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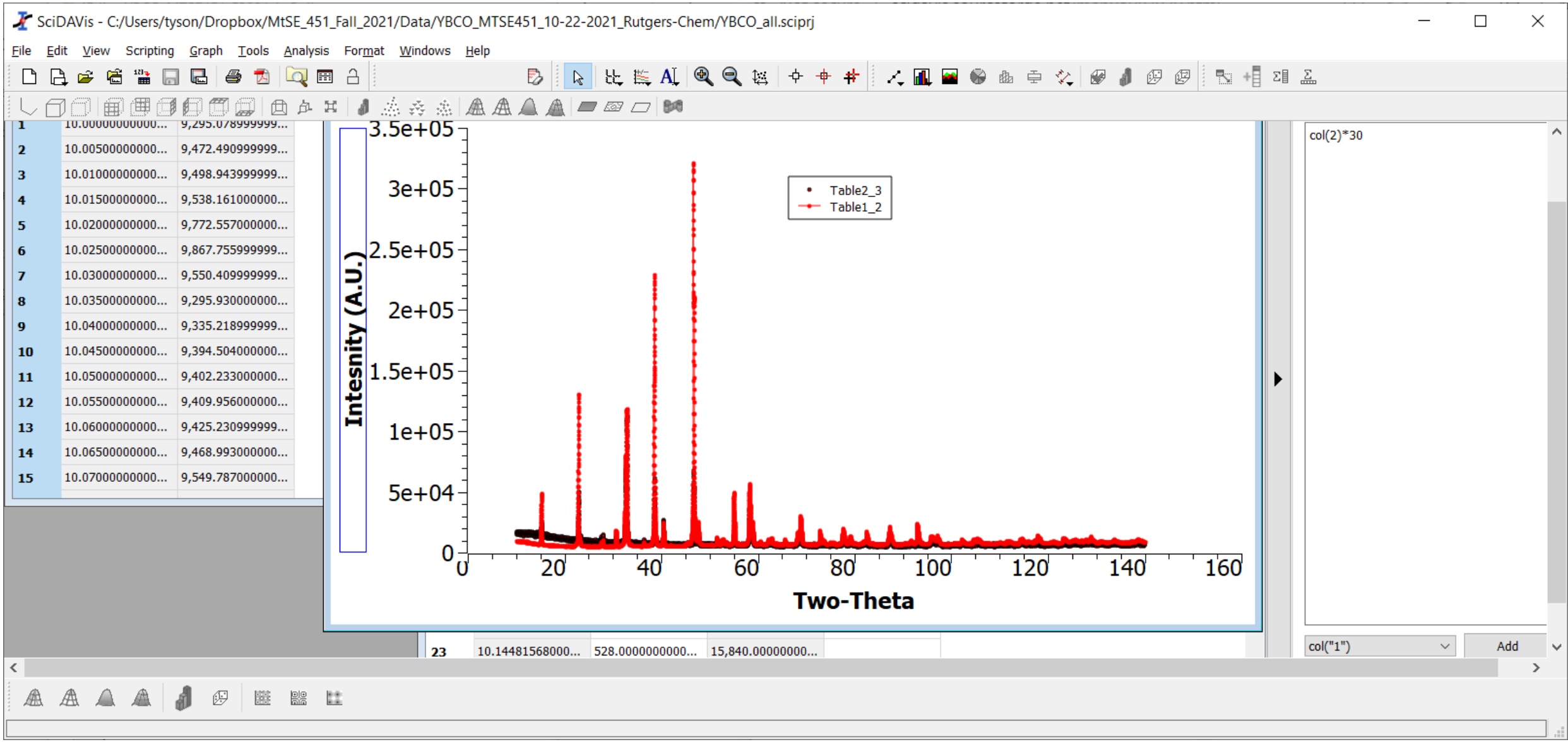


$2d\sin\theta = \lambda$ Cu $K_\alpha \Rightarrow \lambda = 1.5406\text{Å}$

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

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

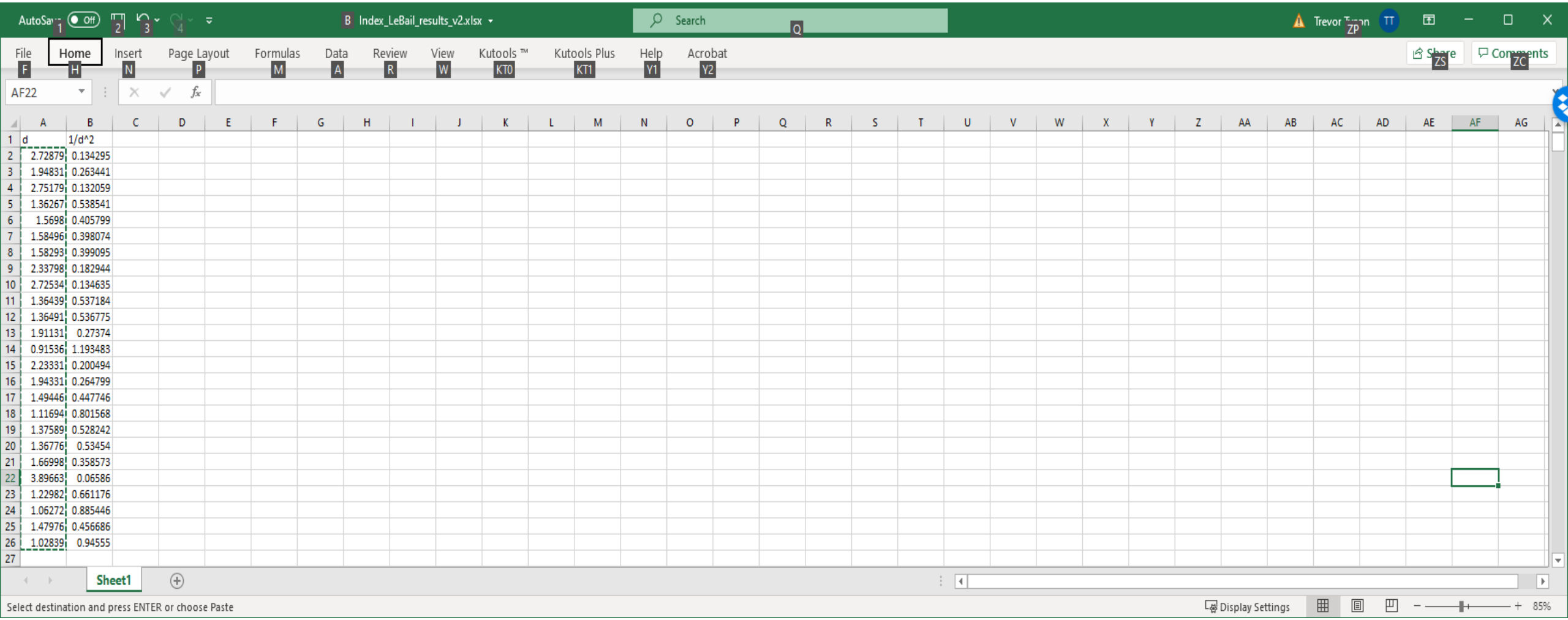
$\Delta\left(\frac{1}{d^2}\right) = (1, 3, 4, 5, 7, 8, 9 \ldots)/c^2$

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

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

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

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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																																	
58																																	
59																																	
60																																	

Sheet1

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D	E	F	G	H	I	J	K	L	M	N
	0.040522									
	0.041946									
	0.047226									
	0.048309									
	0.048649									
	0.04865									
	0.049672									
	0.050885									
	0.050886									
	0.05759									
	0.058612									
	0.060103									
	0.062947									
	0.064304									
	0.065859									
	0.06586									
	0.066199									
	0.066199		1/(1/d^2)	d*sqrt(3)						
	0.068435									
	0.068435									
	0.068775									
	0.071556									
	0.073245									
	0.077854									
	0.080089									
	0.080496	0.080497	3.524601	4.984539	6.104788	7.049202	7.881247	9.969077	10.5738	
	0.080497									
	0.080498									
	0.081855									
	0.081855									
	0.083879									
	0.084833									
	0.086794									
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	0.089173									
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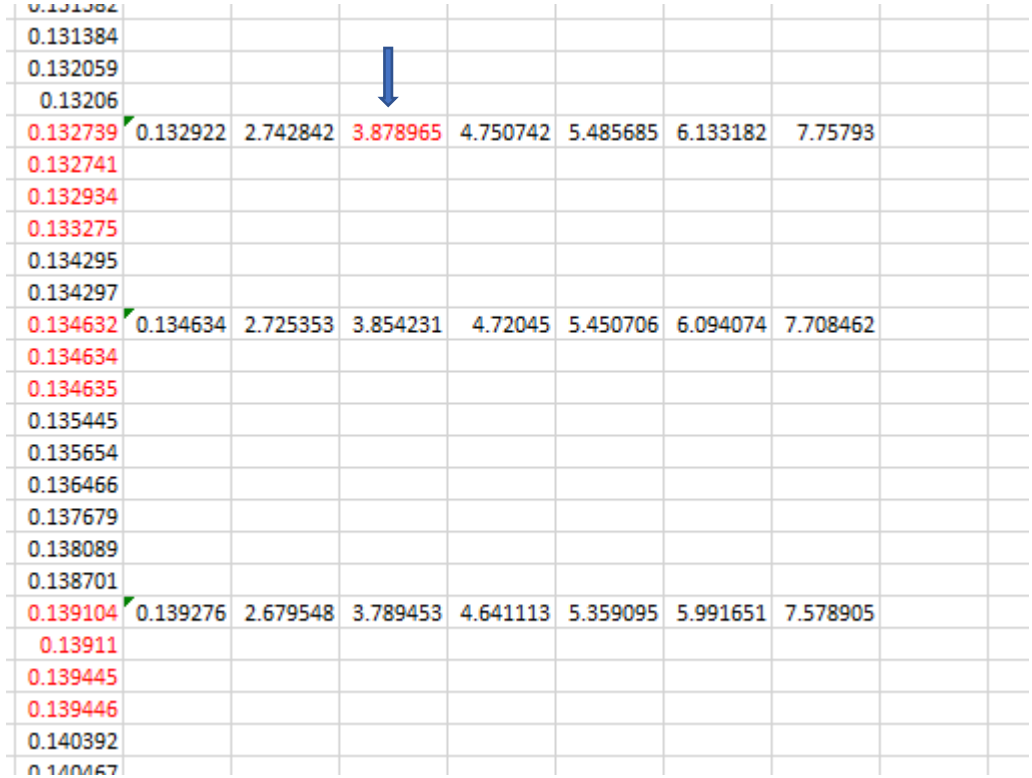
	0.090795									
	0.090796									
	0.093774									



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0.132059								
0.13206								
0.132739	0.132922	2.742842	3.878965	4.750742	5.485685	6.133182	7.75793	
0.132741								
0.132934								
0.133275								
0.134295								
0.134297								
0.134632	0.134634	2.725353	3.854231	4.72045	5.450706	6.094074	7.708462	
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0.134635								
0.135445								
0.135654								
0.136466								
0.137679								
0.138089								
0.138701								
0.139104	0.139276	2.679548	3.789453	4.641113	5.359095	5.991651	7.578905	
0.13911								
0.139445								
0.139446								
0.140392								

0.2608							
0.26208							
0.263027							
0.263035							
0.263102							
0.263438	0.263442	1.948309	2.755324	3.374569	3.896617	4.35655	
0.263441							
0.263443							
0.263444							
0.263779							
0.264384							
0.26446							
0.264793	0.264799	1.943308	2.748253	3.365908	3.886616	4.345369	
0.264799							
0.2648							
0.2648							
0.264801							
0.264802							
0.266014							
0.267028							
0.267036							
0.269741							
0.271099							
0.271164							
0.271504							
0.271976	0.272755	1.914756	2.707874	3.316455	3.829513	4.281525	
0.272385							
0.273326							
0.273333							
0.27374	0.273741	1.911305	2.702993	3.310477	3.82261	4.273807	
0.27374							
0.273742							

Whole powder pattern decomposition methods and applications: A retrospection

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(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

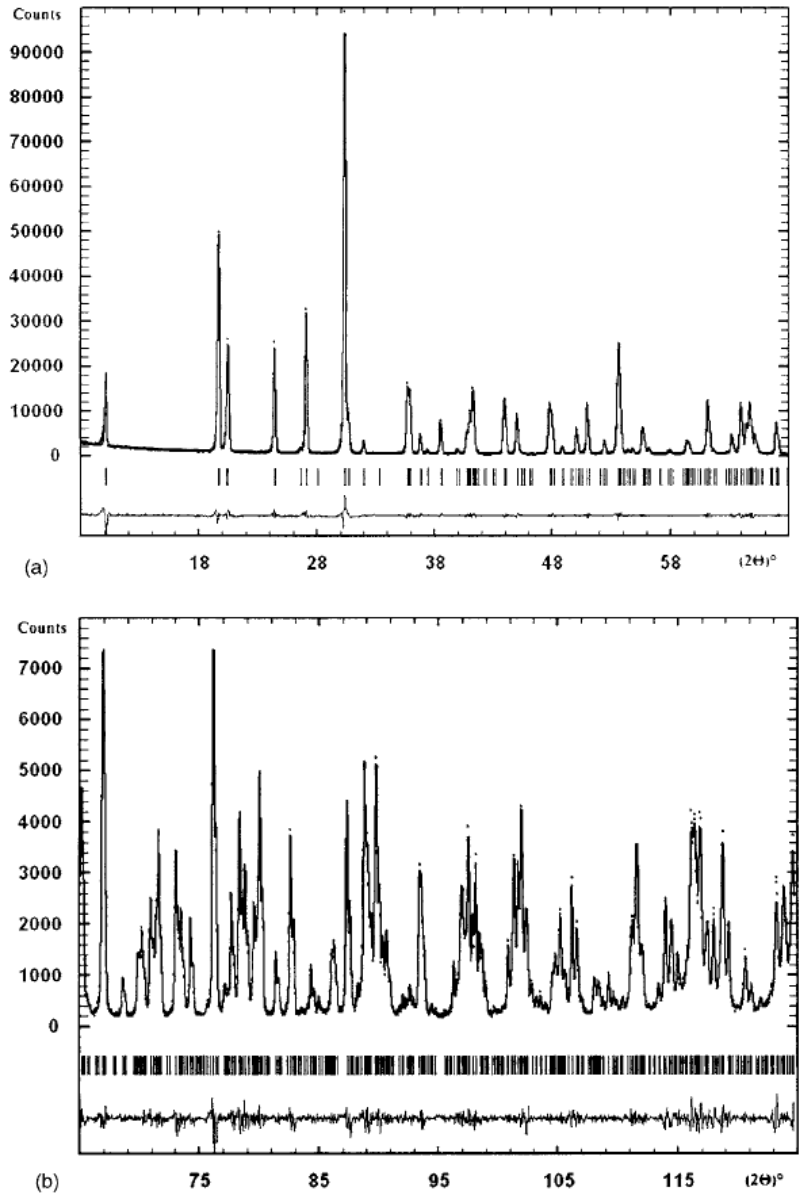

Figure 1. Le Bail fit of the powder pattern of $LiSbWO_6$, the first structure solved (Le Bail *et al.*, 1988) from intensities extracted by iterations of the Rietveld decomposition formula.

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).

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    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"
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        {
               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
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               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
```

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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 δ. 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 δ 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.

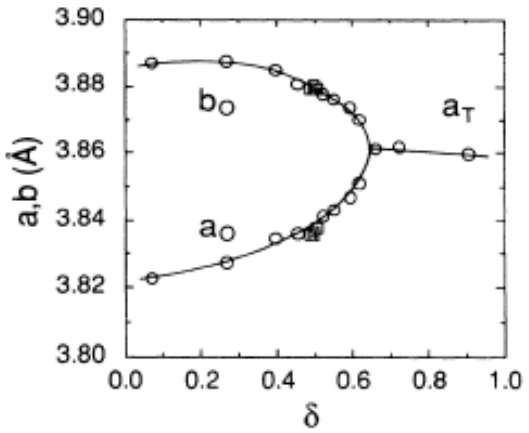

FIG. 5. Lattice parameters, a_O and b_O in the orthorhombic phase and a_T in the tetragonal phase of $YBa_2Cu_3O_{7-\delta}$, determined by Rietveld refinement of neutron powder diffraction data, vs δ. The oxygen compositions, δ, are determined from weight-loss measurements. The open circles are for a consistent set of samples quenched from various controlled oxygen partial pressures at 520°C into liquid nitrogen (Table II). The open squares are for four additional samples made by various quenching and sealed-quartz-tube annealing techniques in order to further investigate the behavior near $\delta = 0.05$ (Table III, see text). Error bars, taken as the statistical standard deviations from the Rietveld refinement, are smaller than the symbols.

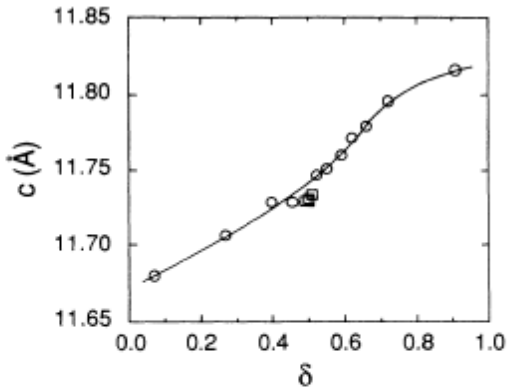

FIG. 6. c-axis lattice parameter vs δ for $YBa_2Cu_3O_{7-\delta}$. Format is the same as for Fig. 5. Error bars are smaller than the symbols.

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*	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_{11}^2 (Å^2)	0.022(3)	0.031(3)	0.033(5)	0.036(5)
	U_{22}^2 (Å^2)	−0.001(2)	0.006(2)	0.012(3)	0.002(3)
	U_{33}^2 (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_{11}^2 (Å^2)	0.009(1)	0.015(1)	0.016(2)	0.011(1)
	U_{22}^2 (Å^2)	0.007(1)	0.18(1)	0.018(2)	0.015(1)
	U_{33}^2 (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

δ (weight loss)		0.52	0.55	0.59	0.62
	a (Å)	3.8415(1)	3.8433(1)	3.8468(1)	3.8510(1)
	b (Å)	3.8778(1)	3.8764(1)	3.8736(1)	3.8700(1)
	c (Å)	11.7470(2)	11.7512(2)	11.7601(2)	11.7711(2)
	V (Å)	174.99	175.07	175.24	175.43
Y:	B (Å^2)	0.23(4)	0.40(4)	0.27(4)	0.38(4)
Ba:	z	0.1896(2)	0.1904(2)	0.1905(2)	0.1915(2)
	B (Å^2)	0.49(5)	0.48(4)	0.49(5)	0.58(5)
Cu(1):	B (Å^2)	0.74(5)	0.79(4)	0.74(4)	0.81(4)
Cu(2):	z	0.3587(2)	0.3588(1)	0.3592(1)	0.3596(1)
	B (Å^2)	0.26(3)	0.23(3)	0.22(3)	0.27(3)
O(1):	U_{11}^2 (Å^2)	0.033(6)	0.036(7)	0.028(7)	0.038(9)
	U_{22}^2 (Å^2)	0.018(5)	−0.001(4)	0.013(5)	−0.009(5)
	U_{33}^2 (Å^2)	0.015(6)	0.047(8)	0.050(9)	0.097(15)
	n	0.56(2)	0.45(2)	0.48(2)	0.38(2)
O(2):	z	0.3787(3)	0.3785(3)	0.3791(3)	0.3794(4)
	B (Å^2)	0.40(5)	0.50(4)	0.39(5)	0.42(6)
O(3):	z	0.3778(3)	0.3787(3)	0.3779(3)	0.3778(4)

Bulk Superconductivity at 91 K in Single-Phase Oxygen-Deficient Perovskite $Ba_2YCu_3O_{9-\delta}$

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(Received 5 March 1987)

We have prepared and identified as a single phase the high-temperature superconducting compound in the chemical system Y-Ba-Cu-O, an orthorhombic, distorted, oxygen-deficient perovskite of stoichiometry $Ba_2YCu_3O_{9-\delta}$ ($\delta \simeq 2.1$). Samples exhibit zero resistance at 91 K, with a transition width of 1.5 K. The Meissner effect attains a value of 76% of the independently measured diamagnetic susceptibility. We estimate parameters that characterize this superconductor, e.g., $\gamma \simeq 3-5$ mJ (mole Cu)$^{-1}$ K^{-2}. The critical current density at 77 K and $H=0$ exceeds 1100 A/cm^2.

PACS numbers: 74.70.Ya, 74.30.Ci

TABLE I. Powder x-ray diffraction pattern for $Ba_2YCu_3O_{6.9}$. Orthorhombic unit cell, $a=3.8218(7)$ Å, $b=3.8913(7)$ Å, $c=11.677(2)$ Å.

h	k	l	d_{OBS}(Å)	I/Io (%)
0	0	2	5.844	2
0	0	3	3.893	11
1	0	0	3.822	3
0	1	2	3.235	3
1	0	2	3.198	5
0	1	3	2.750	60
1	0	3	2.726	100
1	1	0		
1	1	1	2.653	2
1	1	2	2.469	3
0	0	5	2.336	11
1	0	4	2.321	3
1	1	3	2.232	13
0	2	0	1.946	23
0	0	6		
2	0	0	1.911	10
1	1	5	1.775	3
0	1	6	1.741	2
0	2	3		
1	0	6	1.734	2
1	2	0		
2	0	3		
2	1	0	1.716	2
1	2	1		
1	2	2	1.662	1
1	2	3	1.584	24
1	1	6		
2	1	3	1.569	11

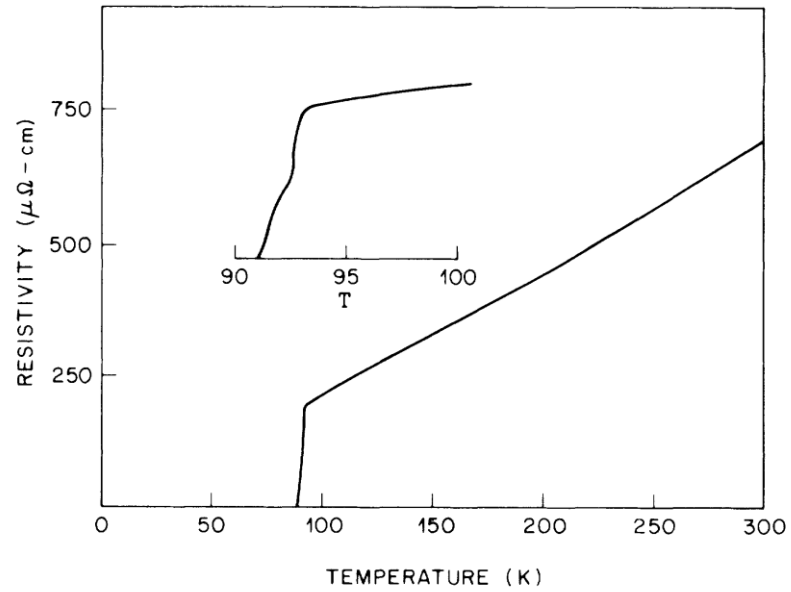


FIG. 1. Temperature dependence of the electrical resistivity.

TABLE II. Material parameters for $Ba_2YCu_3O_{6.9}$. "GL" denotes Ginzburg-Landau.

Measured parameters	
Transition temperature midpoint	$T_c = 92.5$ K
Resistivity in the normal state	$\rho_{300} = 600-700\ \mu\Omega$ cm
	$\rho_{95} = 200-250\ \mu\Omega$ cm
Lower critical field slope	$dH_{c1}/dT = -7$ Oe K^{-1}
Upper critical field slope[a]	$dH_{c2}/dT = -13$ kOe K^{-1}
Critical current density (77 K, $H=0$)	$j_c > 1100$ A cm^{-2}
Dominant carrier type (300 K)	p type
Derived parameters	
Sommerfeld parameter	$\gamma = 3-5$ mJ (mole Cu)$^{-1}$ K^{-2}
GL coherence length	$\xi(0) \sim 22$ Å
GL penetration depth	$\lambda(0) \sim 1400$ Å
GL κ	$\kappa \sim 62$
Thermodynamic critical field	$H_c(0) = 10 \pm 2$ kOe

[a]Reference 6.

Get good data plotting 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)

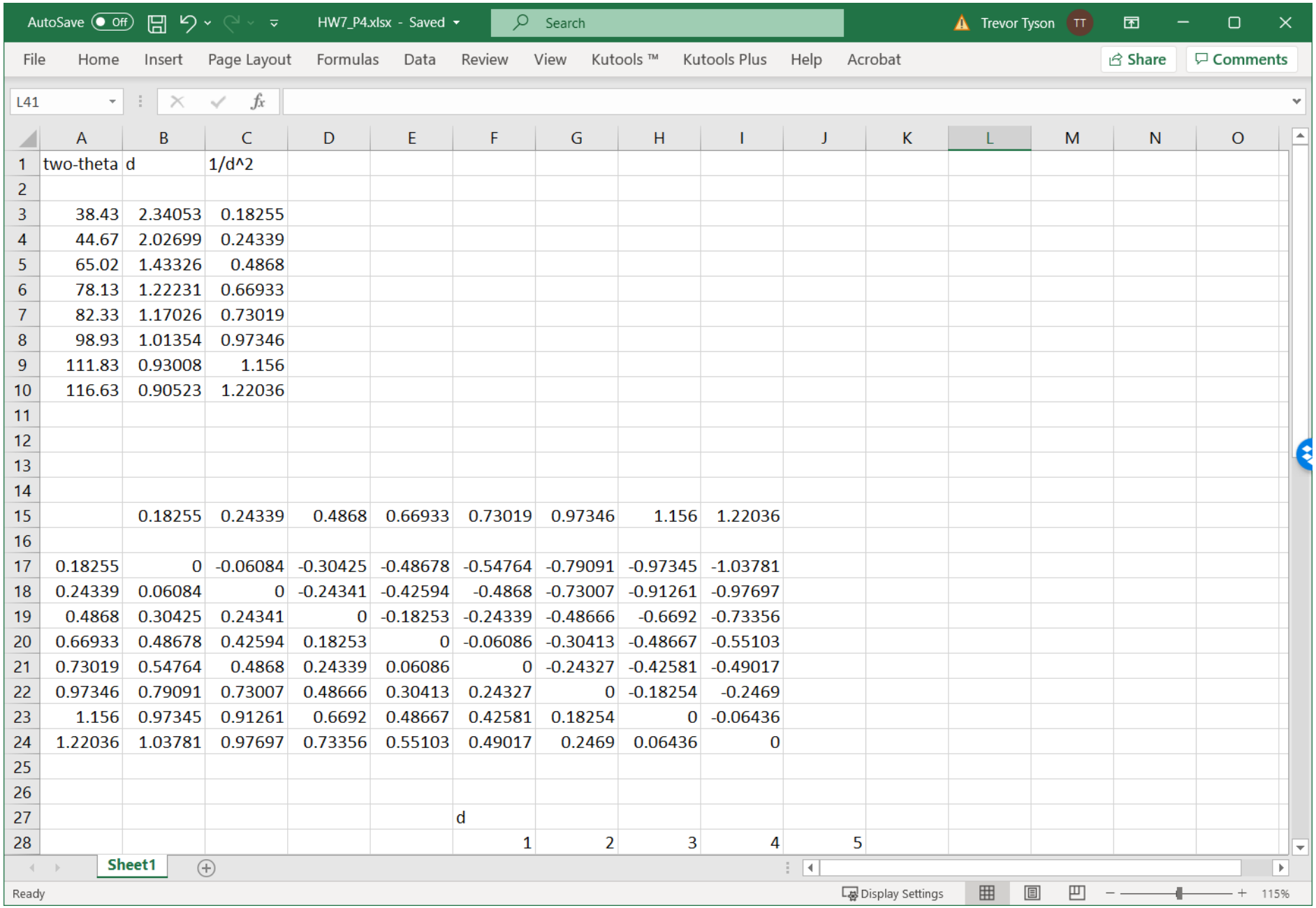
FullProf (https://www.ill.eu/sites/fullprof/php/programs.html_

4. A cubic unit cell has peaks at the angles given in the list below. The data were collected with Cu Kα radiation (λ = 1.5406 Å).

(a) Find the unit cell parameters

(b) Index the peaks (specify the hkl values for each peak)

Peak No.	2θ
1	38.43
2	44.67
3	65.02
4	78.13
5	82.33
6	98.93
7	111.83
8	116.36



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
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4	44.67	2.02699	0.24339												
5	65.02	1.43326	0.4868												
6	78.13	1.22231	0.66933												
7	82.33	1.17026	0.73019												
8	98.93	1.01354	0.97346												
9	111.83	0.93008	1.156												
10	116.63	0.90523	1.22036												
11															
12															
13															
14															
15		0.18255	0.24339	0.4868	0.66933	0.73019	0.97346	1.156	1.22036						
16															
17	0.18255	0	-0.06084	-0.30425	-0.48678	-0.54764	-0.79091	-0.97345	-1.03781						
18	0.24339	0.06084	0	-0.24341	-0.42594	-0.4868	-0.73007	-0.91261	-0.97697						
19	0.4868	0.30425	0.24341	0	-0.18253	-0.24339	-0.48666	-0.6692	-0.73356						
20	0.66933	0.48678	0.42594	0.18253	0	-0.06086	-0.30413	-0.48667	-0.55103						
21	0.73019	0.54764	0.4868	0.24339	0.06086	0	-0.24327	-0.42581	-0.49017						
22	0.97346	0.79091	0.73007	0.48666	0.30413	0.24327	0	-0.18254	-0.2469						
23	1.156	0.97345	0.91261	0.6692	0.48667	0.42581	0.18254	0	-0.06436						
24	1.22036	1.03781	0.97697	0.73356	0.55103	0.49017	0.2469	0.06436	0						
25															
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27						d									
28						1	2	3	4	5					

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30		0.24339		0.06086																	
31		0.4868		0.06436																	
32		0.66933		0.18253																	
33		0.73019		0.18255																	
34		0.97346		0.24327		1	3	4	5	8											
35		1.156		0.24339	0.2434	2.02699	3.51078	**4.0539**	4.5324	5.73308											
36		1.22036		0.24339																	
37		0.06084		0.24341																	
38		0.30425		0.30413																	
39		0.48678		0.30425																	
40		0.54764		0.42581																	
41		0.79091		0.42594		1	2	3	4	5											
42		0.97345		0.48666	0.4867	1.43347	2.48272	2.8668	3.20518	**4.05427**											
43		1.03781		0.48667																	
44		0.24341		0.48678																	
45		0.42594		0.4868																	
46		0.4868		0.4868																	
47		0.73007		0.49017																	
48		0.91261		0.54764																	
49		0.97697		0.55103																	
50		0.18253		0.6692																	
51		0.24339		0.66933																	
52		0.48666		0.73007																	
53		0.6692		0.73019																	
54		0.73356		0.73356																	
55		0.06086		0.79091																	
56		0.30413		0.91261																	
57		0.48667		0.97345																	
58		0.55103		0.97346																	
59		0.24327		0.97697																	
60		0.42581		1.03781																	
61		0.49017		1.156																	
62		0.06436		1.22036																	
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Sheet1

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30		0.24339		0.06086																	
31		0.4868		0.06436																	
32		0.66933		0.18253																	
33		0.73019		0.18255																	
34		0.97346		0.24327		1	3	4	5	8											
35		1.156		0.24339	0.2434	2.02699	3.51078	**4.0539**	4.5324	5.73308											
36		1.22036		0.24339																	
37		0.06084		0.24341																	
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40		0.54764		0.42581																	
41		0.79091		0.42594		1	2	3	4	5											
42		0.97345		0.48666	0.4867	1.43347	2.48272	2.8668	3.20518	**4.05427**											
43		1.03781		0.48667																	
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Rhombohedral, $a = b = c$, $\alpha = \beta = \gamma$:

$$\frac{1}{d_{hkl}^2} = \frac{(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + lh)(\cos^2\alpha - \cos\alpha)}{a^2(1 + 2\cos^3\alpha - 3\cos^2\alpha)}. \quad (2.9)$$

Hexagonal, $a = b$, $\alpha = \beta = 90°$, $\gamma = 120°$:

$$\frac{1}{d_{hkl}^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}. \quad (2.10)$$

Monoclinic, $\alpha = \gamma = 90°$:

$$\frac{1}{d_{hkl}^2} = \frac{1}{\sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right). \quad (2.11)$$

Orthorhombic, $\alpha = \beta = \gamma = 90°$:

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}. \quad (2.12)$$

Tetragonal, $a = b$, $\alpha = \beta = \gamma = 90°$:

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}. \quad (2.13)$$

Cubic, $a = b = c$, $\alpha = \beta = \gamma = 90°$:

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2}. \quad (2.14)$$

$2\,d\sin(\theta) = n\,\lambda$

$d(hkl) = a/(h^2+k^2+l^2)^{1/2}$

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65.02 (202)

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116.63 (420)

13

Symmetry

by

L. S. Dent Glasser

Ibuprofen ≥98% (GC) | 15687-27

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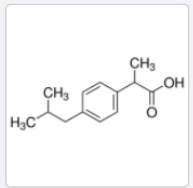

All Photos (4)

Documents

SDS

COO/COA

Specification Sheet

I4883 Sigma-Aldrich.

Ibuprofen

≥98% (GC)

Synonym(s):
(±)-2-(4-Isobutylphenyl)propanoic acid, α-Methyl-4-(isobutyl)phenylacetic acid

Empirical Formula (Hill Notation):
$C_{13}H_{18}O_2$

CAS Number:	15687-27-1	Molecular Weight:	206.28	EC Number:	239-784-6
MDL number:	MFCD00010393	PubChem Substance ID:	24277715	NACRES:	NA.77

SKU	Pack Size	Availability	Price	Quantity
I4883-1G	1 G	Available to ship on November 10, 2021 - FROM	$58.80	– +
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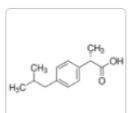

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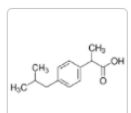
(*S*)-(+)-Ibuprofen



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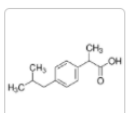

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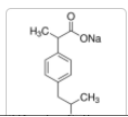


I1892
Ibuprofen sodium salt

Agent Offline

1. Simple Symmetry Operations

The general idea of symmetry is familiar to almost everyone. Formally it can be defined in various ways. The Concise Oxford Dictionary says '1. (Beauty resulting from) right proportion between the parts of the body or any whole, balance, harmony, keeping. 2. Such structure as allows of an object's being divided by a point or line or plane or radiating lines or planes into two or more parts exactly similar in size and shape and in position relative to the dividing point, etc., repetition of exactly similar parts facing each other or a centre, . . .'.

The second of the definitions is the one that relates most closely to crystallography and thus concerns us here, but I have also included the first

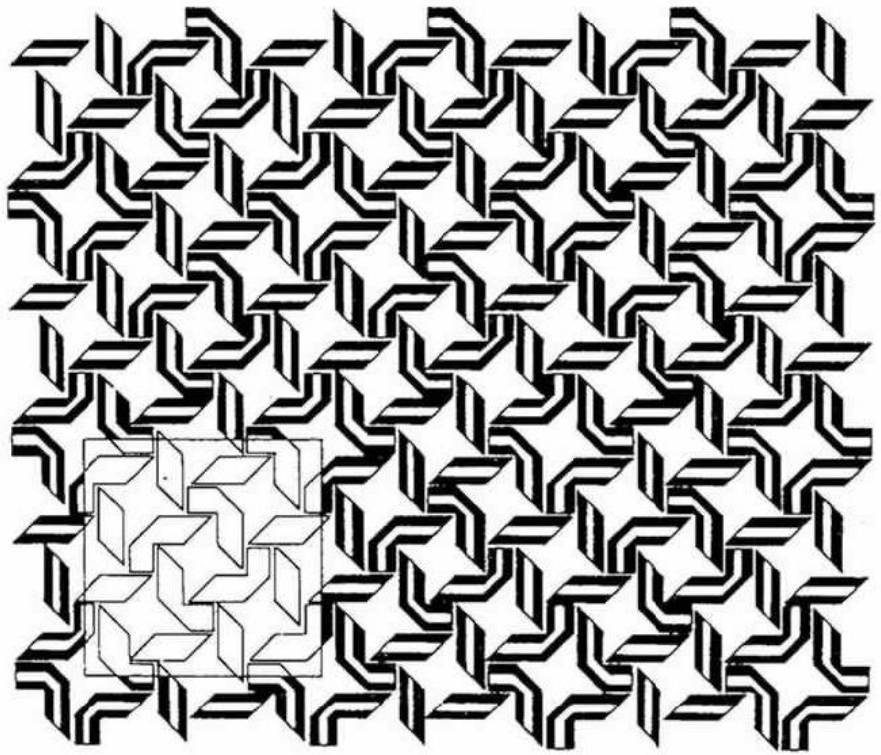


Fig. 1.1. Pattern based on a fourteenth-century Persian tiling design.

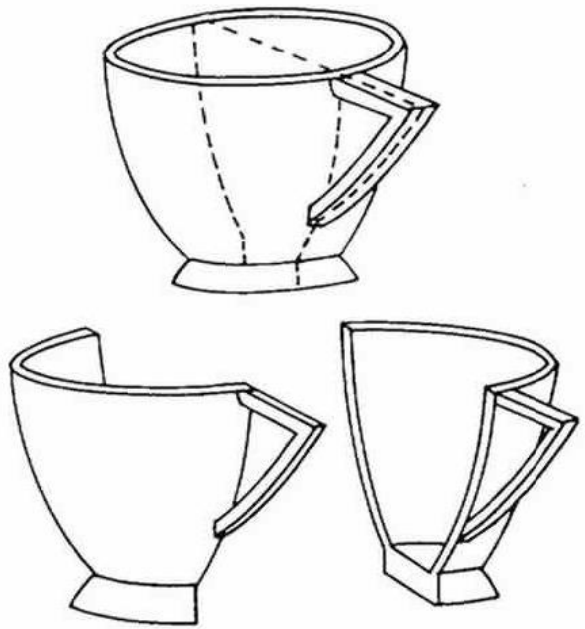


Fig. 1.2. A teacup, showing its mirror plane of symmetry. (After L. S. Dent Glasser, Crystallography & its applications: Van Nostrand Reinhold, 1977.)

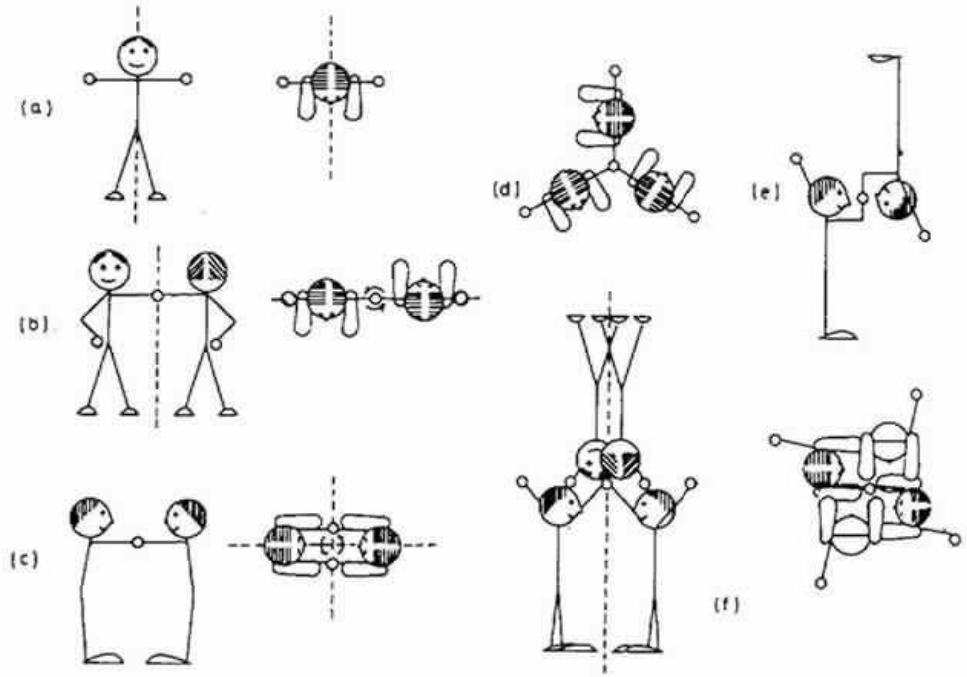


Fig. 1.3. Some symmetry elements, represented by human figures. (a) Mirror plane, shown as dashed line, in elevation and plan. (b) Two-fold axis, lying along broken line in elevation, passing perpendicularly through clasped hands in plan. (c) Combination of two-fold axis with mirror planes; the position of the symmetry elements given only in plan. (d) Three-fold axis, shown in plan only. (e) Centre of symmetry (in centre of clasped hands). (f) Four-fold inversion axis, in elevation and plan, running along the dashed line and through the centre of the clasped hands. (After L. S. Dent Glasser, Chapter 19, The Chemistry of Cements: Academic Press, 1964.)

Even this is inconvenient in written text, in which mirror planes are given the symbol m, while axes and the corresponding inversion axes are referred to as 1, $\bar{1}$; 2, $\bar{2}$ ($\equiv m$); 3, $\bar{3}$; 4, $\bar{4}$; 6, $\bar{6}$. The symbol 1 (for a one-fold axis) means no symmetry at all, while the corresponding inversion axis ($\bar{1}$) is equivalent, as already remarked, to a centre of symmetry.

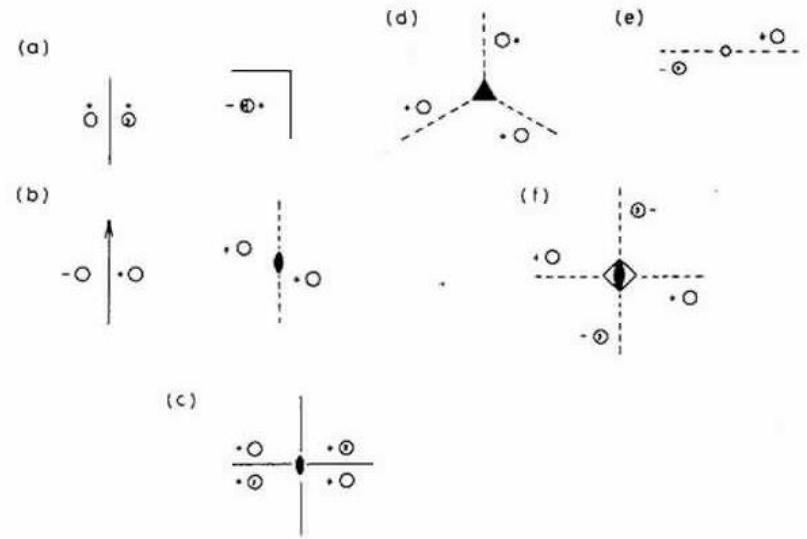


Fig. 1.4. The arrangements in figure 1.3 redrawn using conventional symbols. The right-hand group of (a) is drawn here in a different orientation, and the left-hand groups of (c) and (f) are omitted. Symbols + and − represent equal distances above and below the plane of the paper; open circles represent asymmetric units of one hand, and circles with commas their enantiomorphs. (a) Mirror plane (m), perpendicular to (left) and in the plane of the paper. (b) Two-fold axis (2) in the plane of the paper (left) and perpendicular to it (right). (c) Combination of two-fold axes and mirror planes. Note that the presence of any two of these elements creates the third. (d) Three-fold axis (3). (e) Centre of symmetry (1). (f) Four-fold inversion axis ($\bar{4}$).

Similarly, three mirror planes meeting in a three-fold axis (Fig. 2.1a) are adequately represented by $3m$. The full symbol $3mmm$ is not needed because two of the 'm's are redundant, being created by the action of the three-fold axis on the other one. Figure 2.1b shows a mirror plane perpendicular to a two-fold rotation axis; this is given the symbol $2/m$, the '/' implying 'perpendicular to'. (Note that the combination produces a centre of symmetry at the point where the rotation axis intersects the mirror plane).

This system of nomenclature, which is the one most often used in crystallography is largely self-explanatory, and with very little practice one can

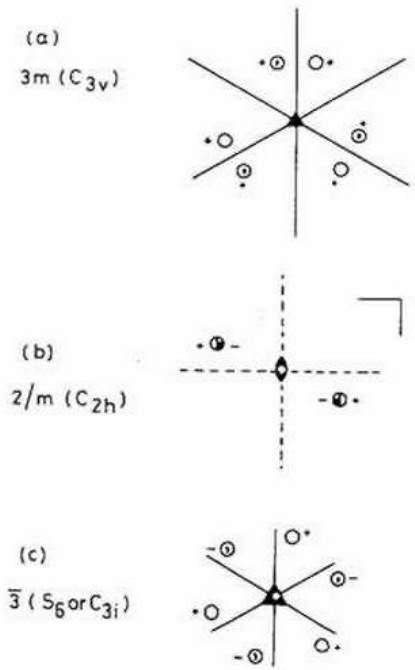


Fig. 2.1. Some combinations of symmetry elements with their point-group symbols. The equivalent Schonflies symbol is given in brackets.

Table 1. Crystal systems and classes (equivalent Schoenflies nomenclature for the latter in brackets)

System	Characteristic symmetry	Unit cell shape	Lattice types	Classes
Triclinic	None	$a \neq b \neq c$ * $\alpha \neq \beta \neq \gamma \neq 90°$	P	$1(C_1)$, $\bar{1}(C_i, S_2)$
Monoclinic	One two-fold axis (2 or $\bar{2} \equiv m$)	$a \neq b \neq c$ $\alpha = \gamma = 90 \neq \beta$	P, C (or A)	$2(C_2)$, $m[=\bar{2}](C_s)$ $2/m(C_{2h})$
Orthorhombic	Three mutually perpendicular two-fold axes	$a \neq b \neq c$ $\alpha = \beta = \gamma \pm 90°$	$P, C,$ (or A or B) I, F	$222(D_2)$, $mm2(C_{2v})$ $mmm(D_{2h})$
Tetragonal	One four-fold axis	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	P, I	$4(C_4)$, $\bar{4}(S_4)$, $4/m(C_{4h})$, $422(D_4)$, $4mm(C_{4v})$ $\bar{4}2m(D_{2d})$, $4/mmm(D_{4h})$
Trigonal	One three-fold-axis	$a = b \neq c$ $\alpha = \beta = 90°$ $\gamma = 120°$	P, R	$3(C_3)$, $\bar{3}(S_6, C_{3i})$, $32(D_3)$ $3m(C_{3v})$, $\bar{3}m(D_{3d})$
Hexagonal	One six-fold axis	$a = b \neq c$ $\alpha = \beta = 90°$ $\gamma = 120°$	P	$6(C_6)$, $\bar{6}(C_{3h})$, $6/m(C_{6h})$ $622(D_6)$, $6mm(C_{6v})$ $\bar{6}m2(D_{3h})$ $\bar{6}/mmm(D_{6h})$
Cubic	Four three-fold axes (along body diagonals of a cube)	$a = b = c$ $\alpha = \beta = \gamma = 90°$	P, I, F	$23(T)$, $m3(T_h)$, $432(O)$ $\bar{4}3m(T_d)$, $m3m(O_h)$

$\neq$ Not necessarily equal to.
* That is, no restrictions.

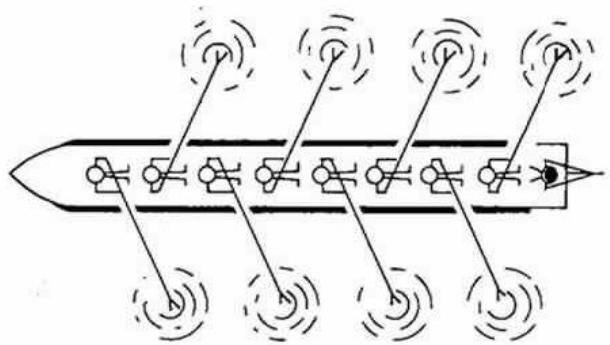
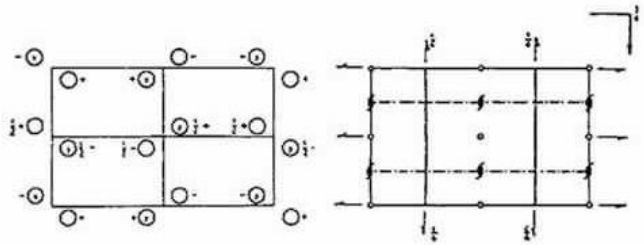


Fig. 3.3. A stylised aerial view of a well-coached 'eight', showing a translational symmetry operation: each rower is related to the next by a combination of translation and reflection.

Orthorhombic $m\,m\,m$ $P\,2_1/n\,2_1/m\,2_1/a$ No. 62 $Pnma$ D_{2h}^{16}



Origin at $\bar{1}$

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
8	d	1	x,y,z; $\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z$; $\bar{x},\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$; $x,\frac{1}{2}-y,z$; $\frac{1}{2}+x,y,\frac{1}{2}-z$.	hkl: No conditions $0kl$: $k+l=2n$ $h0l$: No conditions $hk0$: $h=2n$ $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: $(l=2n)$
				Special: as above, plus
4	c	m	$x,\frac{1}{4},z$; $\bar{x},\frac{3}{4},\bar{z}$; $\frac{1}{2}-x,\frac{3}{4},\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{4},\frac{1}{2}-z$.	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $\frac{1}{2},\frac{1}{2},0$.	hkl: $h+l=2n$; $k=2n$
4	a	$\bar{1}$	$0,0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	

Symmetry of special projections

(001) pgm; $a'=a/2$, $b'=b$ (100) cmm; $b'=b$, $c'=c$ (010) pgg; $c'=c$, $a'=a$

Fig. 5.1. Page 151, Vol. I. reproduced from International Tables for X-Ray Crystallography, 1965 edition (by kind permission of the International Union of Crystallography).

B. E. Warren, Chapter 8

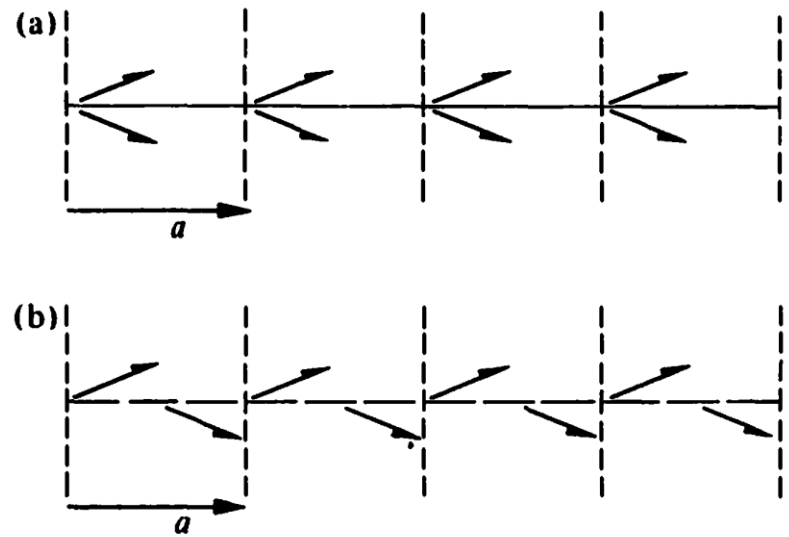


Fig. 8.1 Representation of microscopic symmetry elements. (a) Reflection plane (b) Glide plane.

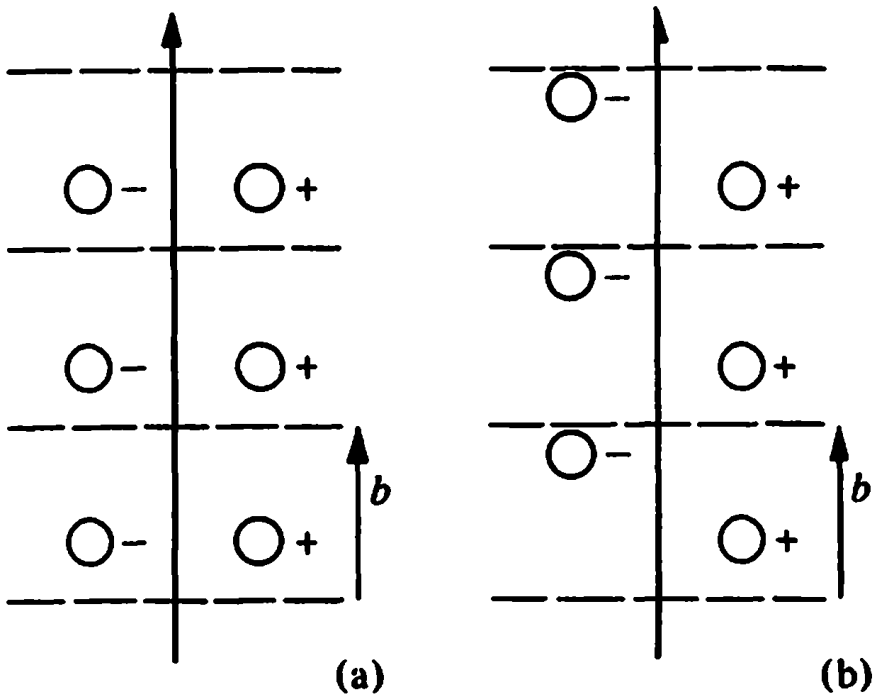


Fig. 8.2 Representation of microscopic symmetry elements. (a) 2-fold rotation axis. (b) 2-fold screw axis.

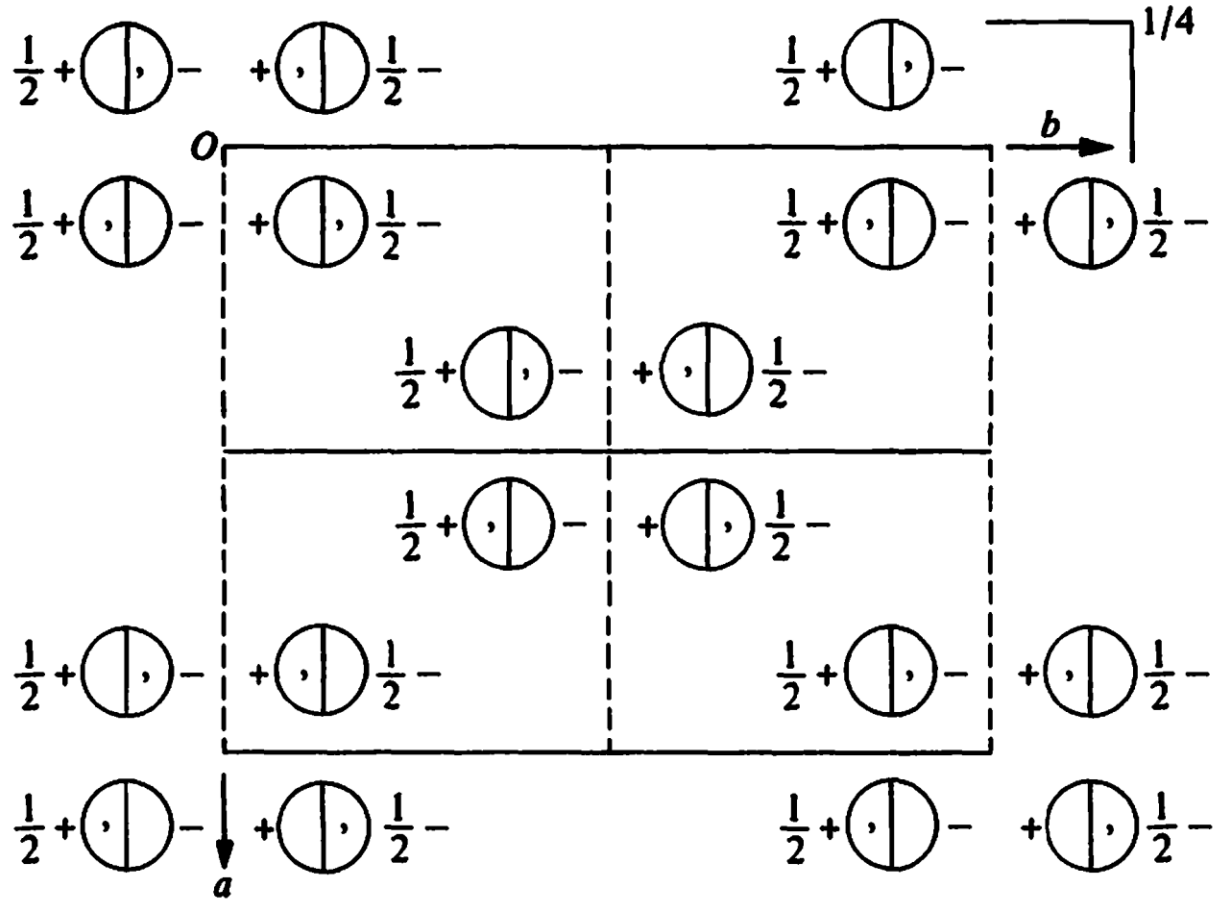


Fig. 8.3 Arrangement of symmetry elements and repeating units in the space group Cmcm.

The first letter in the symbol is a capital letter which gives the type of Bravais lattice. Various capital letters may appear in the first position; P (primitive), F (face-centered), I (body-centered), A (side-centered, additional translation **b**/2 + **c**/2), C (side-centered, additional translation **a**/2 + **b**/2), etc. The next three positions correspond to the *a*-, *b*-, and *c*-axes. A figure "2" in the first of these positions would mean a 2-fold rotation axis parallel to the *a*-axis, and a letter "*m*" in the first position would mean a reflection plane perpendicular to the *a*-axis. The symbol mcm represents reflection planes perpendicular to the *a*- and *c*-axes and a glide plane perpendicular to the *b*-axis with glide of *c*/2.

For the space group Cmcm, the general position is 16 fold. The coordinates of the 16 positions are expressed in terms of the coordinates xyz of the first position in the following 16-fold group of positions:

(16*h*)	x,	y,	z;	x,	$\bar{y}$,	$\bar{z}$;	$\frac{1}{2}+x$,	$\frac{1}{2}+y$,	z;	$\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$\bar{z}$;
	$\bar{x}$,	$\bar{y}$,	$\bar{z}$,	$\bar{x}$,	y,	z	$\frac{1}{2}-x$,	$\frac{1}{2}-y$,	$\bar{z}$;	$\frac{1}{2}-x$,	$\frac{1}{2}+y$,	z
	x,	y,	$\frac{1}{2}-z$;	x,	$\bar{y}$,	$\frac{1}{2}+z$;	$\frac{1}{2}+x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$;	$\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$;
	$\bar{x}$,	$\bar{y}$,	$\frac{1}{2}+z$;	$\bar{x}$,	y,	$\frac{1}{2}-z$	$\frac{1}{2}-x$,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$;	$\frac{1}{2}-x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$

For the space group Cmcm, the general position is 16 fold. The coordinates of the 16 positions are expressed in terms of the coordinates xyz of the first position in the following 16-fold group of positions:

(16*h*)	x,	y,	z;	x,	$\bar{y}$,	$\bar{z}$;		
	$\bar{x}$,	$\bar{y}$,	$\bar{z}$,	$\bar{x}$,	y,	z		
	x,	y,	$\frac{1}{2}-z$;	x,	$\bar{y}$,	$\frac{1}{2}+z$;		
	$\bar{x}$,	$\bar{y}$,	$\frac{1}{2}+z$;	$\bar{x}$,	y,	$\frac{1}{2}-z$		
	$\frac{1}{2}+x$,	$\frac{1}{2}+y$,	z;	$\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$\bar{z}$;		
	$\frac{1}{2}-x$,	$\frac{1}{2}-y$,	$\bar{z}$;	$\frac{1}{2}-x$,	$\frac{1}{2}+y$,	z		
	$\frac{1}{2}+x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$;	$\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$;		
	$\frac{1}{2}-x$,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$;	$\frac{1}{2}-x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$		

The last two terms can be combined by Eq. (8.2) and we obtain finally

$$F/f = 16 \cos^2 \pi\left(\frac{h+k}{2}\right) \cos 2\pi hx \cos 2\pi(ky - l/4) \cos 2\pi(lz + l/4). \quad (8.3)$$

We next work out the conditions for the vanishings. By a vanishing we mean that $F/f = 0$ for certain classes of *hkl*-reflections regardless of the *xyz*-coordinates. Since $\cos^2 (h + k)\pi/2 = 0$ for $h + k =$ odd, the general reflection *hkl* is present only for $h + k =$ even. The term $\cos 2\pi(ky - l/4) = 0$ for $k = 0$ and $l =$ odd. Hence the special reflection *h*0*l* can be present only if $l =$ even and also from the first condition only if $h =$ even. The vanishings for the space group Cmcm are as follows:

The general reflection (*hkl*) is present only for $h + k =$ even.
The reflection (*h*0*l*) is present only for $h =$ even and $l =$ even.

```
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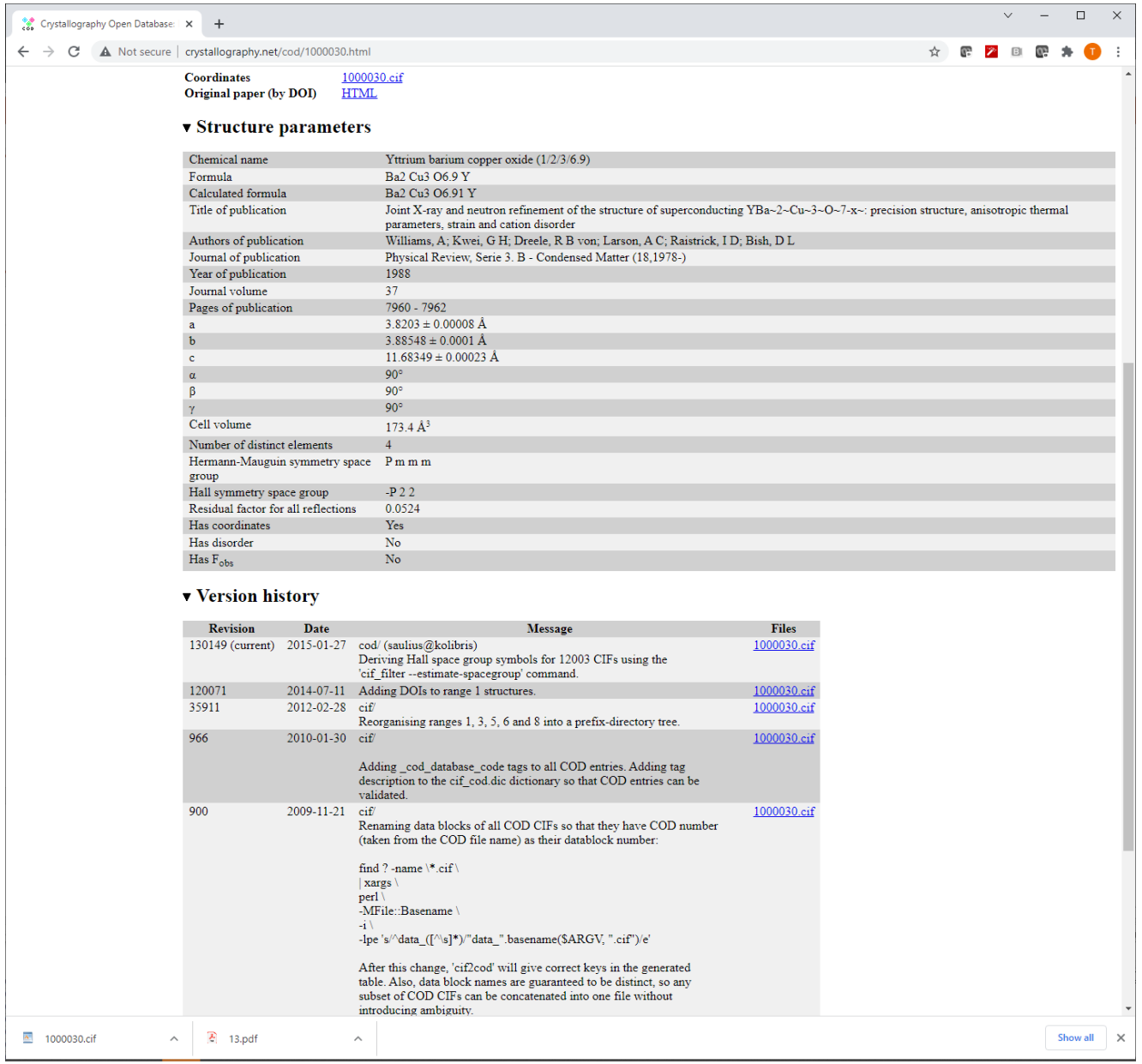
_cell_angle_beta                 90
_cell_angle_gamma                90
_cell_formula_units_Z            1
_cell_length_a                   3.82030(8)
_cell_length_b                   3.88548(10)
_cell_length_c                   11.68349(23)
_cell_volume                     173.4
_refine_ls_R_factor_all          0.0524
_cod_database_code               1000030
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,-y,z
x,-y,-z
-x,y,-z
-x,-y,-z
x,y,-z
-x,y,z
x,-y,z
loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
Y1 0.0085(8) 0.0106(8) 0.0085(6) 0. 0. 0.
Ba1 0.0078(6) 0.0096(7) 0.0198(5) 0. 0. 0.
Cu1 0.0080(9) 0.0115(9) 0.0150(7) 0. 0. 0.
Cu2 0.0033(5) 0.0036(5) 0.0207(5) 0. 0. 0.
O1 0.0161(16) 0.0104(11) 0.0080(14) 0. 0. 0.
O2 0.0039(6) 0.0068(7) 0.0203(11) 0. 0. 0.
O3 0.0109(8) 0.0084(7) 0.0056(11) 0. 0. 0.
O4 0.0162(11) 0.0123(9) 0.0097(7) 0. 0. 0.
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```



Coordinates 1000030.cif
Original paper (by DOI) HTML

▾ Structure parameters

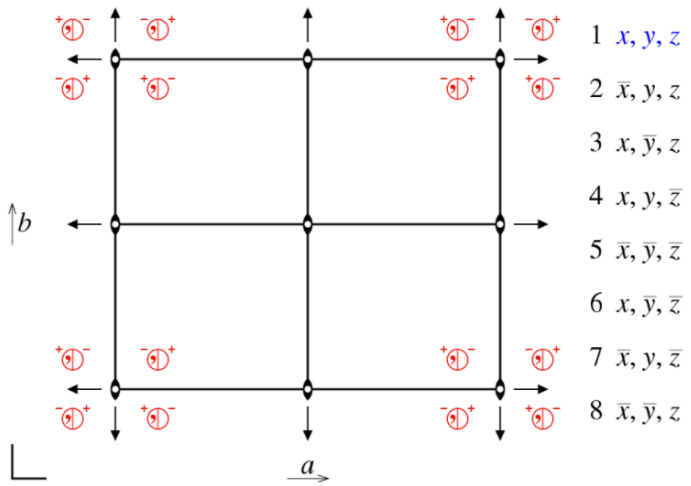
Chemical name	Yttrium barium copper oxide (1/2/3/6.9)
Formula	Ba2 Cu3 O6.9 Y
Calculated formula	Ba2 Cu3 O6.91 Y
Title of publication	Joint X-ray and neutron refinement of the structure of superconducting YBa~2~Cu~3~O~7-x~: precision structure, anisotropic thermal parameters, strain and cation disorder
Authors of publication	Williams, A; Kwei, G H; Dreele, R B von; Larson, A C; Raistrick, I D; Bish, D L
Journal of publication	Physical Review, Serie 3. B - Condensed Matter (18,1978-)
Year of publication	1988
Journal volume	37
Pages of publication	7960 - 7962
a	3.8203 ± 0.00008 Å
b	3.88548 ± 0.0001 Å
c	11.68349 ± 0.00023 Å
α	90°
β	90°
γ	90°
Cell volume	173.4 Å^3
Number of distinct elements	4
Hermann-Mauguin symmetry space group	P m m m
Hall symmetry space group	-P 2 2
Residual factor for all reflections	0.0524
Has coordinates	Yes
Has disorder	No
Has F_{obs}	No

▾ Version history

Revision	Date	Message	Files
130149 (current)	2015-01-27	cod/ (saulius@kolibris) Deriving Hall space group symbols for 12003 CIFs using the 'cif_filter --estimate-spacegroup' command.	1000030.cif
120071	2014-07-11	Adding DOIs to range 1 structures.	1000030.cif
35911	2012-02-28	cif/ Reorganising ranges 1, 3, 5, 6 and 8 into a prefix-directory tree.	1000030.cif
966	2010-01-30	cif/ Adding _cod_database_code tags to all COD entries. Adding tag description to the cif_cod.dic dictionary so that COD entries can be validated.	1000030.cif
900	2009-11-21	cif/ Renaming data blocks of all COD CIFs so that they have COD number (taken from the COD file name) as their datablock number: find ? -name *.cif \ | xargs \ perl \ -MFile::Basename \ -i \ -lpe 's/^data_([^\s]*)/"data_".basename($ARGV, ".cif")/e' After this change, 'cif2cod' will give correct keys in the generated table. Also, data block names are guaranteed to be distinct, so any subset of COD CIFs can be concatenated into one file without introducing ambiguity.	1000030.cif

Not secure | img.chem.ucl.ac.uk/sgp/large/047az1.htm

Pmmm *P 2/m 2/m 2/m* *mmm* No. 47



1 x, y, z
2 $\bar{x}, y, z$
3 $x, \bar{y}, z$
4 $x, y, \bar{z}$
5 $\bar{x}, \bar{y}, \bar{z}$
6 $x, \bar{y}, \bar{z}$
7 $\bar{x}, y, \bar{z}$
8 $\bar{x}, \bar{y}, z$

Pmmm

No. 47

Symmetry Operators

1	x, y, z	1
2	$\bar{x}, y, z$	m $(0, y, z)$
3	$x, \bar{y}, z$	m $(x, 0, z)$
4	$x, y, \bar{z}$	m $(x, y, 0)$
5	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$ $(0, 0, 0)$
6	$x, \bar{y}, \bar{z}$	2 $(x, 0, 0)$
7	$\bar{x}, y, \bar{z}$	2 $(0, y, 0)$
8	$\bar{x}, \bar{y}, z$	2 $(0, 0, z)$

Reflection Conditions

(general)

No conditions

```
# CIF file created by FINDSYM, version 7.1.3

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_cell_length_b    3.8854800000
_cell_length_c    11.6834900000
_cell_angle_alpha 90.0000000000
_cell_angle_beta  90.0000000000
_cell_angle_gamma 90.0000000000
_cell_volume      173.4262116803

_symmetry_space_group_name_H-M "P 2/m 2/m 2/m"
_symmetry_Int_Tables_number 47
_space_group.reference_setting '047:-P 2 2'
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_space_group_symop_operation_xyz
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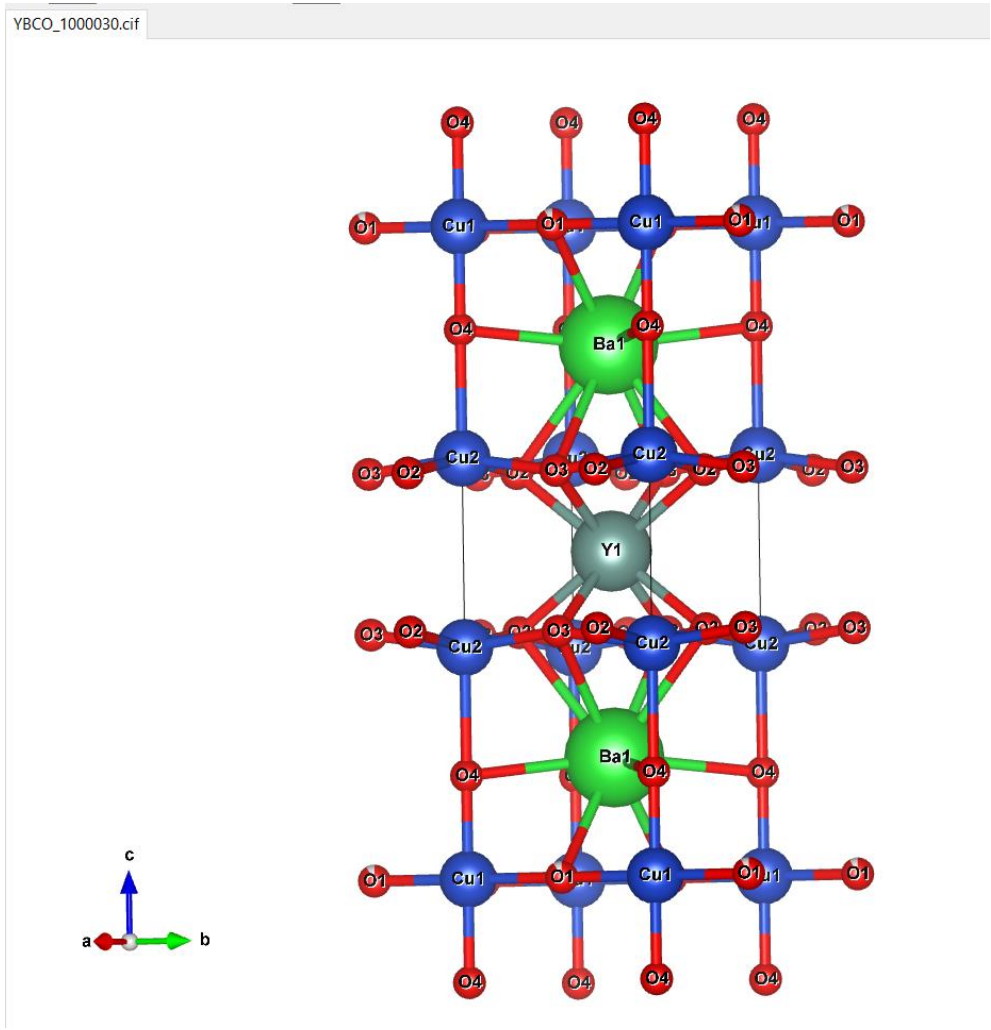
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 -x,-y,-z
6 -x,y,z
7 x,-y,z
8 x,y,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Y3+1  Y3+    1 h 0.50000 0.50000 0.50000 1.00000 0,0,0
Ba2+1 Ba2+   2 t 0.50000 0.50000 0.18393 1.00000 0,0,Dz
Cu2+1 Cu2+   1 a 0.00000 0.00000 0.00000 1.00000 0,0,0
Cu2+2 Cu2+   2 q 0.00000 0.00000 0.35501 1.00000 0,0,Dz
O2-1  O2-    1 e 0.00000 0.50000 0.00000 0.91000 0,0,0
O2-2  O2-    2 s 0.50000 0.00000 0.37819 1.00000 0,0,Dz
O2-3  O2-    2 r 0.00000 0.50000 0.37693 1.00000 0,0,Dz
O2-4  O2-    2 q 0.00000 0.00000 0.15840 1.00000 0,0,Dz
```


YBCO_1000030.cif
O4
Cu1
O1
Ba1
Cu2
O3
O2
Y1
c
a
b

```
# CIF file created by FINDSYM, version 7.1.3

data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a    3.8203000000
_cell_length_b    3.8854800000
_cell_length_c    11.6834900000
_cell_angle_alpha 90.0000000000
_cell_angle_beta  90.0000000000
_cell_angle_gamma 90.0000000000
_cell_volume      173.4262116803

_symmetry_space_group_name_H-M "P 2/m 2/m 2/m"
_symmetry_Int_Tables_number 47
_space_group.reference_setting '047:-P 2 2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 -x,-y,-z
6 -x,y,z
7 x,-y,z
8 x,y,-z

loop_
_atom_site_label
_atom_site_type_symbol
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_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Y3+1  Y3+    1 h 0.50000 0.50000 0.50000 1.00000 0,0,0
Ba2+1 Ba2+   2 t 0.50000 0.50000 0.18393 1.00000 0,0,Dz
Cu2+1 Cu2+   1 a 0.00000 0.00000 0.00000 1.00000 0,0,0
Cu2+2 Cu2+   2 q 0.00000 0.00000 0.35501 1.00000 0,0,Dz
O2-1  O2-    1 e 0.00000 0.50000 0.00000 0.91000 0,0,0
O2-2  O2-    2 s 0.50000 0.00000 0.37819 1.00000 0,0,Dz
O2-3  O2-    2 r 0.00000 0.50000 0.37693 1.00000 0,0,Dz
O2-4  O2-    2 q 0.00000 0.00000 0.15840 1.00000 0,0,Dz
```

YBCO_1000030.vasp - Notepad

File Edit Format View Help

```
Ba2 Cu3 O6.9 Y
1.0
        3.8203001022         0.0000000000         0.0000000000
        0.0000000000         3.8854799271         0.0000000000
        0.0000000000         0.0000000000        11.6834897995
    Y   Ba    Cu    O
    1    2    3    7
Direct
     0.500000000          0.500000000          0.500000000
     0.500000000          0.500000000          0.183929995
     0.500000000          0.500000000          0.816070020
     0.000000000          0.000000000          0.000000000
     0.000000000          0.000000000          0.355010003
     0.000000000          0.000000000          0.644989967
     0.000000000          0.500000000          0.000000000
     0.500000000          0.000000000          0.378190011
     0.500000000          0.000000000          0.621809959
     0.000000000          0.500000000          0.376929998
     0.000000000          0.500000000          0.623070002
     0.000000000          0.000000000          0.158399999
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```

```
# CIF file created by FINDSYM, version 7.1.3

data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a    3.8203000000
_cell_length_b    3.8854800000
_cell_length_c    11.6834900000
_cell_angle_alpha 90.0000000000
_cell_angle_beta  90.0000000000
_cell_angle_gamma 90.0000000000
_cell_volume      173.4262116803

_symmetry_space_group_name_H-M "P 2/m 2/m 2/m"
_symmetry_Int_Tables_number 47
_space_group.reference_setting '047:-P 2 2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 -x,-y,-z
6 -x,y,z
7 x,-y,z
8 x,y,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Y3+1  Y3+    1 h 0.50000 0.50000 0.50000 1.00000 0,0,0
Ba2+1 Ba2+   2 t 0.50000 0.50000 0.18393 1.00000 0,0,Dz
Cu2+1 Cu2+   1 a 0.00000 0.00000 0.00000 1.00000 0,0,0
Cu2+2 Cu2+   2 q 0.00000 0.00000 0.35501 1.00000 0,0,Dz
O2-1  O2-    1 e 0.00000 0.50000 0.00000 0.91000 0,0,0
O2-2  O2-    2 s 0.50000 0.00000 0.37819 1.00000 0,0,Dz
O2-3  O2-    2 r 0.00000 0.50000 0.37693 1.00000 0,0,Dz
O2-4  O2-    2 q 0.00000 0.00000 0.15840 1.00000 0,0,Dz
```