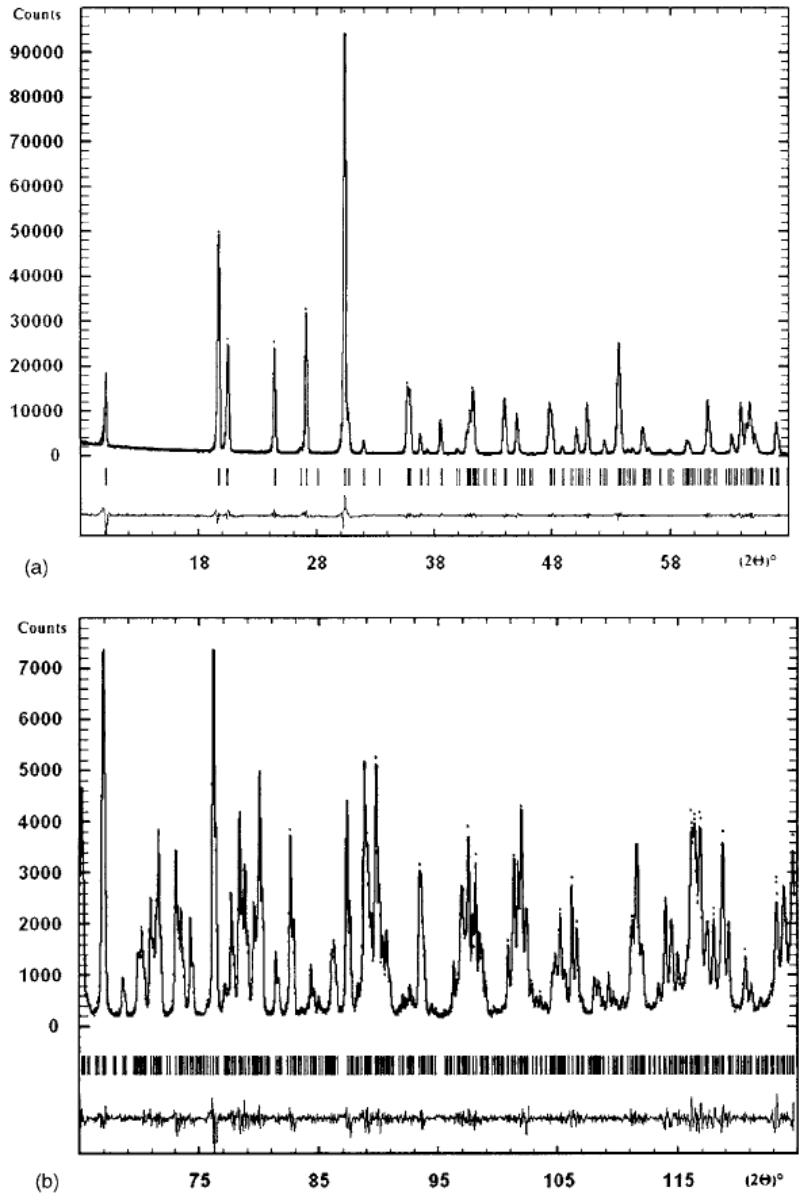


Figure 1. Le Bail fit of the powder pattern of $LiSbWO_6$, the first structure solved (Le Bail *et al.*, 1988) from intensities extracted by iterations of the Rietveld decomposition formula.

B. The Le Bail method

In order to be able to estimate R factors related to integrated intensities, Rietveld (1969) stated [see also the book edited by Young (1993)]: "a fair approximation to the observed integrated intensity can be made by separating the peaks according to the calculated values of the integrated intensities, i.e."

$$I_K(\text{obs}) = \sum_j \{w_{j.K} \,.\, S_K^2(\text{calc}) \,.\, y_j(\text{obs})/y_j(\text{calc})\}, \qquad (1)$$

where $w_{j.K}$ is a measure of the contribution of the Bragg peak at position $2\theta_K$ to the diffraction profile y_j at position $2\theta_j$. The sum is over all y_j(obs) which can theoretically contribute to the integrated intensity I_K(obs). So that there is a bias introduced here by the apportioning according to the calculated intensities, this is why the observed intensities are in fact said to be "observed," under quotes, in the Rietveld method. These "observed" intensities are used in the R_B and R_F calculations (reliabilities on intensities and structure factor amplitudes). They are also required for

Young, R. A. (**1993**). *The Rietveld Method* (Oxford University Press, New York).

jEdit - YBCO_MTSE451_F2021_LeBail.out

File Edit Search Markers Folding View Utilities Macros Plugins Help

YBCO_MTSE451_F2021_LeBail.out (%USERPROFILE%\Dropbox\Topas_old_version_Runs_9-24-2011_DropBox\YBCO_MTSE451_10-22-2021_Rutgers-Chem\)

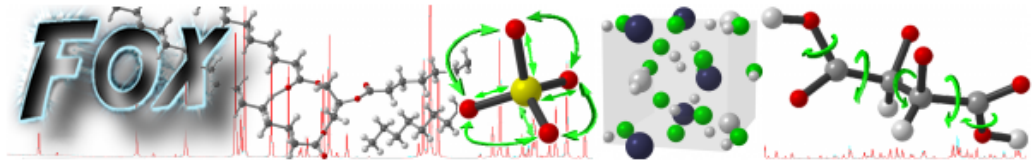
File Browser

```
'-------------------------------------
  XY(ybco_10-20-2021, 0.005)
    CuKa5(0.001)
   Radius(200.5)
  LP_Factor(17)
  Divergence(1)
  Full_Axial_Model(12, 20, 12, 5.1, 5.1)
  Slit_Width(.15)
  ZE(@,  0.104056709`)


  ' Note 1st bkg parameter starting value, this helps the Le Bail refinement
    bkg @  7179.26297`  641.906682`  855.729576` -626.467955`  789.170963` -610.274848`  270.453263` -89.1638798`  89.5631321`  31.2514135`  11.842618`  89.791371` -103.

  hkl_Is

   a   @  3.825348`
   b   @  3.889308`
   c   @  11.695510`
       al  90.0
       be  90.0
       ga  90.0

     lebail 1 ' The LeBail method

    space_group "Pmmm"
      load hkl_m_d_th2 I
      {
             0   0   2   2    5.84776       15.13862  1.23239393
             0   0   3   2    3.89850       22.79191  9.32490314
             0   1   0   2    3.88931       22.84652  0.214154015
             1   0   0   2    3.82535       23.23379  0.378833954
             0   1   1   4    3.69059       24.09464  0.0778195881
             1   0   1   4    3.63581       24.46325  0.0288400417
             0   1   2   4    3.23845       27.52057  0.508764984
             1   0   2   4    3.20124       27.84681  0.762418836
             0   0   4   2    2.92388       30.54984  2.04130461
             0   1   3   4    2.75340       32.49204  17.1508646
             1   0   3   4    2.73043       32.77311  22.5743199
             1   1   0   4    2.72726       32.81222  4.46807094
             1   1   1   8    2.65600       33.71847  0.251767396
             1   1   2   8    2.47167       36.31746  0.681346243
             0   0   5   2    2.33910       38.45423  52.745479
             0   1   4   4    2.33711       38.48828  12.6580279
             1   0   4   4    2.32301       38.73117  1.30196611
             1   1   3   8    2.23472       40.32652  7.20145869
             0   1   5   4    2.00451       45.19845  1.05538607
```

1,1 (0/14469) Input/output complete (text,none,Cp1252) l n m r o UG 71/76MB 4:00 PM

Install/Windows - FOX, Free Obje

Not secure | fox.vincefn.net/Install/Windows



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Features Requests
ObjCryst++ API
Getting FOX from git
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Installing Fox on Windows

To install F.O.X. under windows (this should work for win 98 or above), just download the `Fox-DATE.zip` package from GitHub.

Then unzip the package, and voilà, you have Fox on your computer.

If you want to **compile Fox yourself**, you can download the Linux `Fox-DATE.tar.bz2` package, which includes the full source code, including project files for compiling with the (free as a beer) VC++ 2005 Express edition. Follow these instructions to compile under windows.

None: Install/Windows (last edited 2018-09-26 14:02:55 by VincentFavreNicolin)

Fox-2017-06-28.zip

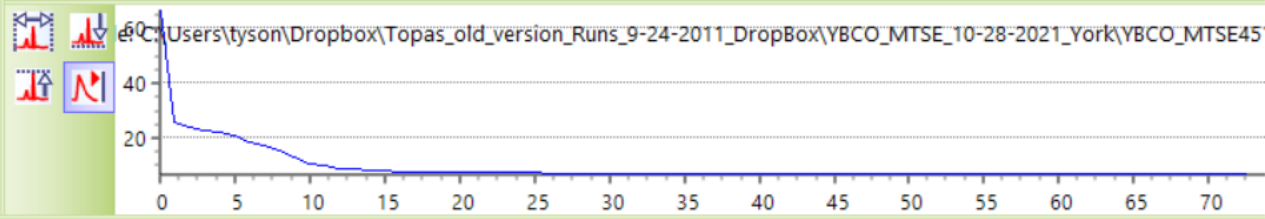
Show all

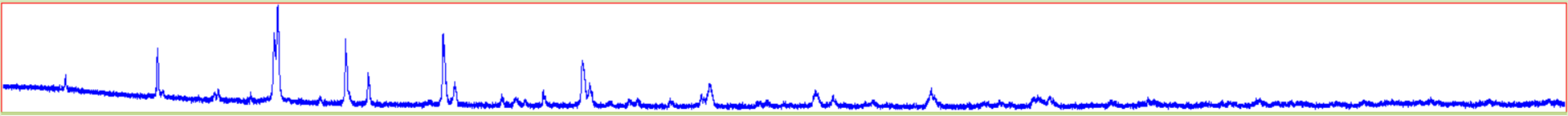
TOPAS-Academic-64 V7.12 - [YBCO_MtSE451_XRD_York.xy]

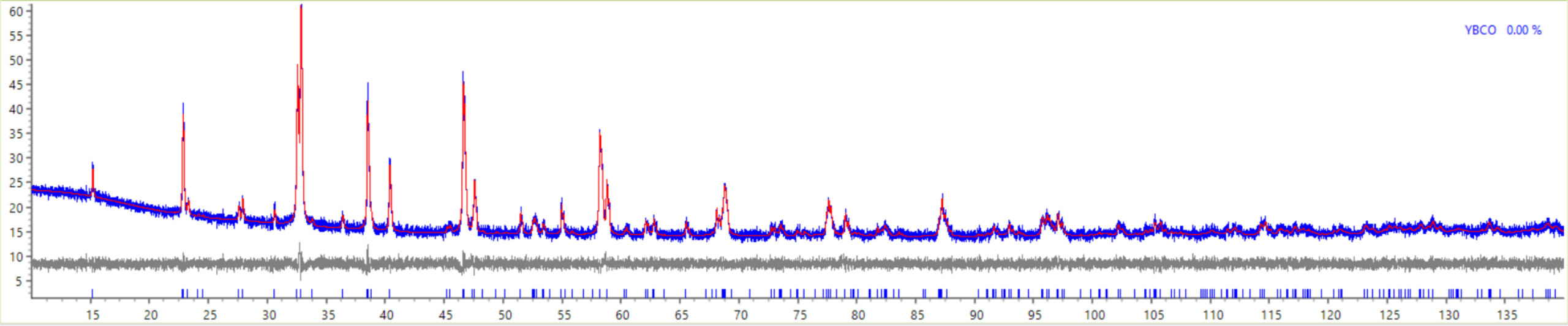
File View Fit Launch Tools Window Help

Global
YBCO_MtSE451_XRD_York.xy

```
 71  Time    2.82  Rwp     6.853    -0.001 MC      0.00 1
 72  Time    2.85  Rwp     6.852    -0.001 MC      0.00 1
 73  Time    2.89  Rwp     6.851    -0.001 MC      0.00 1
--- 2.891 seconds ---
File C:\Users\tyson\Dropbox\Topas_old_version_Runs_9-24-2011_DropBox\YBCO_MTSE_10-28-2021_York\YBCO_MTSE4
    with parameters from last iteration
```







x = 77.29364 Sqrt(y) = 56.62114 d = 1.233428

jEdit - YBCO_MTSE451_2021_LeBail.out

File Edit Search Markers Folding View Utilities Macros Plugins Help

YBCO_MTSE451_2021_LeBail.out (%USERPROFILE%\Dropbox\Topas_old_version_Runs_9-24-2011_DropBox\YBCO_MTSE_10-28-2021_York\)

File Browser

```
'-------------------------------------
  XY(YBCO_MtSE451_XRD_York, 0.005)


  '  Full_Axial_Model(12, 12, 12, 0,  @ 0.92652225)
   Zero_Error(zero, 0.0445386448`)

   CuKa2(0.001)
   LP_Factor(27)
   Radius(200.5)


  ' Note 1st bkg parameter starting value, this helps the Le Bail refinement
    bkg @  276.319851` -115.357946`  100.063704` -50.2034219`  23.6923221` -6.50070139` -2.88746245`  4.80657682` -5.02113692`  3.92389952` -3.55609351`  3.40198648` -1.

  hkl_Is

   a   @  3.822614`
   b   @  3.886621`
   c   @  11.689883`
       al  90.0
       be  90.0
       ga  90.0

     lebail 1 ' The LeBail method

    space_group "Pmmm"
       load hkl_m_d_th2 I
       {
              0   0   2   2    5.84494       15.14595  1.69349422
              0   0   3   2    3.89663       22.80303  18.4497257
              0   1   0   2    3.88662       22.86253  0.98754451
              1   0   0   2    3.82261       23.25064  1.93066495
              0   1   1   4    3.68812       24.11103  0.349548149
              1   0   1   4    3.63329       24.48046  0.231164732
              0   1   2   4    3.23642       27.53816  2.82889871
              1   0   2   4    3.19918       27.86514  4.55220019
              0   0   4   2    2.92247       30.56491  3.2888288
              0   1   3   4    2.75179       32.51163  78.7396059
              1   0   3   4    2.72879       32.79335  111.475728
              1   1   0   4    2.72534       32.83595  33.2355873
              1   1   1   8    2.65417       33.74250  1.58656539
              1   1   2   8    2.47003       36.34240  1.32187
              0   0   5   2    2.33798       38.47347  43.55836
              0   1   4   4    2.33581       38.51057  9.92827083
              1   0   4   4    2.32169       38.75403  4.22533032
              1   1   3   8    2.23331       40.35305  24.5712449
```

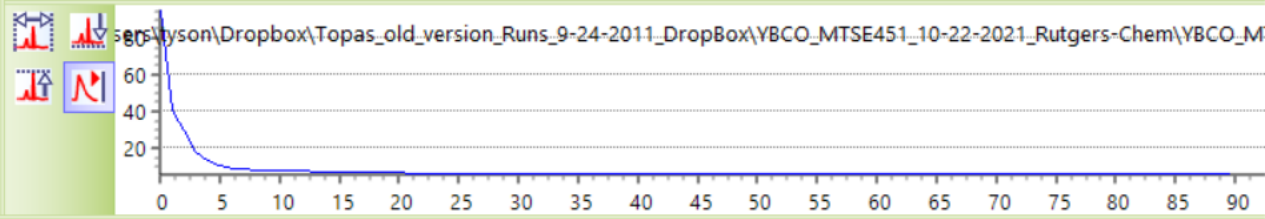
1,1 (0/15006) (text,none,Cp1252) I n m r o UG 64/76MB 3:51 PM

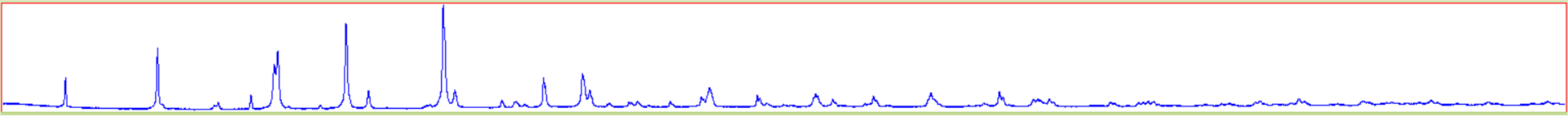
TOPAS-Academic-64 V7.12 - [ybco_10-20-2021.xy]

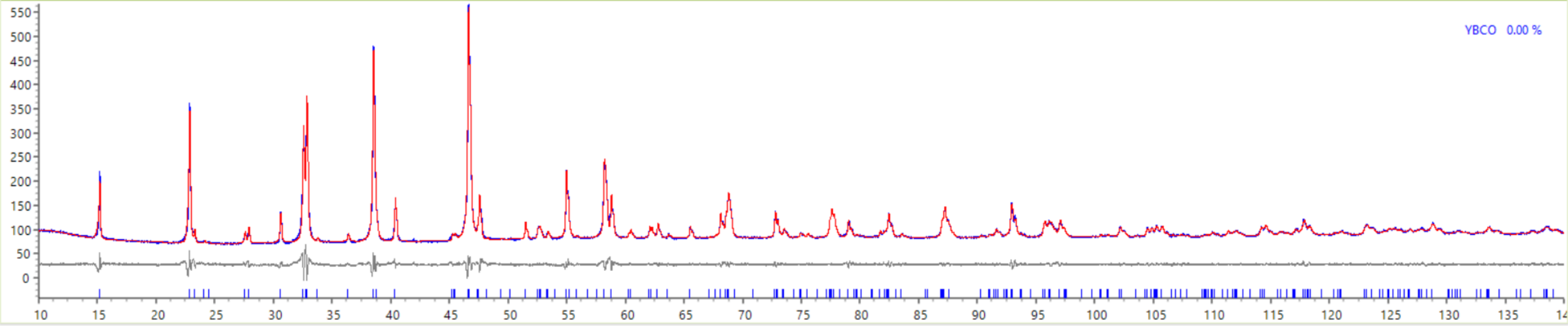
File View Fit Launch Tools Window Help

Global
ybco_10-20-2021.xy

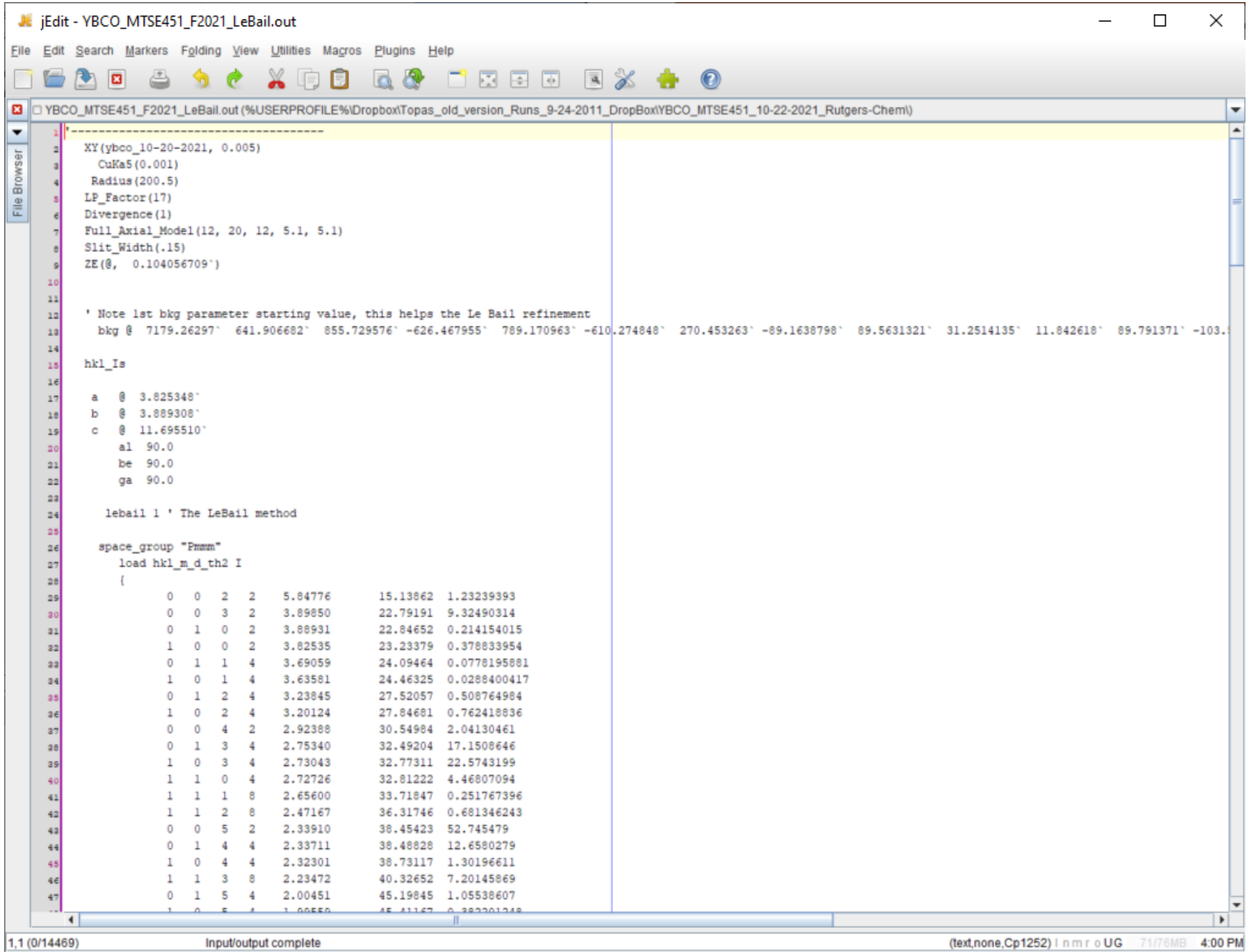
```
--- 4.281 seconds ---

*** Parameter(s) close to limit(s).
    Check for LIMIT_MIN and LIMIT_MAX in Grid/Text
File C:\Users\tyson\Dropbox\Topas_old_version_Runs_9-24-2011_DropBox\YBCO_MTSE451_10-22-2021_Rutgers-Chem
    with parameters from last iteration
```







x = 78.82865 Sqrt(y) = 503.7592 d = 1.213214


jEdit - YBCO_MTSE451_F2021_LeBail.out
File Edit Search Markers Folding View Utilities Macros Plugins Help
YBCO_MTSE451_F2021_LeBail.out (%USERPROFILE%\Dropbox\Topas_old_version_Runs_9-24-2011_DropBox\YBCO_MTSE451_10-22-2021_Rutgers-Chem\)
File Browser
'--------------------------------------
XY(ybco_10-20-2021, 0.005)
CuKa5(0.001)
Radius(200.5)
LP_Factor(17)
Divergence(1)
Full_Axial_Model(12, 20, 12, 5.1, 5.1)
Slit_Width(.15)
ZE(@, 0.104056709`)
' Note 1st bkg parameter starting value, this helps the Le Bail refinement
bkg @ 7179.26297` 641.906682` 855.729576` -626.467955` 789.170963` -610.274848` 270.453263` -89.1638798` 89.5631321` 31.2514135` 11.842618` 89.791371` -103.
hkl_Is
a @ 3.825348`
b @ 3.889308`
c @ 11.695510`
al 90.0
be 90.0
ga 90.0
lebail 1 ' The LeBail method
space_group "Pmmm"
load hkl_m_d_th2 I
{
0 0 2 2 5.84776 15.13862 1.23239393
0 0 3 2 3.89850 22.79191 9.32490314
0 1 0 2 3.88931 22.84652 0.214154015
1 0 0 2 3.82535 23.23379 0.378833954
0 1 1 4 3.69059 24.09464 0.0778195881
1 0 1 4 3.63581 24.46325 0.0288400417
0 1 2 4 3.23845 27.52057 0.508764984
1 0 2 4 3.20124 27.84681 0.762418836
0 0 4 2 2.92388 30.54984 2.04130461
0 1 3 4 2.75340 32.49204 17.1508646
1 0 3 4 2.73043 32.77311 22.5743199
1 1 0 4 2.72726 32.81222 4.46807094
1 1 1 8 2.65600 33.71847 0.251767396
1 1 2 8 2.47167 36.31746 0.681346243
0 0 5 2 2.33910 38.45423 52.745479
0 1 4 4 2.33711 38.48828 12.6580279
1 0 4 4 2.32301 38.73117 1.30196611
1 1 3 8 2.23472 40.32652 7.20145869
0 1 5 4 2.00451 45.19845 1.05538607
1,1 (0/14469)
Input/output complete
(text,none,Cp1252)
4:00 PM

Get good data program
SciDAVis (http://scidavis.sourceforge.net/)
OriginLab (not free)

LeBail Pattern Fitting Programs
Topas5 (6, 7, …) (http://www.topas-academic.net/)
GSAS II (https://subversion.xray.aps.anl.gov/trac/pyGSAS)
Fox (http://fox.vincefn.net/Manual/ProfileFitting)
FullProf (https://www.ill.eu/sites/fullprof/php/programs.html_