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CRISTAL·LOQUÍMICA DE PEROVSKITES COMPLEXES DE COURE I TITANI. RELACIÓ ENTRE SÍNTESI, ESTRUCTURA I PROPIETATS SUPERCONDUCTORES

Memòria presentada per Maria Rosa Palacín i Peiró
per a optar al grau de Doctora en Ciències Químiques.

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APÈNDIX 1

APPENDIX 1

DEFINICIÓ DELS FACTORS D'ACORD D'UN AFINAMENT (PROGRAMA FULLPROF)

En el programa FULLPROF (88) els factors d'acord d'un afinament a partir de dades experimentals es defineixen de la següent manera:

$$R_p = 100 \cdot (\Sigma |Yi_{obs} - Yi_{calc}|) \; / \; \Sigma |Yi_{obs}|$$

$$R_{wp} = 100 \cdot \sqrt{(\Sigma \; w \; |Yi_{obs} - Yi_{calc}|^2) \; / \; \Sigma \; w \; |Yi_{obs}|^2}$$

on Yi representa el nombre de comptes per segon (c.p.s) de cada punt experimental mentre que χ^2 i $R_{expected}$ són els paràmetres de bondat de l'ajust:

$$\chi^2 = [R_{wp} \; / \; R_{expected}]^2$$

$$R_{expected} = 100 \cdot \sqrt{(N-P+C) \; / \; \Sigma \; w \; |Yi_{obs}|^2}$$

(N-P+C) és el nombre de graus de llibertat en realitzar l'afinament, on N és el nombre de punts experimentals, P el nombre de paràmetres afinats i C el nombre de restriccions imposades en dur a terme l'afinament.

APÈNDIX 2

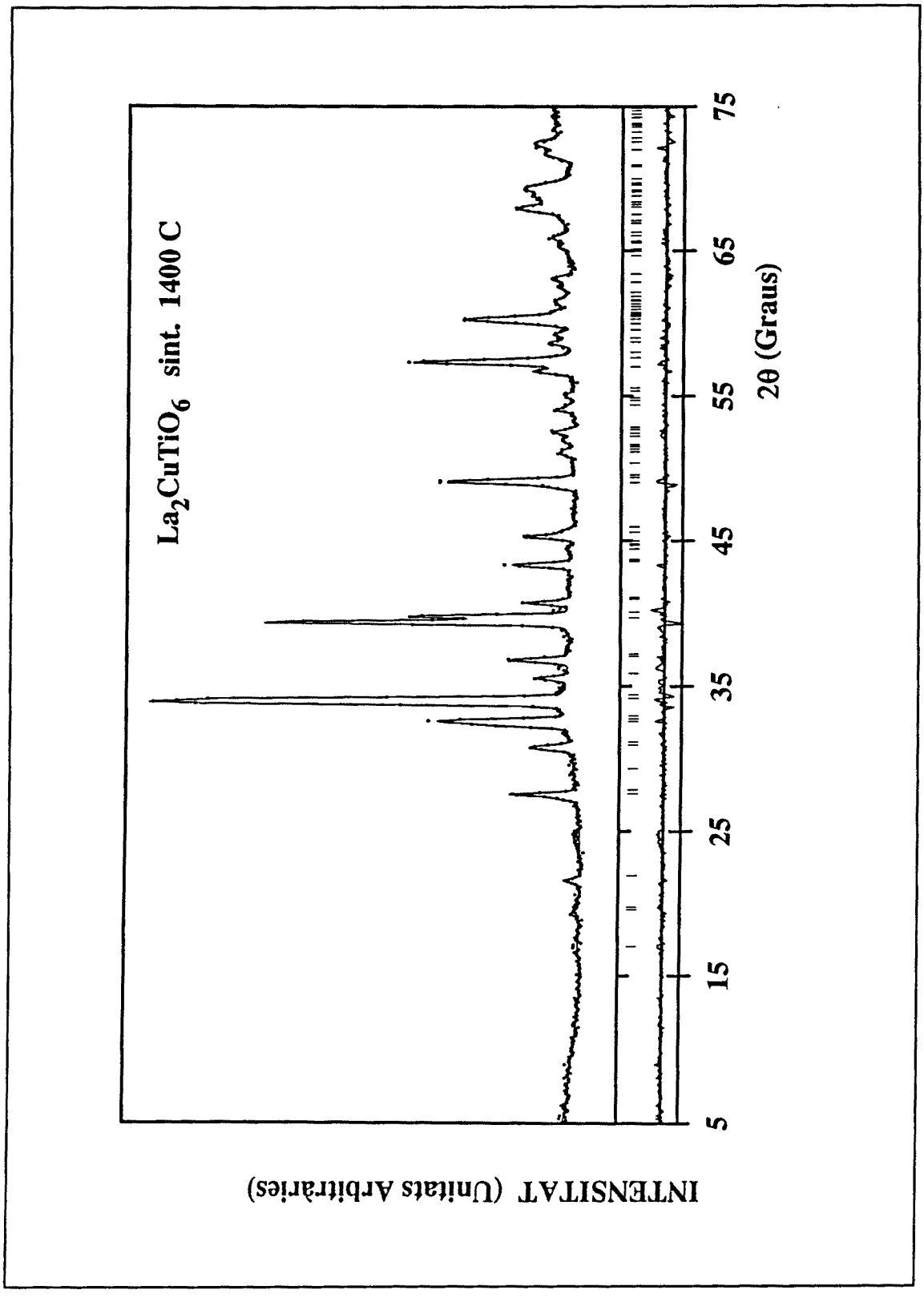
DADES ADDICIONALS SOBRE ELS AFINAMENTS RIETVELD REALITZATS

Hom presenta en aquest apèndix la sortida d'ordinador dels afinaments Rietveld descrits en aquesta memòria. Aquests afinaments han estat realitzats amb el programa FULLPROF (88), i les taules següents mostren les dades per a cada reflexió permesa. HW representa l'amplada del pic, ETA/M és un paràmetre que ajusta la forma dels pics a una combinació linial entre una corba Lorentziana i una Gaussiana, POSN indica la posició (2θ) i ICALC i IOBS són les intensitats calculada i observada respectivament. Després de cada taula de valors es mostra el difractograma observat com punts discrets i el calculat com una línia que s'hi superposa; la línia base representa IOBS-ICALC (Yi_{obs}-Yi_{calc}) i les barres verticals indiquen la posició de les reflexions de Bragg permeses pel grup espacial.

La_2CuTiO_6 sint. 1400°C (AFINAMENT PER DIFRACCIÓ DE NEUTRONS)

Grup espacial: Pnma (lambda=1.3428Å $2\theta_{in}$=5°, step=0.1°, $2\theta_{fin}$=75°)

H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
0	1	1	4	0.281	0.219	17.006	6.	20.
1	0	1	4	0.271	0.219	19.531	23.	16.
0	2	0	2	0.271	0.219	19.725	17.	25.
1	1	1	8	0.264	0.219	21.907	64.	58.
2	0	0	2	0.253	0.219	27.616	70.	75.
1	2	1	8	0.253	0.219	27.898	230.	231.
0	0	2	2	0.253	0.219	27.899	34.	34.
2	1	0	4	0.252	0.219	29.378	9.	10.
2	0	1	4	0.251	0.219	31.017	94.	91.
1	0	2	4	0.251	0.219	31.208	135.	135.
2	1	1	8	0.252	0.219	32.611	176.	186.
1	1	2	8	0.252	0.219	32.794	292.	293.
0	3	1	4	0.252	0.219	32.974	390.	404.
2	2	0	4	0.254	0.219	34.168	1464	1456.
0	2	2	4	0.254	0.219	34.402	1255	1265.
1	3	1	8	0.256	0.219	35.861	130.	167.
2	2	1	8	0.259	0.219	37.028	187.	233.
1	2	2	8	0.259	0.219	37.192	117.	138.
2	0	2	4	0.266	0.219	39.660	1305	1296.
0	4	0	2	0.267	0.219	40.067	679.	712.
2	1	2	8	0.270	0.219	40.959	99.	104.
2	3	0	4	0.271	0.219	41.057	107.	108.
2	3	1	8	0.281	0.219	43.532	98.	105.
0	1	3	4	0.281	0.219	43.629	90.	93.
1	3	2	8	0.282	0.219	43.675	101.	102.
3	0	1	4	0.285	0.219	44.389	15.	10.
2	2	2	8	0.286	0.219	44.670	1.	1.
1	0	3	4	0.287	0.219	44.765	22.	21.
1	4	1	8	0.288	0.219	44.947	7.	5.
3	1	1	8	0.291	0.219	45.578	241.	228.
1	1	3	8	0.293	0.219	45.946	62.	57.
3	2	1	8	0.310	0.219	49.010	94.	78.
2	4	0	4	0.313	0.219	49.355	164.	162.
1	2	3	8	0.313	0.219	49.358	421.	417.
0	4	2	4	0.314	0.219	49.529	119.	122.
2	3	2	8	0.319	0.219	50.370	0.	0.
3	0	2	4	0.324	0.219	51.139	17.	16.
2	0	3	4	0.326	0.219	51.350	57.	57.
2	4	1	8	0.327	0.219	51.515	13.	14.
1	4	2	8	0.328	0.219	51.641	29.	29.
3	1	2	8	0.332	0.219	52.210	57.	60.
2	1	3	8	0.333	0.219	52.418	16.	21.
0	3	3	4	0.335	0.219	52.666	5.	6.
0	5	1	4	0.336	0.219	52.828	111.	131.
3	3	1	8	0.347	0.219	54.367	95.	106.
1	3	3	8	0.350	0.219	54.691	25.	29.
1	5	1	8	0.351	0.219	54.849	0.	0.
3	2	2	8	0.355	0.219	55.336	49.	61.
2	2	3	8	0.356	0.219	55.536	8.	13.
4	0	0	2	0.369	0.219	57.023	220.	223.
2	4	2	8	0.374	0.219	57.647	779.	801.
0	0	4	2	0.374	0.219	57.650	142.	146.
4	1	0	4	0.377	0.219	58.020	62.	66.
2	5	0	4	0.383	0.219	58.712	7.	11.
4	0	1	4	0.385	0.219	58.987	140.	154.
1	0	4	4	0.390	0.219	59.562	98.	108.
4	1	1	8	0.394	0.219	59.962	1.	1.
3	3	2	8	0.397	0.219	60.303	133.	125.
2	3	3	8	0.399	0.219	60.492	199.	198.
1	1	4	8	0.399	0.219	60.532	103.	103.
2	5	1	8	0.400	0.219	60.640	299.	301.
1	5	2	8	0.401	0.219	60.754	105.	107.
4	2	0	4	0.403	0.219	60.947	5.	6.
3	0	3	4	0.405	0.219	61.174	79.	78.
3	4	1	8	0.406	0.219	61.321	6.	6.
0	2	4	4	0.408	0.219	61.549	3.	3.
1	4	3	8	0.409	0.219	61.621	38.	40.
0	6	0	2	0.411	0.219	61.842	69.	73.
3	1	3	8	0.414	0.219	62.129	42.	42.
4	2	1	8	0.420	0.219	62.834	94.	82.
1	2	4	8	0.426	0.219	63.389	136.	103.
4	0	2	4	0.438	0.219	64.655	17.	8.
3	2	3	8	0.441	0.219	64.946	19.	16.
2	0	4	4	0.443	0.219	65.092	3.	3.
1	6	1	8	0.447	0.219	65.520	54.	55.
4	1	2	8	0.448	0.219	65.581	24.	25.
4	3	0	4	0.448	0.219	65.652	3.	4.
2	1	4	8	0.452	0.219	66.015	23.	26.
2	5	2	8	0.454	0.219	66.227	116.	135.
3	4	2	8	0.461	0.219	66.875	4.	5.
2	4	3	8	0.463	0.219	67.055	30.	31.
4	3	1	8	0.467	0.219	67.467	73.	67.
1	3	4	8	0.473	0.219	68.001	140.	137.
0	5	3	4	0.475	0.219	68.176	133.	132.
4	2	2	8	0.477	0.219	68.322	197.	194.
2	2	4	8	0.481	0.219	68.747	124.	124.
2	6	0	4	0.484	0.219	69.024	116.	119.
0	6	2	4	0.486	0.219	69.165	90.	93.
3	3	3	8	0.490	0.219	69.505	160.	166.
3	5	1	8	0.491	0.219	69.642	142.	147.
1	5	3	8	0.494	0.219	69.923	140.	154.
2	6	1	8	0.504	0.219	70.796	2.	5.
1	6	2	8	0.505	0.219	70.901	0.	0.
4	4	0	4	0.518	0.219	71.965	190.	205.
0	4	4	4	0.524	0.219	72.519	114.	121.
4	3	2	8	0.527	0.219	72.780	205.	192.
2	3	4	8	0.532	0.219	73.194	62.	58.
4	0	3	4	0.537	0.219	73.574	10.	10.
4	4	1	8	0.538	0.219	73.708	63.	64.
3	0	4	4	0.539	0.219	73.814	40.	41.
1	4	4	8	0.544	0.219	74.223	35.	35.
4	1	3	8	0.547	0.219	74.448	43.	39.
3	1	4	8	0.550	0.219	74.687	96.	83.
3	5	2	8	0.553	0.219	74.888	4.	4.
5	0	1	4	0.554	0.219	74.995	1.	0.
0	1	5	4	0.554	0.219	74.995	0.	0.
2	5	3	8	0.555	0.219	75.059	12.	11.


La2CuTiO6 sint. 1400 C
INTENSITAT (Unitats Arbitràries)
5
15
25
35
45
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65
75
2θ (Graus)

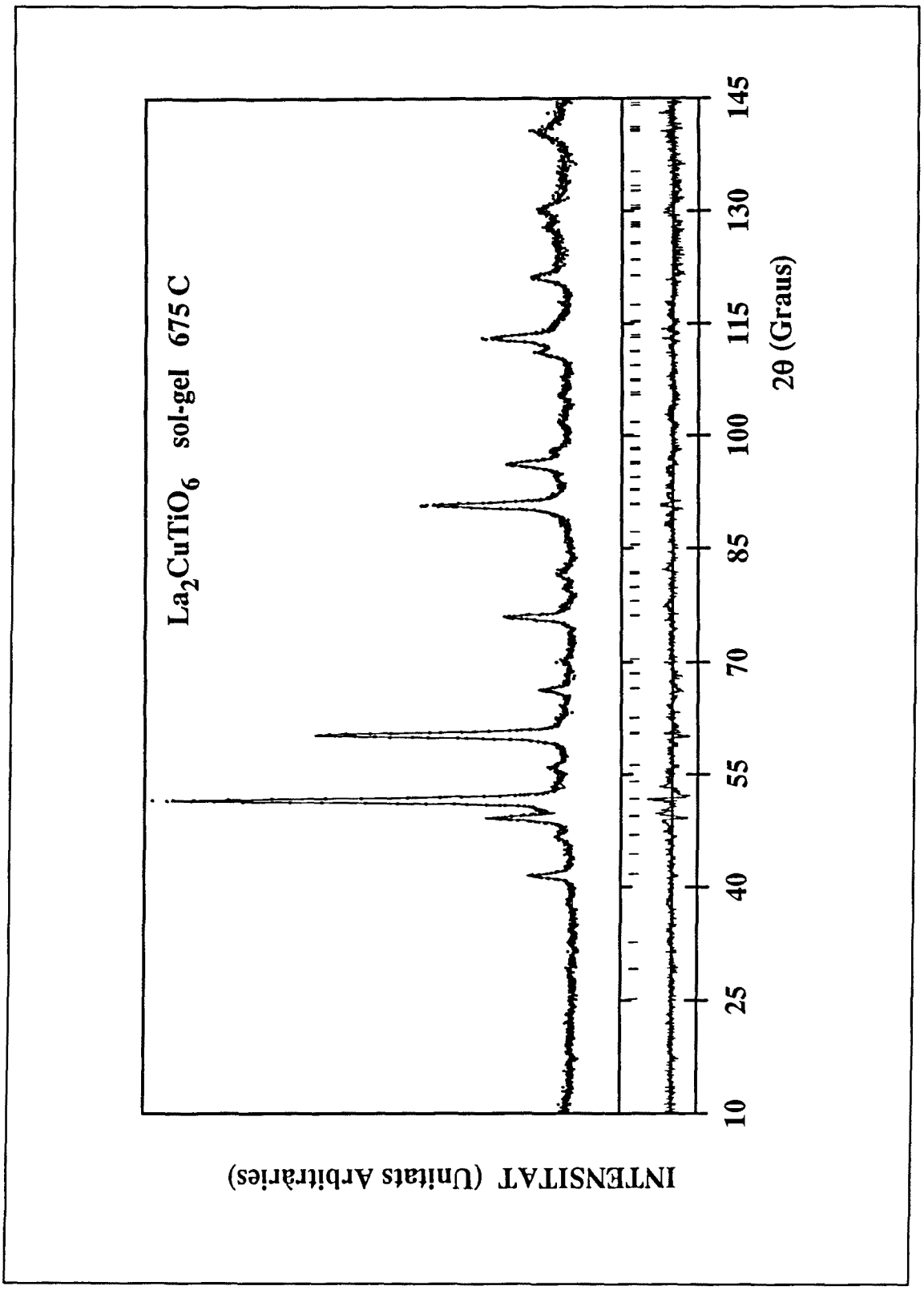
La_2CuTiO_6 sint. 675°C (AFINAMENT PER DIFRACCIÓ DE NEUTRONS)

Grup espacial: Pnma (lambda=1.9845Å $2\theta_{in}$=1°, step=0.05°, $2\theta_{fin}$=160°)

H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs	H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
0	1	1	4	0.636	0.760	25.189	0.	0.	3	0	2	4	0.762	0.760	79.817	2.	3.
1	0	1	4	0.635	0.760	29.146	3.	2.	1	4	2	8	0.762	0.760	79.956	3.	3.
0	2	0	2	0.635	0.760	29.226	3.	2.	2	4	1	8	0.763	0.760	79.970	1.	1.
1	1	1	8	0.635	0.760	32.695	1.	1.	2	1	3	8	0.773	0.760	81.640	4.	5.
0	0	2	2	0.639	0.760	41.674	6.	6.	3	1	2	8	0.773	0.760	81.664	6.	7.
2	0	0	2	0.639	0.760	41.703	9.	9.	0	3	3	4	0.774	0.760	81.710	0.	0.
1	2	1	8	0.639	0.760	41.747	30.	30.	0	5	1	4	0.775	0.760	81.886	9.	12.
2	1	0	4	0.642	0.760	44.375	1.	1.	1	3	3	8	0.800	0.760	85.363	3.	2.
1	0	2	4	0.645	0.760	46.875	12.	16.	3	3	1	8	0.800	0.760	85.401	1.	1.
2	0	1	4	0.645	0.760	46.895	4.	6.	1	5	1	8	0.801	0.760	85.539	0.	0.
1	1	2	8	0.649	0.760	49.325	22.	24.	2	2	3	8	0.813	0.760	87.139	1.	1.
2	1	1	8	0.649	0.760	49.344	22.	25.	3	2	2	8	0.813	0.760	87.163	4.	6.
0	3	1	4	0.649	0.760	49.434	44.	49.	0	0	4	2	0.843	0.760	90.703	23.	25.
0	2	2	4	0.653	0.760	51.710	188.	189.	4	0	0	2	0.844	0.760	90.778	45.	48.
2	2	0	4	0.653	0.760	51.734	228.	228.	2	4	2	8	0.845	0.760	90.896	121.	128.
1	3	1	8	0.658	0.760	54.058	5.	15.	4	1	0	4	0.860	0.760	92.602	3.	4.
1	2	2	8	0.663	0.760	56.200	12.	14.	2	5	0	4	0.862	0.760	92.808	0.	0.
2	2	1	8	0.663	0.760	56.217	6.	7.	1	0	4	4	0.877	0.760	94.336	7.	11.
2	0	2	4	0.674	0.760	60.426	197.	191.	4	0	1	4	0.878	0.760	94.407	4.	6.
0	4	0	2	0.675	0.760	60.606	90.	87.	1	1	4	8	0.896	0.760	96.167	11.	12.
2	1	2	8	0.681	0.760	62.502	3.	3.	4	1	1	8	0.896	0.760	96.238	0.	0.
2	3	0	4	0.681	0.760	62.601	4.	4.	2	3	3	8	0.897	0.760	96.270	30.	33.
0	1	3	4	0.695	0.760	66.498	15.	12.	3	3	2	8	0.897	0.760	96.293	8.	9.
1	3	2	8	0.695	0.760	66.599	9.	7.	1	5	2	8	0.899	0.760	96.431	7.	7.
2	3	1	8	0.696	0.760	66.614	10.	8.	2	5	1	8	0.899	0.760	96.445	33.	35.
1	0	3	4	0.703	0.760	68.454	3.	2.	3	0	3	4	0.916	0.760	98.021	6.	5.
3	0	1	4	0.703	0.760	68.494	0.	0.	0	2	4	4	0.916	0.760	98.022	0.	0.
2	2	2	8	0.703	0.760	68.516	2.	1.	4	2	0	4	0.917	0.760	98.098	2.	2.
1	4	1	8	0.704	0.760	68.641	1.	0.	1	4	3	8	0.917	0.760	98.159	5.	4.
1	1	3	8	0.711	0.760	70.401	3.	3.	3	4	1	8	0.918	0.760	98.197	0.	0.
3	1	1	8	0.712	0.760	70.441	7.	8.	0	6	0	2	0.920	0.760	98.376	8.	7.
1	2	3	8	0.740	0.760	76.116	33.	37.	3	1	3	8	0.937	0.760	99.867	1.	1.
3	2	1	8	0.740	0.760	76.155	11.	12.	1	2	4	8	0.959	0.760	101.707	11.	12.
0	4	2	4	0.741	0.760	76.246	16.	18.	4	2	1	8	0.960	0.760	101.779	4.	5.
2	4	0	4	0.741	0.760	76.265	21.	23.	2	0	4	4	1.008	0.760	105.406	1.	1.
2	3	2	8	0.751	0.760	78.046	0.	0.	4	0	2	4	1.009	0.760	105.464	4.	3.
2	0	3	4	0.761	0.760	79.793	1.	1.	3	2	3	8	1.009	0.760	105.476	8.	6.

H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
1	6	1	8	1.014	0.760	105.800	5.	5.
2	1	4	8	1.036	0.760	107.306	1.	1.
4	1	2	8	1.037	0.760	107.365	1.	1.
4	3	0	4	1.038	0.760	107.457	0.	0.
2	5	2	8	1.040	0.760	107.581	4.	4.
2	4	3	8	1.068	0.760	109.389	1.	0.
3	4	2	8	1.068	0.760	109.414	1.	1.
1	3	4	8	1.098	0.760	111.225	11.	11.
4	3	1	8	1.099	0.760	111.300	13.	13.
0	5	3	4	1.101	0.760	111.407	18.	19.
2	2	4	8	1.132	0.760	113.138	34.	35.
4	2	2	8	1.133	0.760	113.200	67.	68.
0	6	2	4	1.138	0.760	113.499	19.	19.
2	6	0	4	1.139	0.760	113.519	24.	25.
3	3	3	8	1.171	0.760	115.211	9.	11.
1	5	3	8	1.174	0.760	115.363	8.	10.
3	5	1	8	1.174	0.760	115.404	5.	7.
1	6	2	8	1.217	0.760	117.521	0.	0.
2	6	1	8	1.218	0.760	117.537	0.	0.
0	4	4	4	1.306	0.760	121.429	22.	17.
4	4	0	4	1.308	0.760	121.517	45.	36.
2	3	4	8	1.358	0.760	123.509	2.	1.
4	3	2	8	1.360	0.760	123.577	8.	4.
3	0	4	4	1.416	0.760	125.619	5.	2.
4	0	3	4	1.417	0.760	125.660	1.	1.

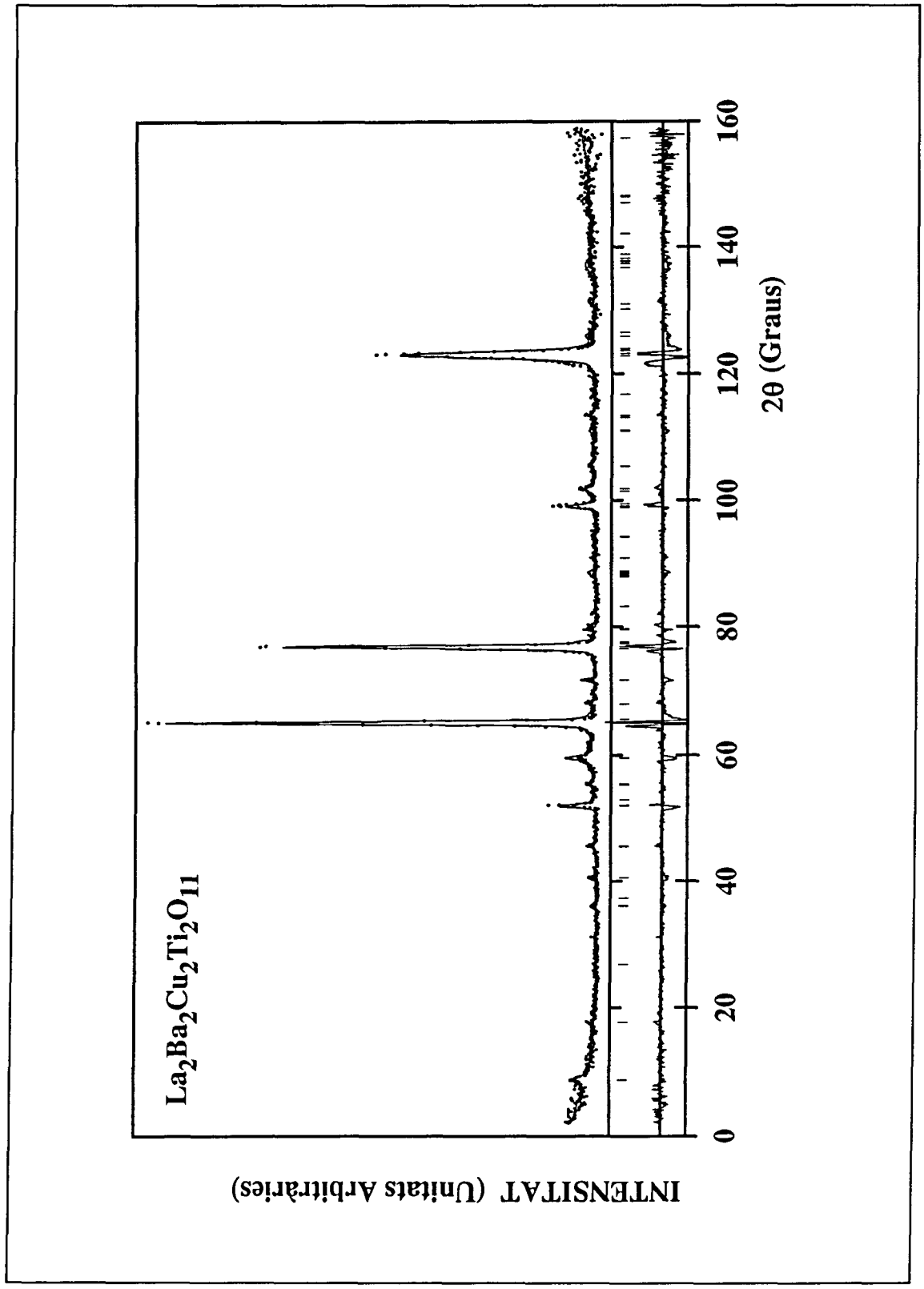
H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
1	4	4	8	1.421	0.760	125.788	3.	2.
4	4	1	8	1.423	0.760	125.875	2.	1.
0	1	5	4	1.482	0.760	127.842	2.	1.
3	1	4	8	1.483	0.760	127.895	10.	8.
4	1	3	8	1.485	0.760	127.937	10.	7.
2	5	3	8	1.493	0.760	128.199	0.	0.
3	5	2	8	1.494	0.760	128.228	2.	2.
0	7	1	4	1.503	0.760	128.509	14.	11.
1	0	5	4	1.557	0.760	130.166	12.	13.
5	0	1	4	1.563	0.760	130.314	0.	0.
3	4	3	8	1.567	0.760	130.445	7.	7.
2	6	2	8	1.576	0.760	130.702	19.	19.
1	1	5	8	1.645	0.760	132.597	0.	0.
5	1	1	8	1.651	0.760	132.750	6.	1.
1	7	1	8	1.672	0.760	133.313	2.	0.
3	2	4	8	1.750	0.760	135.210	6.	3.
4	2	3	8	1.752	0.760	135.257	4.	2.
1	2	5	8	2.010	0.760	140.561	32.	35.
5	2	1	8	2.020	0.760	140.739	1.	1.
2	4	4	8	2.023	0.760	140.790	9.	10.
4	4	2	8	2.028	0.760	140.880	20.	22.
1	6	3	8	2.041	0.760	141.115	15.	17.
3	6	1	8	2.044	0.760	141.175	4.	5.
4	5	0	4	2.220	0.760	144.015	5.	7.
2	7	0	4	2.243	0.760	144.367	1.	2.


La2CuTiO6 sol-gel 675 C
INTENSITAT (Unitats Arbitràries)
2θ (Graus)
10
25
40
55
70
85
100
115
130
145

$La_2Ba_2Cu_2Ti_2O_{11-\delta}$ (AFINAMENT PER DIFRACCIÓ DE NEUTRONS)

Grup espacial: P4/mmm (lambda=2.4497Å $2\theta_{in}$=1°, step=0.1°, $2\theta_{fin}$=160°)

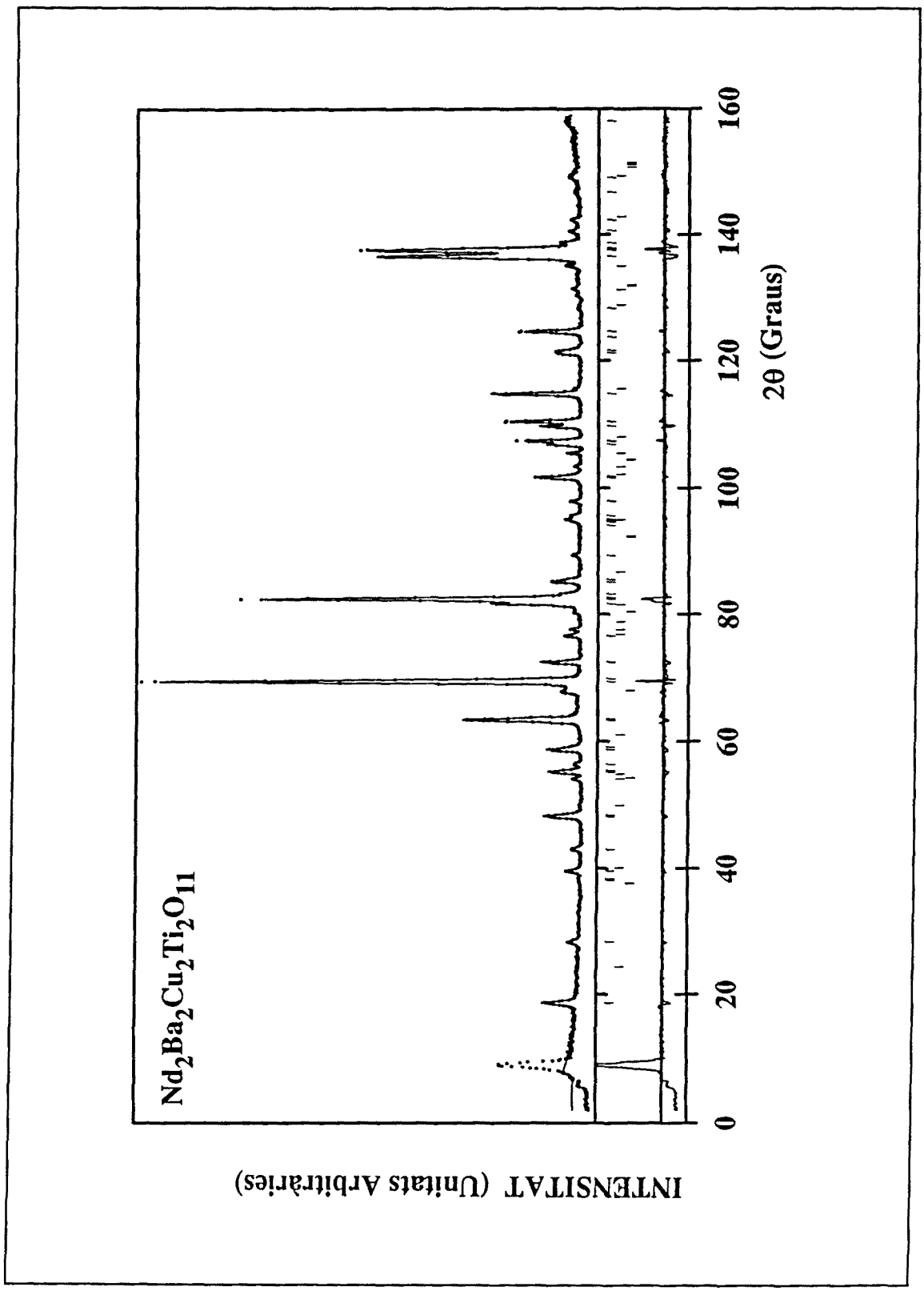
H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
0	0	1	2	0.851	0.457	8.890	7.	10.
0	0	2	2	0.788	0.457	17.833	1.	4.
0	0	3	2	0.724	0.457	26.888	0.	0.
0	0	4	2	0.660	0.457	36.118	2.	2.
1	0	0	4	0.659	0.457	36.253	0.	0.
1	0	1	8	0.652	0.457	37.401	1.	0.
1	0	2	8	0.629	0.457	40.679	4.	2.
0	0	5	2	0.596	0.457	45.597	3.	4.
1	0	3	8	0.595	0.457	45.708	1.	2.
1	0	4	8	0.554	0.457	52.104	23.	17.
1	1	0	4	0.553	0.457	52.205	2.	2.
1	1	1	8	0.548	0.457	53.071	0.	0.
0	0	6	2	0.533	0.457	55.419	3.	2.
1	1	2	8	0.532	0.457	55.612	3.	2.
1	0	5	8	0.508	0.457	59.594	5.	7.
1	1	3	8	0.508	0.457	59.687	3.	3.
1	1	4	8	0.479	0.457	65.125	257.	255.
0	0	7	2	0.476	0.457	65.706	0.	0.
1	0	6	8	0.465	0.457	68.038	5.	3.
1	1	5	8	0.450	0.457	71.788	2.	2.
0	0	8	2	0.437	0.457	76.630	48.	48.
2	0	0	4	0.437	0.457	76.958	166.	169.
1	0	7	8	0.436	0.457	77.418	0.	0.
2	0	1	8	0.436	0.457	77.663	0.	0.
1	1	6	8	0.434	0.457	79.607	4.	5.
2	0	2	8	0.433	0.457	79.769	0.	1.
2	0	3	8	0.434	0.457	83.248	0.	0.
1	0	8	8	0.445	0.457	87.842	1.	1.
2	0	4	8	0.446	0.457	88.081	1.	0.
2	1	0	8	0.446	0.457	88.161	1.	0.
0	0	9	2	0.447	0.457	88.451	0.	0.
1	1	7	8	0.448	0.457	88.610	2.	2.
2	1	1	16	0.449	0.457	88.850	0.	0.
2	1	2	16	0.459	0.457	90.914	2.	2.
2	0	5	8	0.481	0.457	94.280	4.	3.
2	1	3	16	0.482	0.457	94.360	1.	1.
1	1	8	8	0.525	0.457	98.971	4.	4.
2	1	4	16	0.528	0.457	99.213	23.	27.
1	0	9	8	0.532	0.457	99.587	0.	0.
0	0	10	2	0.557	0.457	101.607	7.	7.
2	0	6	8	0.561	0.457	101.932	5.	7.
2	1	5	16	0.614	0.457	105.558	5.	4.
1	1	9	8	0.715	0.457	111.108	0.	0.
2	0	7	8	0.718	0.457	111.279	1.	1.
1	0	10	8	0.761	0.457	113.252	0.	0.
2	1	6	16	0.768	0.457	113.599	6.	5.
0	0	11	2	0.850	0.457	116.965	1.	0.
2	0	8	8	1.023	0.457	122.894	138.	139.
2	2	0	4	1.035	0.457	123.275	120.	117.
2	1	7	16	1.053	0.457	123.814	1.	0.
2	2	1	8	1.063	0.457	124.102	0.	0.
1	1	10	8	1.132	0.457	126.040	0.	0.
2	2	2	8	1.154	0.457	126.634	0.	0.
1	0	11	8	1.304	0.457	130.318	0.	0.
2	2	3	8	1.337	0.457	131.053	0.	0.
0	0	12	2	1.637	0.457	136.863	0.	0.
2	1	8	16	1.672	0.457	137.449	6.	5.
2	2	4	8	1.694	0.457	137.804	0.	0.
3	0	0	4	1.701	0.457	137.922	1.	1.
2	0	9	8	1.728	0.457	138.356	1.	0.
3	0	1	8	1.767	0.457	138.960	0.	0.
3	0	2	8	1.996	0.457	142.212	1.	2.
1	1	11	8	2.436	0.457	147.204	3.	6.
2	2	5	8	2.530	0.457	148.098	4.	8.
3	0	3	8	2.546	0.457	148.249	0.	1.
1	0	12	8	3.938	0.457	157.413	16.	10.


La2Ba2Cu2Ti2O11
INTENSITAT (Unitats Arbitràries)
0
20
40
60
80
100
120
140
160
2θ (Graus)

$Nd_2Ba_2Cu_2Ti_2O_{11-\delta}$ (AFINAMENT PER DIFRACCIÓ DE NEUTRONS)

Grup espacial: P4/mmm (lambda=2.5795Å $2\theta_{in}$=1°, step=0.1°, $2\theta_{fin}$=160°)

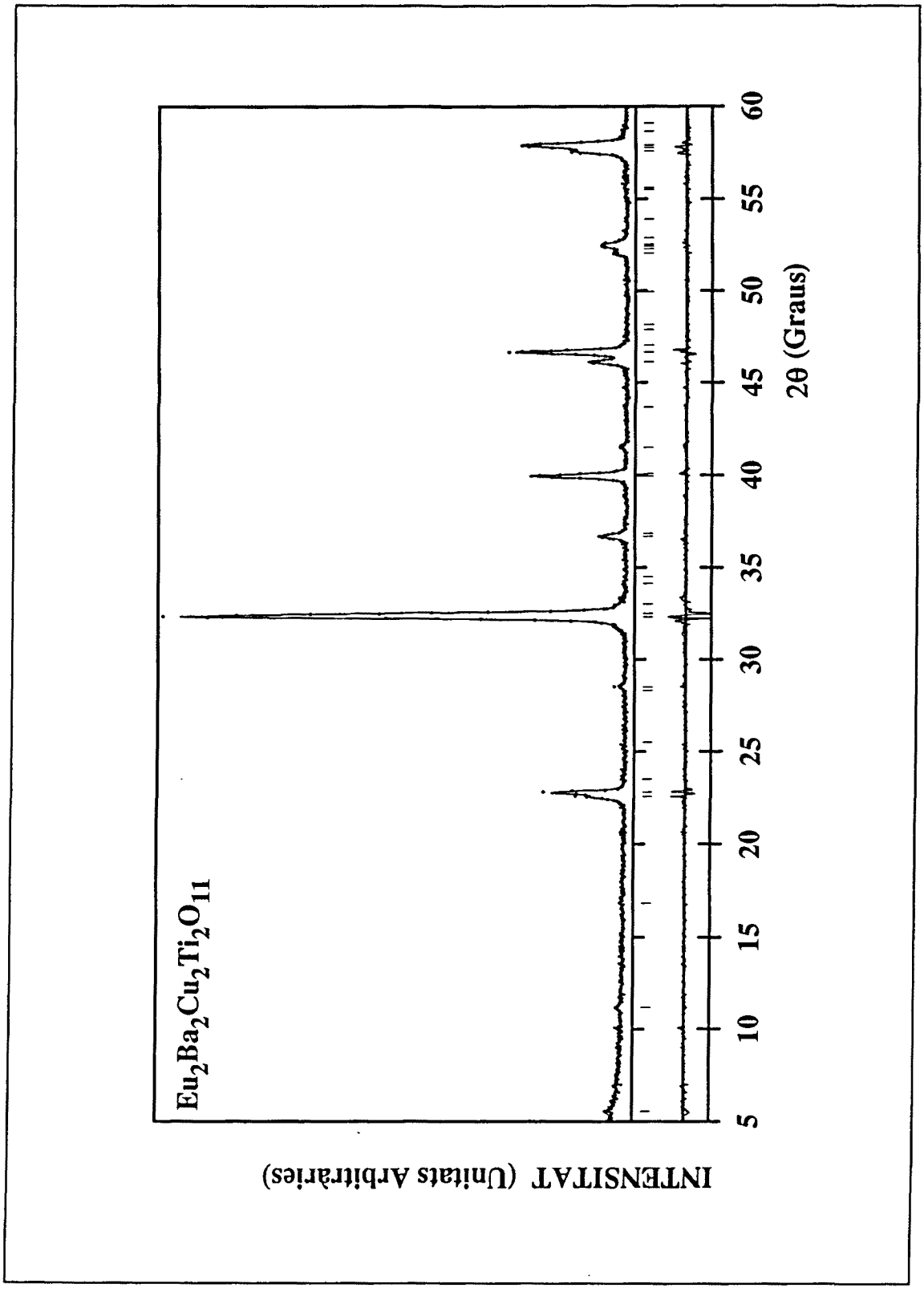
H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
0	0	2	2	0.662	0.259	18.837	127.	112.
0	0	3	2	0.634	0.259	28.419	39.	37.
0	0	4	2	0.606	0.259	38.209	5.	5.
1	0	0	4	0.605	0.259	38.492	0.	0.
1	0	1	8	0.601	0.259	39.708	50.	44.
1	0	2	8	0.591	0.259	43.186	30.	33.
0	0	5	2	0.576	0.259	48.298	61.	56.
1	0	3	8	0.575	0.259	48.533	65.	62.
1	0	4	8	0.555	0.259	55.357	90.	74.
1	1	0	4	0.554	0.259	55.570	7.	6.
1	1	1	8	0.551	0.259	56.695	20.	15.
0	0	6	2	0.544	0.259	58.804	89.	69.
1	1	2	8	0.543	0.259	59.214	15.	13.
1	0	5	8	0.530	0.259	63.388	204.	194.
1	1	3	8	0.530	0.259	63.584	124.	122.
1	1	4	8	0.512	0.259	69.442	959.	958.
0	0	7	2	0.510	0.259	69.886	21.	18.
1	0	6	8	0.503	0.259	72.503	93.	75.
1	1	5	8	0.490	0.259	76.665	37.	34.
0	0	8	2	0.475	0.259	81.776	169.	179.
2	0	0	4	0.473	0.259	82.484	703.	772.
1	0	7	8	0.472	0.259	82.727	8.	9.
2	0	1	8	0.471	0.259	83.257	37.	37.
1	1	6	8	0.465	0.259	85.218	54.	55.
2	0	2	8	0.464	0.259	85.570	27.	29.
2	0	3	8	0.454	0.259	89.410	15.	20.
1	0	8	8	0.442	0.259	94.258	1.	1.
2	0	4	8	0.441	0.259	94.786	8.	7.
0	0	9	2	0.441	0.259	94.852	8.	7.
2	1	0	8	0.441	0.259	94.962	0.	0.
1	1	7	8	0.440	0.259	95.204	24.	26.
2	1	1	16	0.439	0.259	95.733	19.	21.
2	1	2	16	0.434	0.259	98.051	18.	20.
2	0	5	8	0.429	0.259	101.768	76.	85.
2	1	3	16	0.428	0.259	101.947	29.	34.
1	1	8	8	0.424	0.259	106.951	66.	61.
2	1	4	16	0.424	0.259	107.502	110	114.
1	0	9	8	0.424	0.259	107.571	1.	1.
0	0	10	2	0.425	0.259	109.815	78.	75.
2	0	6	8	0.425	0.259	110.563	145.	159.
2	1	5	16	0.432	0.259	114.914	174	190.
1	1	9	8	0.457	0.259	121.277	42.	46.
2	0	7	8	0.460	0.259	121.689	45.	45.
1	0	10	8	0.474	0.259	123.799	0.	0.
2	1	6	16	0.480	0.259	124.648	117	124.
0	0	11	2	0.515	0.259	128.329	11.	5.
2	0	8	8	0.640	0.259	136.565	507.	478.
2	2	0	4	0.661	0.259	137.596	552.	537.
2	1	7	16	0.669	0.259	137.954	10.	9.
2	2	1	8	0.687	0.259	138.746	43.	35.
1	1	10	8	0.735	0.259	140.677	31.	21.
2	2	2	8	0.782	0.259	142.369	26.	18.
1	0	11	8	0.938	0.259	146.875	16.	9.
2	2	3	8	1.040	0.259	149.195	14.	24.
0	0	12	2	1.657	0.259	158.147	41.	40.


$Nd_2Ba_2Cu_2Ti_2O_{11}$
0
20
40
60
80
100
120
140
160
2θ (Graus)
INTENSITAT (Unitats Arbitràries)

$Eu_2Ba_2Cu_2Ti_2O_{11-\delta}$ (AFINAMENT PER DIFRACCIÓ DE RAIGS X)

Grup espacial: P4/mmm (lambda=1.5418Å $2\theta_{in}$=2°, step=0.025°, $2\theta_{fin}$=60°)

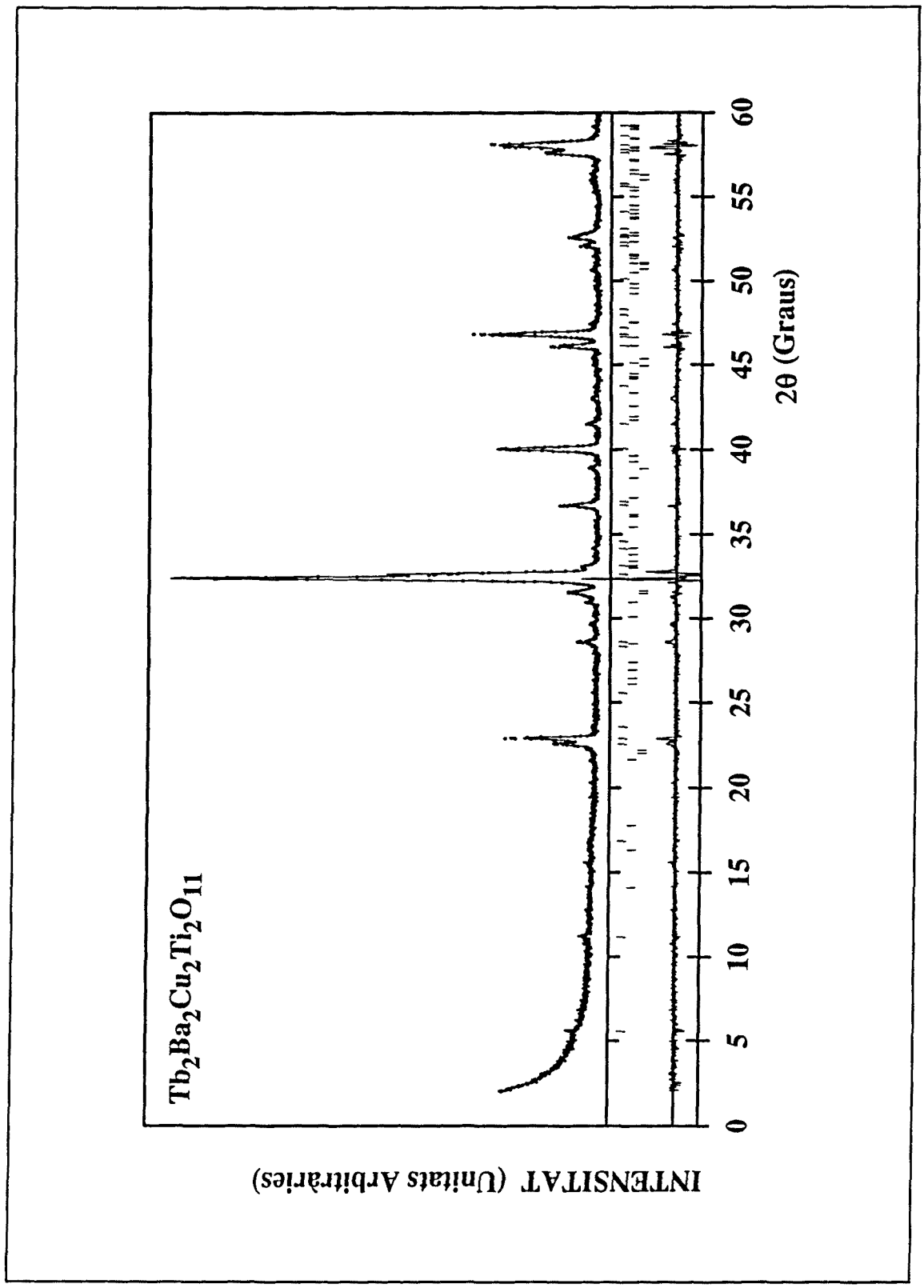
H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
0	0	1	2	0.233	0.546	5.620	18.	5.
0	0	2	2	0.221	0.546	11.253	15.	13.
0	0	3	2	0.212	0.546	16.914	5.	6.
0	0	4	2	0.207	0.546	22.617	59.	66.
1	0	0	4	0.207	0.546	22.867	145.	141.
1	0	1	8	0.207	0.546	23.565	2.	2.
1	0	2	8	0.206	0.546	25.553	1.	1.
0	0	5	2	0.206	0.546	28.377	0.	1.
1	0	3	8	0.207	0.546	28.579	13.	25.
1	0	4	8	0.209	0.546	32.380	840.	839.
1	1	0	4	0.209	0.546	32.560	394.	378.
1	1	1	8	0.210	0.546	33.069	1.	3.
0	0	6	2	0.211	0.546	34.211	5.	7.
1	1	2	8	0.211	0.546	34.553	1.	2.
1	0	5	8	0.214	0.546	36.750	54.	65.
1	1	3	8	0.215	0.546	36.911	8.	10.
1	1	4	8	0.220	0.546	40.011	206.	206.
0	0	7	2	0.220	0.546	40.138	12.	12.
1	0	6	8	0.223	0.546	41.549	9.	17.
1	1	5	8	0.229	0.546	43.725	1.	3.
0	0	8	2	0.236	0.546	46.180	86.	88.
1	0	7	8	0.237	0.546	46.693	8.	8.
2	0	0	4	0.237	0.546	46.713	252.	252.
2	0	1	8	0.238	0.546	47.090	1.	1.
1	1	6	8	0.241	0.546	47.949	4.	1.
2	0	2	8	0.242	0.546	48.208	1.	0.
2	0	3	8	0.248	0.546	50.030	1.	0.
1	0	8	8	0.256	0.546	52.135	30.	24.
0	0	9	2	0.256	0.546	52.361	4.	4.
2	0	4	8	0.257	0.546	52.501	29.	29.
1	1	7	8	0.257	0.546	52.604	10.	10.
2	1	0	8	0.257	0.546	52.623	35.	35.
2	1	1	16	0.259	0.546	52.968	0.	0.
2	1	2	16	0.263	0.546	53.996	0.	0.
2	0	5	8	0.269	0.546	55.564	1.	0.
2	1	3	16	0.270	0.546	55.681	3.	1.
1	1	8	8	0.278	0.546	57.641	119.	125.
1	0	9	8	0.279	0.546	57.853	9.	9.
2	1	4	16	0.280	0.546	57.984	272.	275.
0	0	10	2	0.283	0.546	58.710	6.	2.
2	0	6	8	0.285	0.546	59.161	2.	0.


$Eu_2Ba_2Cu_2Ti_2O_{11}$
INTENSITAT (Unitats Arbitràries)
2θ (Graus)
5
10
15
20
25
30
35
40
45
50
55
60

$Tb_2Ba_2Cu_2Ti_2O_{11-\delta}$ (AFINAMENT PER DIFRACCIÓ DE RAIGS X)

Grup espacial: P4/mmm (lambda=1.5418Å $2\theta_{in}$=2°, step=0.025°, $2\theta_{fin}$=60°)

H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs	H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
0	0	1	2	0.237	0.358	5.617	28.	10.	1	0	7	8	0.249	0.358	46.716	8.	8.
0	0	2	2	0.219	0.358	11.248	22.	21.	2	0	0	4	0.249	0.358	46.867	333.	327.
0	0	3	2	0.206	0.358	16.907	10.	7.	2	0	1	8	0.251	0.358	47.243	2.	2.
0	0	4	2	0.199	0.358	22.607	72.	85.	1	1	6	8	0.255	0.358	48.013	5.	0.
1	0	0	4	0.198	0.358	22.939	172.	190.	2	0	2	8	0.256	0.358	48.357	2.	1.
1	0	1	8	0.198	0.358	23.635	3.	2.	2	0	3	8	0.265	0.358	50.173	2.	1.
1	0	2	8	0.198	0.358	25.616	0.	2.	1	0	8	8	0.276	0.358	52.151	36.	29.
0	0	5	2	0.199	0.358	28.364	1.	3.	0	0	9	2	0.277	0.358	52.337	8.	7.
1	0	3	8	0.199	0.358	28.634	18.	44.	2	0	4	8	0.279	0.358	52.637	39.	37.
1	0	4	8	0.203	0.358	32.426	1021.	1062.	1	1	7	8	0.279	0.358	52.661	20.	19.
1	1	0	4	0.204	0.358	32.664	489.	463.	2	1	0	8	0.280	0.358	52.799	46.	42.
1	1	1	8	0.205	0.358	33.171	3.	4.	2	1	1	16	0.282	0.358	53.143	1.	1.
0	0	6	2	0.206	0.358	34.196	7.	4.	2	1	2	16	0.288	0.358	54.168	0.	0.
1	1	2	8	0.207	0.358	34.650	1.	0.	2	0	5	8	0.297	0.358	55.692	2.	4.
1	0	5	8	0.212	0.358	36.787	79.	83.	2	1	3	16	0.298	0.358	55.848	4.	7.
1	1	3	8	0.213	0.358	37.001	8.	8.	1	1	8	8	0.309	0.358	57.690	163.	166.
1	1	4	8	0.222	0.358	40.092	263.	262.	1	0	9	8	0.310	0.358	57.863	17.	18.
0	0	7	2	0.222	0.358	40.121	17.	17.	2	1	4	16	0.312	0.358	58.144	373.	389.
1	0	6	8	0.227	0.358	41.579	16.	27.	0	0	10	2	0.316	0.358	58.683	9.	6.
1	1	5	8	0.236	0.358	43.798	3.	8.	2	0	6	8	0.320	0.358	59.282	4.	3.
0	0	8	2	0.246	0.358	46.159	108.	108.									


$Tb_2Ba_2Cu_2Ti_2O_{11}$
INTENSITAT (Unitats Arbitràries)
0
5
10
15
20
25
30
35
40
45
50
55
60
2θ (Graus)

$Tb_2Ba_2Cu_2Ti_2O_{11-\delta}$ (AFINAMENT PER DIFRACCIÓ DE NEUTRONS)

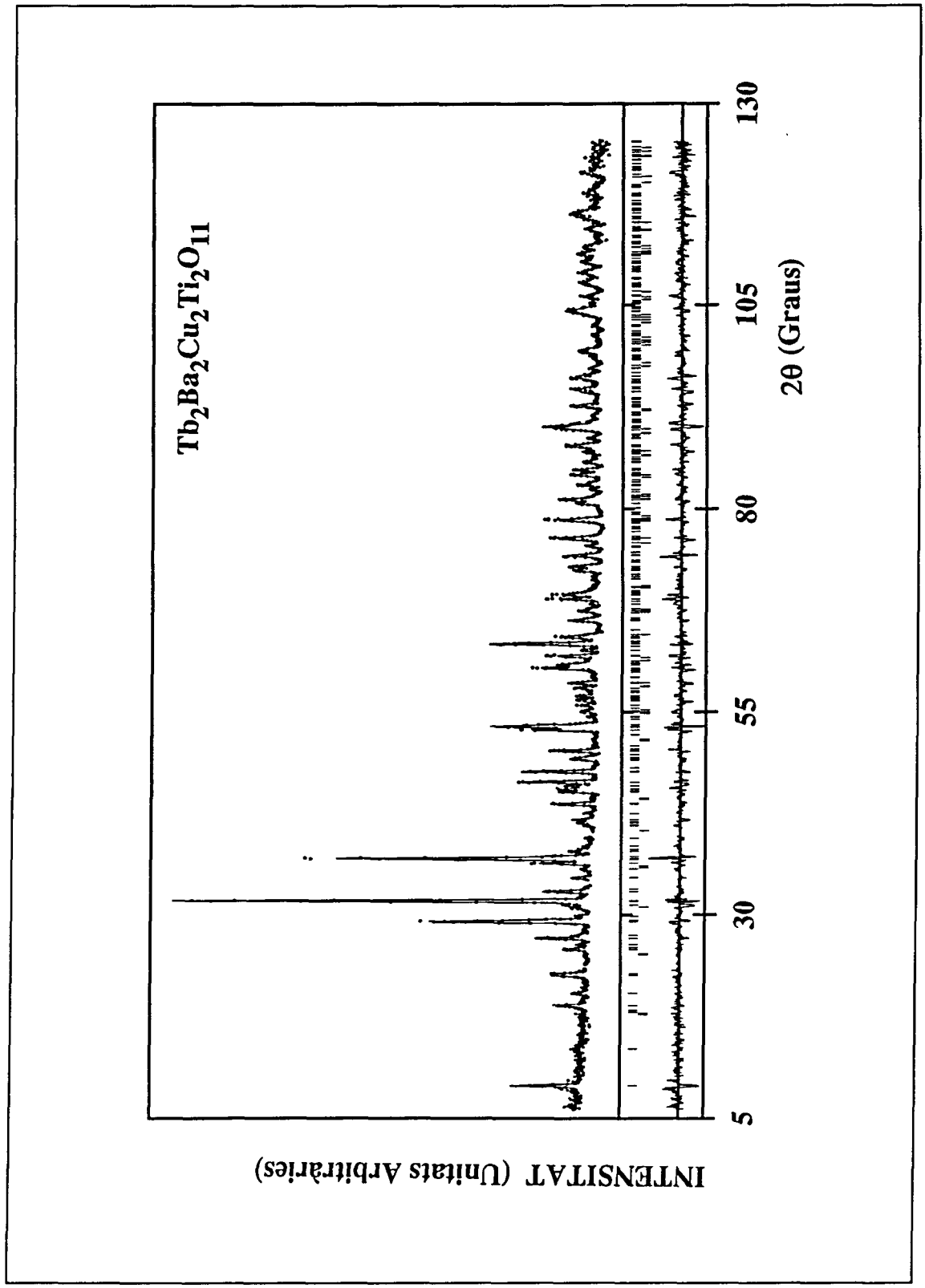
Grup espacial: I4/mcm (lambda=1.2272Å $2\theta_{in}$=1°, step=0.05°, $2\theta_{fin}$=126°)

H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
0	0	4	2	0.271	0.194	8.934	23.	21.
0	0	6	2	0.265	0.194	13.418	4.	3.
0	0	8	2	0.260	0.194	17.922	0.	0.
1	1	0	4	0.260	0.194	18.192	0.	0.
1	1	2	8	0.259	0.194	18.741	10.	10.
1	1	4	8	0.258	0.194	20.301	3.	3.
0	0	10	2	0.256	0.194	22.455	9.	10.
1	1	6	8	0.256	0.194	22.673	9.	9.
1	1	8	8	0.255	0.194	25.646	7.	7.
2	0	0	4	0.255	0.194	25.838	1.	1.
2	0	2	8	0.254	0.194	26.234	3.	3.
0	0	12	2	0.254	0.194	27.024	16.	15.
2	0	4	8	0.254	0.194	27.390	4.	4.
2	1	1	16	0.254	0.194	29.041	2.	2.
1	1	10	8	0.254	0.194	29.050	41.	43.
2	0	6	8	0.254	0.194	29.222	19.	19.
2	1	3	16	0.254	0.194	29.749	3.	4.
2	1	5	16	0.254	0.194	31.121	5.	3.
2	0	8	8	0.254	0.194	31.625	124.	124.
0	0	14	2	0.254	0.194	31.637	5.	5.
1	1	12	8	0.254	0.194	32.772	14.	13.
2	1	7	16	0.254	0.194	33.083	2.	2.
2	0	10	8	0.254	0.194	34.492	6.	5.
2	1	9	16	0.254	0.194	35.549	0.	1.
0	0	16	2	0.255	0.194	36.303	15.	16.
1	1	14	8	0.255	0.194	36.736	2.	2.
2	2	0	4	0.255	0.194	36.865	79.	83.
2	2	2	8	0.255	0.194	37.153	11.	9.
2	0	12	8	0.255	0.194	37.735	6.	6.
2	2	4	8	0.256	0.194	38.008	3.	3.
2	1	11	16	0.256	0.194	38.437	1.	2.
2	2	6	8	0.256	0.194	39.398	2.	1.
1	1	16	8	0.258	0.194	40.895	0.	1.
0	0	18	2	0.258	0.194	41.032	0.	1.
2	2	8	8	0.258	0.194	41.277	0.	0.
2	0	14	8	0.258	0.194	41.287	4.	5.
3	1	0	8	0.258	0.194	41.404	0.	0.
3	1	2	16	0.258	0.194	41.666	3.	2.
2	1	13	16	0.258	0.194	41.678	3.	2.
3	1	4	16	0.259	0.194	42.444	2.	2.
2	2	10	8	0.260	0.194	43.595	12.	10.
3	1	6	16	0.260	0.194	43.716	3.	2.
2	0	16	8	0.262	0.194	45.096	10.	10.
2	1	15	16	0.262	0.194	45.216	1.	1.
1	1	18	8	0.262	0.194	45.223	0.	0.
3	1	8	16	0.262	0.194	45.449	11.	12.
0	0	20	2	0.263	0.194	45.836	10.	9.
2	2	12	8	0.264	0.194	46.301	22.	21.
3	2	1	16	0.265	0.194	47.598	0.	0.
3	1	10	16	0.265	0.194	47.604	24.	23.
3	2	3	16	0.266	0.194	48.067	0.	1.
3	2	5	16	0.268	0.194	48.994	1.	1.
2	1	17	16	0.268	0.194	49.011	0.	0.
2	0	18	8	0.268	0.194	49.128	8.	7.
2	2	14	8	0.268	0.194	49.349	5.	5.
1	1	20	8	0.269	0.194	49.705	0.	0.
3	1	12	16	0.270	0.194	50.142	16.	16.
3	2	7	16	0.270	0.194	50.362	0.	1.
0	0	22	2	0.271	0.194	50.726	1.	1.
3	2	9	16	0.273	0.194	52.144	0.	0.
2	2	16	8	0.274	0.194	52.703	21.	22.
3	1	14	16	0.275	0.194	53.026	2.	2.
2	1	19	16	0.275	0.194	53.036	0.	0.
4	0	0	4	0.275	0.194	53.122	32.	30.
4	0	2	8	0.276	0.194	53.339	9.	10.
2	0	20	8	0.276	0.194	53.363	1.	1.
4	0	4	8	0.277	0.194	53.986	1.	0.
3	2	11	16	0.278	0.194	54.314	0.	0.
1	1	22	8	0.278	0.194	54.336	1.	2.
4	1	1	16	0.279	0.194	54.945	1.	3.
4	0	6	8	0.279	0.194	55.053	2.	3.
4	1	3	16	0.280	0.194	55.369	1.	1.
0	0	24	2	0.281	0.194	55.718	5.	5.
4	1	5	16	0.282	0.194	56.209	3.	2.
3	1	16	16	0.282	0.194	56.223	0.	0.
2	2	18	8	0.282	0.194	56.331	4.	3.
4	0	8	8	0.283	0.194	56.524	0.	0.
3	3	0	4	0.283	0.194	56.624	1.	1.
3	3	2	8	0.283	0.194	56.832	3.	5.
3	2	13	16	0.283	0.194	56.842	1.	1.
2	1	21	16	0.284	0.194	57.271	1.	1.
3	3	4	8	0.285	0.194	57.453	1.	1.
4	1	7	16	0.285	0.194	57.455	1.	1.
2	0	22	8	0.286	0.194	57.788	7.	6.
4	0	10	8	0.287	0.194	58.380	8.	7.
3	3	6	8	0.287	0.194	58.478	1.	1.
4	1	9	16	0.289	0.194	59.089	0.	0.
1	1	24	8	0.289	0.194	59.117	0.	0.
3	2	15	16	0.291	0.194	59.702	0.	0.
3	1	18	16	0.291	0.194	59.708	0.	0.
3	3	8	8	0.291	0.194	59.894	1.	1.
4	2	0	8	0.291	0.194	59.991	2.	1.
4	2	2	16	0.292	0.194	60.191	1.	1.
2	2	20	8	0.292	0.194	60.214	18.	18.
4	0	12	8	0.293	0.194	60.598	13.	12.
4	2	4	16	0.294	0.194	60.790	3.	3.
0	0	26	2	0.294	0.194	60.827	0.	0.
4	1	11	16	0.295	0.194	61.094	0.	0.
3	3	10	8	0.296	0.194	61.686	11.	12.
2	1	23	16	0.296	0.194	61.710	0.	0.
4	2	6	16	0.297	0.194	61.781	3.	3.
2	0	24	8	0.298	0.194	62.400	6.	5.
3	2	17	16	0.300	0.194	62.873	0.	0.
4	2	8	16	0.301	0.194	63.153	37.	37.
4	0	14	8	0.301	0.194	63.160	2.	2.
4	1	13	16	0.302	0.194	63.450	3.	3.
3	1	20	16	0.302	0.194	63.463	0.	0.
3	3	12	8	0.303	0.194	63.836	4.	4.

H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
1	1	26	8	0.304	0.194	64.058	12.	12.
2	2	22	8	0.304	0.194	64.337	3.	2.
4	2	10	16	0.306	0.194	64.893	0.	0.
4	0	16	8	0.310	0.194	66.046	10.	10.
0	0	28	2	0.310	0.194	66.074	1.	1.
4	1	15	16	0.310	0.194	66.139	1.	1.
3	3	14	8	0.311	0.194	66.327	2.	2.
3	2	19	16	0.311	0.194	66.336	0.	0.
2	1	25	16	0.311	0.194	66.350	0.	0.
4	2	12	16	0.313	0.194	66.986	1.	1.
2	0	26	8	0.314	0.194	67.203	7.	8.
3	1	22	16	0.315	0.194	67.475	2.	3.
4	3	1	16	0.317	0.194	68.012	1.	2.
4	3	3	16	0.318	0.194	68.386	0.	1.
2	2	24	8	0.320	0.194	68.696	14.	18.
4	3	5	16	0.321	0.194	69.132	1.	1.
3	3	16	8	0.321	0.194	69.144	1.	2.
4	1	17	16	0.321	0.194	69.146	0.	0.
1	1	28	8	0.321	0.194	69.171	7.	8.
4	0	18	8	0.322	0.194	69.240	5.	5.
4	2	14	16	0.322	0.194	69.419	4.	4.
5	1	0	8	0.323	0.194	69.502	0.	0.
5	1	2	16	0.323	0.194	69.687	3.	4.
3	2	21	16	0.325	0.194	70.079	0.	1.
5	1	4	16	0.326	0.194	70.242	1.	2.
4	3	7	16	0.326	0.194	70.244	1.	1.
5	1	6	16	0.329	0.194	71.163	2.	3.
2	1	27	16	0.329	0.194	71.198	0.	0.
0	0	30	2	0.331	0.194	71.482	1.	2.
4	3	9	16	0.331	0.194	71.714	0.	0.
3	1	24	16	0.332	0.194	71.740	0.	0.
4	2	16	16	0.333	0.194	72.180	10.	9.
2	0	28	8	0.334	0.194	72.207	0.	0.
3	3	18	8	0.334	0.194	72.274	0.	0.
5	1	8	16	0.334	0.194	72.443	4.	4.
4	1	19	16	0.335	0.194	72.458	0.	0.
4	0	20	8	0.336	0.194	72.733	11.	11.
2	2	26	8	0.338	0.194	73.292	0.	0.
4	3	11	16	0.339	0.194	73.535	0.	0.
5	2	1	16	0.341	0.194	74.071	0.	0.
5	1	10	16	0.342	0.194	74.076	14.	17.
3	2	23	16	0.342	0.194	74.098	0.	0.
5	2	3	16	0.343	0.194	74.432	0.	0.
1	1	30	8	0.343	0.194	74.477	0.	0.
5	2	5	16	0.346	0.194	75.153	0.	0.
4	2	18	16	0.347	0.194	75.257	6.	7.
4	3	13	16	0.349	0.194	75.698	1.	1.
3	3	20	8	0.349	0.194	75.710	0.	0.
5	1	12	16	0.350	0.194	76.055	7.	6.
4	1	21	16	0.351	0.194	76.070	2.	1.
5	2	7	16	0.351	0.194	76.229	0.	0.
3	1	26	16	0.351	0.194	76.260	14.	14.
2	1	29	16	0.351	0.194	76.268	0.	0.
4	0	22	8	0.353	0.194	76.518	2.	2.
0	0	32	2	0.355	0.194	77.080	0.	0.
2	0	30	8	0.357	0.194	77.430	0.	0.
5	2	9	16	0.358	0.194	77.656	0.	0.
2	2	28	8	0.360	0.194	78.135	2.	2.
4	3	15	16	0.361	0.194	78.195	0.	0.
5	1	14	16	0.362	0.194	78.371	2.	2.
3	2	25	16	0.362	0.194	78.393	0.	0.
4	4	0	4	0.362	0.194	78.450	12.	13.
4	4	2	8	0.363	0.194	78.627	8.	9.
4	2	20	16	0.363	0.194	78.647	0.	0.
4	4	4	8	0.366	0.194	79.159	0.	0.
5	2	11	16	0.367	0.194	79.429	0.	0.
3	3	22	8	0.367	0.194	79.447	1.	1.
4	1	23	16	0.370	0.194	79.978	0.	0.
1	1	32	8	0.370	0.194	80.003	1.	1.
4	4	6	8	0.370	0.194	80.042	1.	0.
4	0	24	8	0.373	0.194	80.597	11.	10.
5	1	16	16	0.375	0.194	81.021	1.	2.
4	3	17	16	0.375	0.194	81.022	0.	0.
3	1	28	16	0.375	0.194	81.047	14.	15.
4	4	8	8	0.377	0.194	81.275	0.	0.
5	3	0	8	0.377	0.194	81.359	0.	0.
5	3	2	16	0.378	0.194	81.535	1.	2.
5	2	13	16	0.378	0.194	81.543	0.	0.
2	1	31	16	0.378	0.194	81.582	0.	0.
5	3	4	16	0.381	0.194	82.062	1.	0.
4	2	22	16	0.382	0.194	82.348	5.	3.
4	4	10	8	0.385	0.194	82.854	4.	4.
2	0	32	8	0.385	0.194	82.899	3.	3.
0	0	34	2	0.386	0.194	82.906	1.	1.
5	3	6	16	0.386	0.194	82.938	0.	0.
3	2	27	16	0.386	0.194	82.972	0.	0.
2	2	30	8	0.387	0.194	83.243	3.	4.
3	3	24	8	0.389	0.194	83.489	0.	0.
5	2	15	16	0.392	0.194	83.996	0.	0.
5	1	18	16	0.392	0.194	84.001	0.	0.
5	3	8	16	0.393	0.194	84.162	8.	9.
4	3	19	16	0.393	0.194	84.177	0.	0.
4	1	25	16	0.393	0.194	84.190	0.	0.
6	0	0	4	0.393	0.194	84.246	1.	1.
6	0	2	8	0.394	0.194	84.421	0.	0.
4	4	12	8	0.396	0.194	84.777	8.	9.
6	0	4	8	0.397	0.194	84.945	1.	1.
4	0	26	8	0.397	0.194	84.977	0.	0.
6	1	1	16	0.402	0.194	85.728	1.	1.
5	3	10	16	0.402	0.194	85.732	6.	6.
1	1	34	8	0.402	0.194	85.784	2.	2.
6	0	6	8	0.402	0.194	85.816	0.	0.
6	1	3	16	0.404	0.194	86.076	0.	0.
3	1	30	16	0.404	0.194	86.120	0.	0.
4	2	24	16	0.406	0.194	86.365	3.	3.
6	1	5	16	0.408	0.194	86.772	1.	1.
5	2	17	16	0.408	0.194	86.785	0.	0.
6	0	8	8	0.410	0.194	87.035	8.	6.
4	4	14	8	0.410	0.194	87.042	0.	0.
2	1	33	16	0.411	0.194	87.172	0.	0.
5	1	20	16	0.412	0.194	87.312	0.	0.
5	3	12	16	0.414	0.194	87.647	9.	9.
4	3	21	16	0.414	0.194	87.662	1.	1.
6	1	7	16	0.415	0.194	87.816	1.	1.
3	3	26	8	0.415	0.194	87.847	7.	8.
3	2	29	16	0.415	0.194	87.855	0.	0.
6	0	10	8	0.420	0.194	88.600	0.	0.
2	2	32	8	0.420	0.194	88.645	0.	0.
2	0	34	8	0.420	0.194	88.652	6.	4.
4	1	27	16	0.421	0.194	88.718	0.	0.
0	0	36	2	0.423	0.194	89.006	1.	1.
6	1	9	16	0.424	0.194	89.207	0.	0.
4	4	16	8	0.427	0.194	89.649	3.	4.
4	0	28	8	0.427	0.194	89.675	2.	2.
5	3	14	16	0.429	0.194	89.907	1.	1.
5	2	19	16	0.429	0.194	89.915	0.	0.
6	2	0	8	0.429	0.194	89.984	18.	16.
6	2	2	16	0.430	0.194	90.158	14.	14.
6	0	12	8	0.433	0.194	90.512	0.	0.
6	2	4	16	0.434	0.194	90.679	0.	0.
4	2	26	16	0.434	0.194	90.711	3.	4.
6	1	11	16	0.436	0.194	90.945	0.	0.
5	1	22	16	0.436	0.194	90.962	2.	2.

H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
5	4	1	16	0.439	0.194	91.460	0.	0.
4	3	23	16	0.439	0.194	91.485	0.	0.
3	1	32	16	0.440	0.194	91.510	2.	2.
6	2	6	16	0.440	0.194	91.548	1.	1.
5	4	3	16	0.442	0.194	91.807	0.	0.
1	1	36	8	0.442	0.194	91.870	0.	0.
5	4	5	16	0.447	0.194	92.503	0.	0.
5	3	16	16	0.447	0.194	92.514	1.	0.
3	3	28	8	0.447	0.194	92.540	5.	4.
4	4	18	8	0.447	0.194	92.604	6.	5.
6	2	8	16	0.449	0.194	92.766	1.	1.
6	0	14	8	0.449	0.194	92.772	1.	1.
6	1	13	16	0.451	0.194	93.031	1.	1.
3	2	31	16	0.451	0.194	93.070	0.	0.
2	1	35	16	0.451	0.194	93.083	0.	0.
5	2	21	16	0.453	0.194	93.392	0.	0.
5	4	7	16	0.454	0.194	93.547	0.	0.
4	1	29	16	0.455	0.194	93.586	0.	1.
6	2	10	16	0.460	0.194	94.333	8.	6.
2	2	34	8	0.461	0.194	94.384	1.	1.
4	0	30	8	0.463	0.194	94.720	3.	3.
2	0	36	8	0.463	0.194	94.739	6.	6.
5	4	9	16	0.465	0.194	94.941	0.	0.
5	1	24	16	0.465	0.194	94.965	0.	0.
6	0	16	8	0.468	0.194	95.385	4.	3.
4	2	28	16	0.468	0.194	95.411	0.	0.
0	0	38	2	0.469	0.194	95.443	0.	0.
6	1	15	16	0.469	0.194	95.471	0.	0.
5	3	18	16	0.469	0.194	95.476	0.	0.
4	3	25	16	0.470	0.194	95.665	0.	0.
4	4	20	8	0.472	0.194	95.916	5.	6.
6	2	12	16	0.475	0.194	96.252	12.	12.
5	4	11	16	0.479	0.194	96.688	0.	0.
6	3	1	16	0.483	0.194	97.207	0.	0.
5	2	23	16	0.483	0.194	97.232	0.	0.
3	1	34	16	0.483	0.194	97.263	3.	3.
6	3	3	16	0.486	0.194	97.557	0.	0.
3	3	30	8	0.486	0.194	97.601	0.	0.
6	3	5	16	0.491	0.194	98.259	0.	0.
6	1	17	16	0.492	0.194	98.272	0.	0.
1	1	38	8	0.492	0.194	98.329	1.	1.
6	0	18	8	0.492	0.194	98.361	2.	2.
6	2	14	16	0.494	0.194	98.530	1.	1.
3	2	33	16	0.495	0.194	98.662	0.	0.
5	4	13	16	0.496	0.194	98.792	0.	0.
5	3	20	16	0.496	0.194	98.804	0.	0.
4	1	31	16	0.496	0.194	98.831	0.	0.
6	3	7	16	0.500	0.194	99.314	0.	0.
5	1	26	16	0.501	0.194	99.345	11.	12.
2	1	37	16	0.501	0.194	99.379	0.	0.
4	4	22	8	0.503	0.194	99.599	2.	2.
4	0	32	8	0.508	0.194	100.154	1.	1.
4	3	27	16	0.508	0.194	100.228	0.	0.
4	2	30	16	0.511	0.194	100.501	0.	0.
2	2	36	8	0.511	0.194	100.521	2.	2.
6	3	9	16	0.513	0.194	100.725	0.	0.
6	2	16	16	0.517	0.194	101.176	6.	4.
2	0	38	8	0.517	0.194	101.235	0.	0.
5	4	15	16	0.518	0.194	101.263	0.	0.
6	1	19	16	0.519	0.194	101.447	0.	0.
5	2	25	16	0.519	0.194	101.460	0.	0.
6	0	20	8	0.522	0.194	101.715	0.	0.
0	0	40	2	0.527	0.194	102.307	2.	2.
6	3	11	16	0.529	0.194	102.500	0.	0.
5	3	22	16	0.529	0.194	102.518	2.	2.
3	3	32	8	0.534	0.194	103.079	2.	1.
3	1	36	16	0.538	0.194	103.449	0.	0.
4	4	24	8	0.540	0.194	103.681	7.	7.
5	4	17	16	0.544	0.194	104.113	0.	0.
5	1	28	16	0.545	0.194	104.138	10.	9.
6	2	18	16	0.545	0.194	104.205	12.	12.
7	1	0	8	0.548	0.194	104.457	0.	0.
5	5	0	4	0.548	0.194	104.457	1.	1.
4	1	33	16	0.548	0.194	104.512	0.	0.
7	1	2	16	0.550	0.194	104.637	1.	1.
5	5	2	8	0.550	0.194	104.637	2.	2.
6	3	13	16	0.550	0.194	104.645	1.	1.
3	2	35	16	0.550	0.194	104.698	0.	0.
6	1	21	16	0.553	0.194	105.018	1.	1.
7	1	4	16	0.555	0.194	105.176	0.	0.
5	5	4	8	0.555	0.194	105.176	1.	1.
4	3	29	16	0.555	0.194	105.218	0.	0.
1	1	40	8	0.556	0.194	105.256	3.	3.
6	0	22	8	0.558	0.194	105.470	1.	1.
4	2	32	16	0.564	0.194	106.038	3.	5.
4	0	34	8	0.564	0.194	106.045	0.	0.
7	1	6	16	0.564	0.194	106.078	1.	1.
5	5	6	8	0.564	0.194	106.078	0.	0.
5	2	27	16	0.565	0.194	106.113	0.	0.
2	1	39	16	0.565	0.194	106.154	0.	0.
5	3	24	16	0.570	0.194	106.648	0.	0.
2	2	38	8	0.575	0.194	107.146	0.	0.
6	3	15	16	0.576	0.194	107.175	0.	0.
7	1	8	16	0.578	0.194	107.348	4.	4.
5	5	8	8	0.578	0.194	107.348	2.	1.
5	4	19	16	0.578	0.194	107.363	0.	0.
6	4	0	8	0.578	0.194	107.436	1.	1.
6	4	2	16	0.580	0.194	107.618	1.	1.
6	2	20	16	0.581	0.194	107.638	8.	8.
6	4	4	16	0.586	0.194	108.166	2.	2.
4	4	26	8	0.587	0.194	108.200	0.	0.
2	0	40	8	0.587	0.194	108.247	3.	4.
7	2	1	16	0.596	0.194	108.989	0.	0.
7	1	10	16	0.596	0.194	108.994	8.	9.
5	5	10	8	0.596	0.194	108.994	4.	5.
6	1	23	16	0.596	0.194	109.016	0.	0.
3	3	34	8	0.596	0.194	109.049	1.	1.
6	4	6	16	0.597	0.194	109.083	0.	0.
7	2	3	16	0.600	0.194	109.357	0.	0.
5	1	30	16	0.600	0.194	109.403	0.	0.
6	0	24	8	0.603	0.194	109.663	1.	1.
0	0	42	2	0.604	0.194	109.724	1.	1.
7	2	5	16	0.608	0.194	110.096	0.	0.
6	3	17	16	0.608	0.194	110.109	0.	0.
3	1	38	16	0.609	0.194	110.169	3.	4.
6	4	8	16	0.611	0.194	110.375	8.	10.
4	3	31	16	0.615	0.194	110.700	0.	0.
4	1	35	16	0.615	0.194	110.714	0.	0.
7	1	12	16	0.619	0.194	111.029	5.	5.
5	5	12	8	0.619	0.194	111.029	3.	3.
5	4	21	16	0.619	0.194	111.044	0.	0.
7	2	7	16	0.621	0.194	111.210	0.	0.
5	3	26	16	0.622	0.194	111.243	6.	7.
5	2	29	16	0.622	0.194	111.251	0.	0.
3	2	37	16	0.622	0.194	111.279	0.	0.
6	2	22	16	0.625	0.194	111.512	3.	4.
6	4	10	16	0.631	0.194	112.053	1.	1.
4	2	34	16	0.632	0.194	112.108	11.	10.
4	0	36	8	0.637	0.194	112.491	2.	1.
7	2	9	16	0.640	0.194	112.709	0.	0.

H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs	H	K	L	Mult	Hw	ETA/M	2tetha	Icalc	Iobs
1	1	42	8	0.641	0.194	112.798	2.	1.	3	1	40	16	0.705	0.194	117.586	4.	5.
4	4	28	8	0.646	0.194	113.217	2.	1.	0	0	44	2	0.710	0.194	117.898	1.	1.
7	1	14	16	0.649	0.194	113.470	1.	1.	7	3	6	16	0.719	0.194	118.483	1.	1.
5	5	14	8	0.649	0.194	113.470	1.	1.	6	1	27	16	0.719	0.194	118.521	0.	0.
6	3	19	16	0.649	0.194	113.478	0.	0.	3	2	39	16	0.720	0.194	118.565	0.	0.
6	1	25	16	0.650	0.194	113.492	0.	0.	4	4	30	8	0.724	0.194	118.827	2.	2.
2	1	41	16	0.650	0.194	113.549	0.	0.	7	3	10	16	0.769	0.194	121.697	9.	11.
6	4	12	16	0.658	0.194	114.131	0.	0.	6	3	23	16	0.770	0.194	121.721	0.	0.
6	0	26	8	0.661	0.194	114.350	1.	1.	5	1	34	16	0.770	0.194	121.757	1.	2.
2	2	40	8	0.661	0.194	114.399	7.	9.	2	1	43	16	0.771	0.194	121.797	0.	0.
7	2	11	16	0.664	0.194	114.606	0.	0.	6	5	3	16	0.776	0.194	122.100	0.	0.
5	4	23	16	0.672	0.194	115.202	0.	0.	5	3	30	16	0.777	0.194	122.151	0.	0.
5	1	32	16	0.672	0.194	115.229	3.	3.	2	2	42	8	0.783	0.194	122.509	2.	2.
3	3	36	8	0.678	0.194	115.628	0.	0.	6	5	5	16	0.790	0.194	122.924	0.	0.
6	2	24	16	0.681	0.194	115.878	14.	13.	7	2	17	16	0.790	0.194	122.940	0.	0.
2	0	42	8	0.682	0.194	115.942	1.	1.	3	3	38	8	0.792	0.194	123.007	2.	2.
7	1	16	16	0.688	0.194	116.344	1.	1.	6	4	18	16	0.792	0.194	123.045	6.	5.
5	5	16	8	0.688	0.194	116.344	2.	2.	5	2	33	16	0.798	0.194	123.401	0.	0.
5	3	28	16	0.688	0.194	116.373	14.	13.	7	1	20	16	0.801	0.194	123.569	0.	0.
6	4	14	16	0.692	0.194	116.631	3.	3.	5	5	20	8	0.801	0.194	123.569	0.	0.
7	3	0	8	0.693	0.194	116.718	1.	1.	4	3	35	16	0.802	0.194	123.617	0.	0.
4	3	33	16	0.694	0.194	116.777	0.	0.	7	3	12	16	0.809	0.194	123.972	4.	3.
7	3	2	16	0.696	0.194	116.913	3.	2.	6	5	7	16	0.812	0.194	124.176	0.	0.
7	2	13	16	0.696	0.194	116.922	0.	0.	6	1	29	16	0.813	0.194	124.222	0.	0.
5	2	31	16	0.696	0.194	116.965	0.	0.	2	0	44	8	0.820	0.194	124.602	0.	0.
6	3	21	16	0.702	0.194	117.327	1.	1.	4	4	32	8	0.831	0.194	125.183	1.	2.
7	3	4	16	0.704	0.194	117.499	0.	1.	5	4	27	16	0.833	0.194	125.272	0.	0.
4	1	37	16	0.705	0.194	117.573	0.	0.	4	1	39	16	0.833	0.194	125.319	0.	0.


$Tb_2Ba_2Cu_2Ti_2O_{11}$
INTENSITAT (Unitats Arbitràries)
5
30
55
80
105
130
2θ (Graus)