Supplementary material

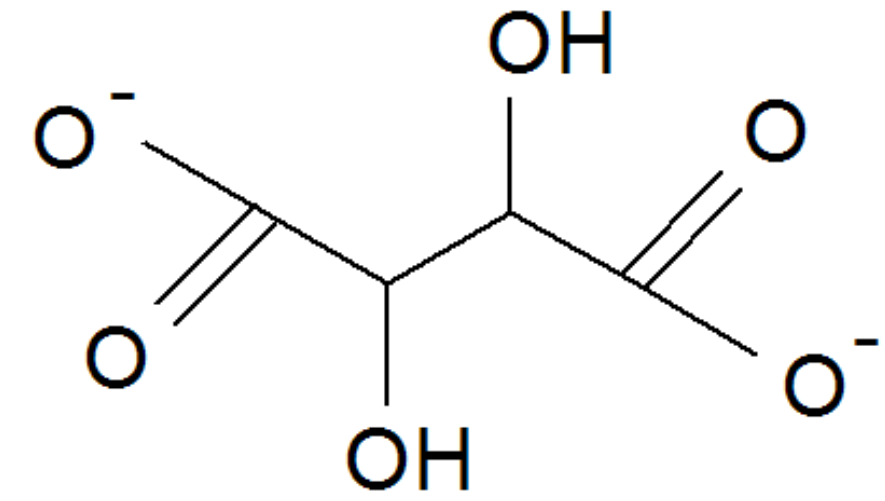
Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	Uiso*/Ueq
Ca1	0.34040(16)	0.19006(12)	0.27379(10)	0.0191(3)
O1	0.3163(6)	-.0233(4)	0.0927(3)	0.0232(7)
O2	1.1726(6)	-.0267(5)	0.3928(4)	0.0273(8)
O3	0.9111(6)	0.0269(4)	0.1676(3)	0.0223(7)
O4	0.6207(6)	0.0217(4)	0.3327(3)	0.0217(7)
O5	0.9267(7)	-.2925(5)	0.3736(4)	0.0301(8)
O6	0.2977(6)	-.2968(5)	0.0343(4)	0.0260(8)
C1	0.9834(8)	-.1508(6)	0.3352(5)	0.0186(9)
C2	0.3817(8)	-.1506(6)	0.1127(5)	0.0194(9)
C3	0.8071(8)	-.1289(6)	0.2081(4)	0.0166(9)
C4	0.5809(8)	-.1332(6)	0.2429(5)	0.0182(9)
OW1	0.6007(6)	0.3134(5)	0.5045(4)	0.0312(9)
OW2	0.1417(6)	0.3464(5)	0.3836(4)	0.0285(8)
OW3	0.6889(7)	0.3761(5)	0.2295(4)	0.0296(8)
OW4	0.1896(7)	0.3524(5)	0.1016(4)	0.0350(9)
H1W1	0.686(12)	0.424(4)	0.540(8)	0.074(10)*
H2W1	0.683(12)	0.244(8)	0.498(9)	0.074(10)*
H1W2	0.118(13)	0.307(11)	0.458(5)	0.074(10)*
H2W2	0.006(9)	0.327(11)	0.317(5)	0.074(10)*
H1W3	0.679(15)	0.347(9)	0.143(4)	0.074(10)*
H2W3	0.758(13)	0.494(4)	0.255(7)	0.074(10)*
H1W4	0.033(5)	0.332(10)	0.068(8)	0.074(10)*
H2W4	0.268(11)	0.462(5)	0.095(9)	0.074(10)*
HC3	0.781(8)	-.210(5)	0.135(4)	0.036(6)*
HC4	0.534(8)	-.210(5)	0.293(4)	0.036(6)*
HO4	0.669(8)	-.003(6)	0.414(3)	0.036(6)*
HO3	0.822(7)	0.015(6)	0.084(3)	0.036(6)*

*B factors common to several H atoms

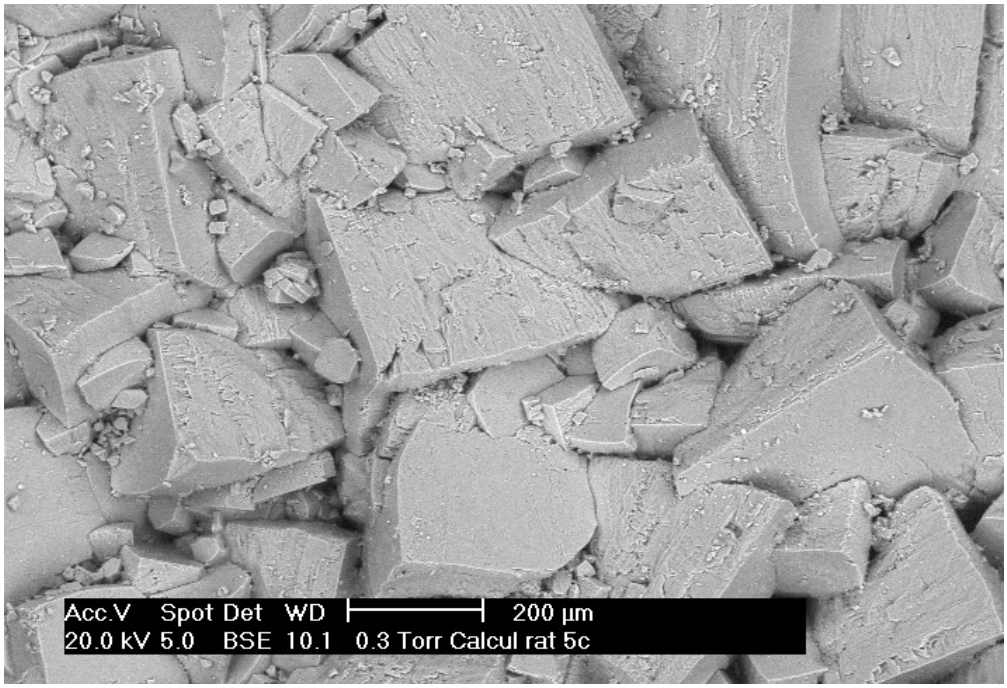
Anisotropic atomic displacement parameters (Å²)

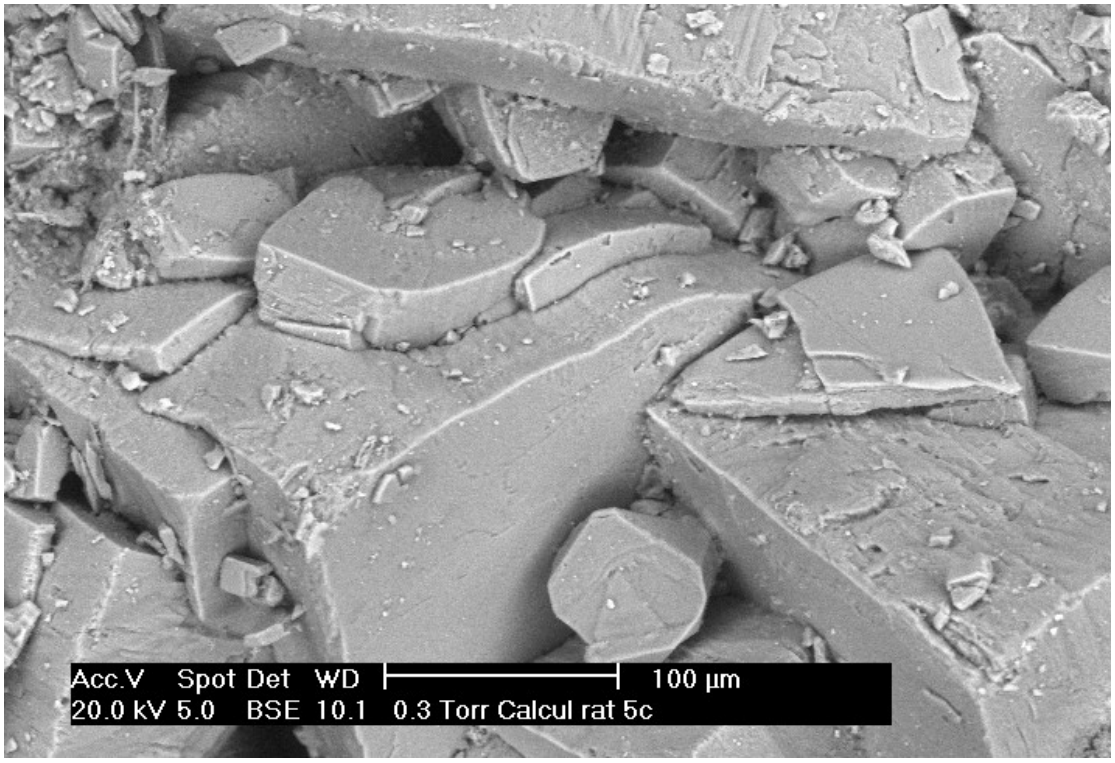
	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0153 (4)	0.0188 (5)	0.0208 (5)	0.0052 (3)	0.0030 (3)	0.0036 (3)
O1	0.0248 (17)	0.0240 (17)	0.0187 (17)	0.0131 (14)	-0.0011 (13)	0.0025 (13)
O2	0.0172 (17)	0.0295 (19)	0.0267 (19)	0.0019 (14)	-0.0011 (14)	0.0113 (15)
O3	0.0155 (16)	0.0246 (17)	0.0221 (18)	0.0019 (13)	0.0020 (13)	0.0120 (14)
O4	0.0228 (17)	0.0256 (17)	0.0179 (17)	0.0123 (14)	0.0043 (14)	0.0018 (14)
O5	0.033 (2)	0.0243 (18)	0.031 (2)	0.0114 (15)	0.0042 (16)	0.0095 (15)
O6	0.0213 (17)	0.0220 (17)	0.0255 (19)	0.0037 (14)	-0.0003 (14)	-0.0043 (14)
C1	0.016 (2)	0.024 (2)	0.016 (2)	0.0100 (17)	0.0026 (17)	0.0011 (18)
C2	0.0121 (19)	0.023 (2)	0.020 (2)	0.0024 (17)	0.0027 (17)	0.0050 (18)
C3	0.017 (2)	0.019 (2)	0.011 (2)	0.0061 (17)	0.0004 (16)	-0.0001 (16)
C4	0.015 (2)	0.018 (2)	0.021 (2)	0.0061 (17)	0.0031 (17)	0.0055 (18)
OW1	0.0249 (19)	0.033 (2)	0.029 (2)	0.0126 (16)	-0.0040 (15)	-0.0030 (17)
OW2	0.0233 (18)	0.034 (2)	0.028 (2)	0.0133 (16)	0.0037 (15)	0.0079 (16)
OW3	0.0300 (19)	0.0250 (18)	0.027 (2)	0.0018 (15)	0.0077 (16)	0.0016 (15)
OW4	0.0238 (19)	0.035 (2)	0.040 (2)	0.0067 (16)	0.0005 (17)	0.0178 (18)

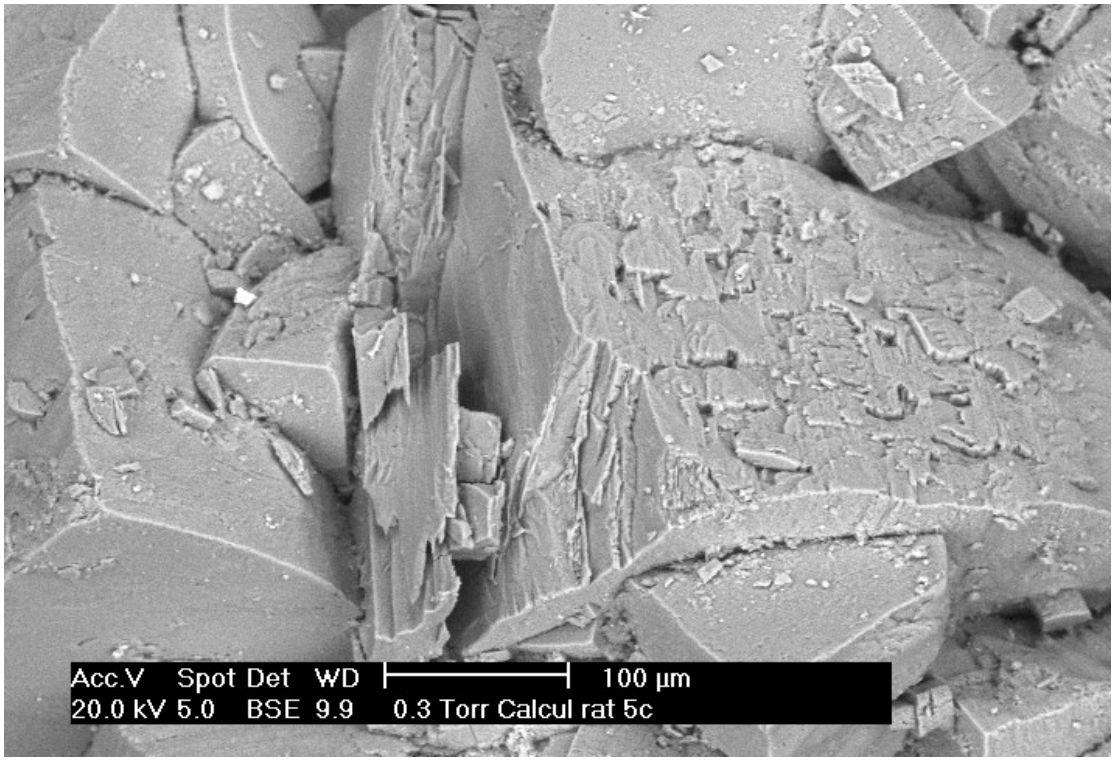


Ca^{2+} $4H_2O$

More views of the interpenetrated crystals forming a calculus inside of the rat kidney.

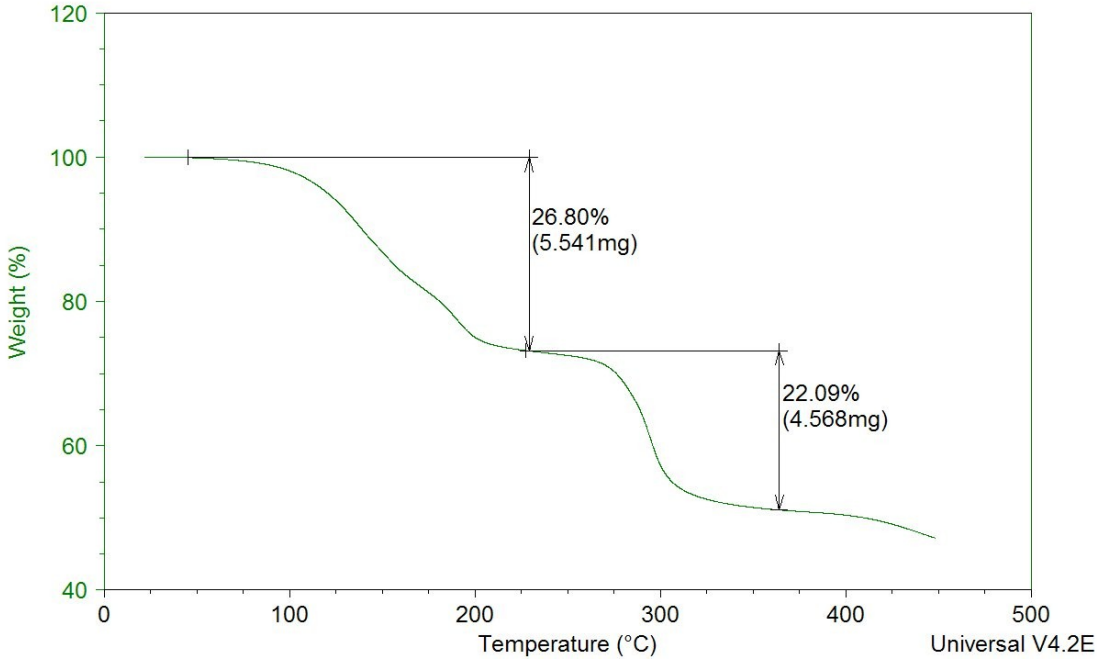





Acc.V Spot Det WD 100 µm
20.0 kV 5.0 BSE 9.9 0.3 Torr Calcul rat 5c

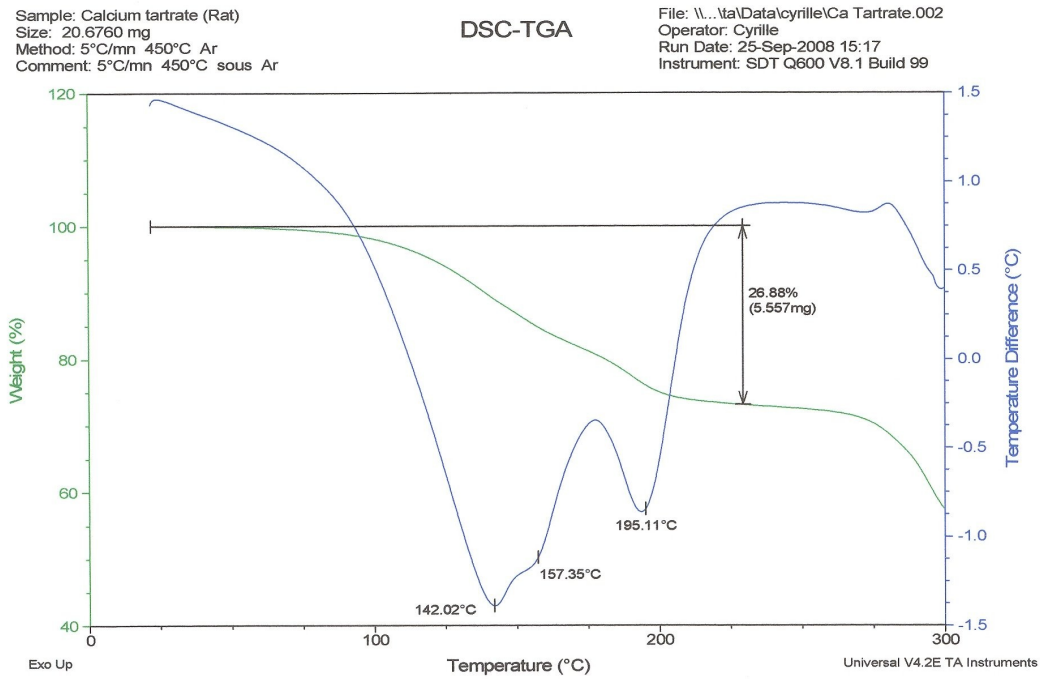
TGA (5°C/mn)

theoretical weight loss for $4H_2O$: 27.7% (water of hydration) ;
for 2C and $2H_2O$: 23.1% (decomposition into calcium oxalate)



TGA/DTA (5°C/mn)

3 peaks at 142, 157 and 195°C are close to the peaks at 149 and 189°C on Fig. 3 in Menahem & Mastai (2008), though they were said to correspond to water loss and decomposition of the anhydrous calcium tartrate into calcium oxalate. In fact, these endothermic peaks occur during the water loss, the decomposition into oxalate is later, in the 230-350°C range.



Peak position extraction by using the EVA-Bruker software

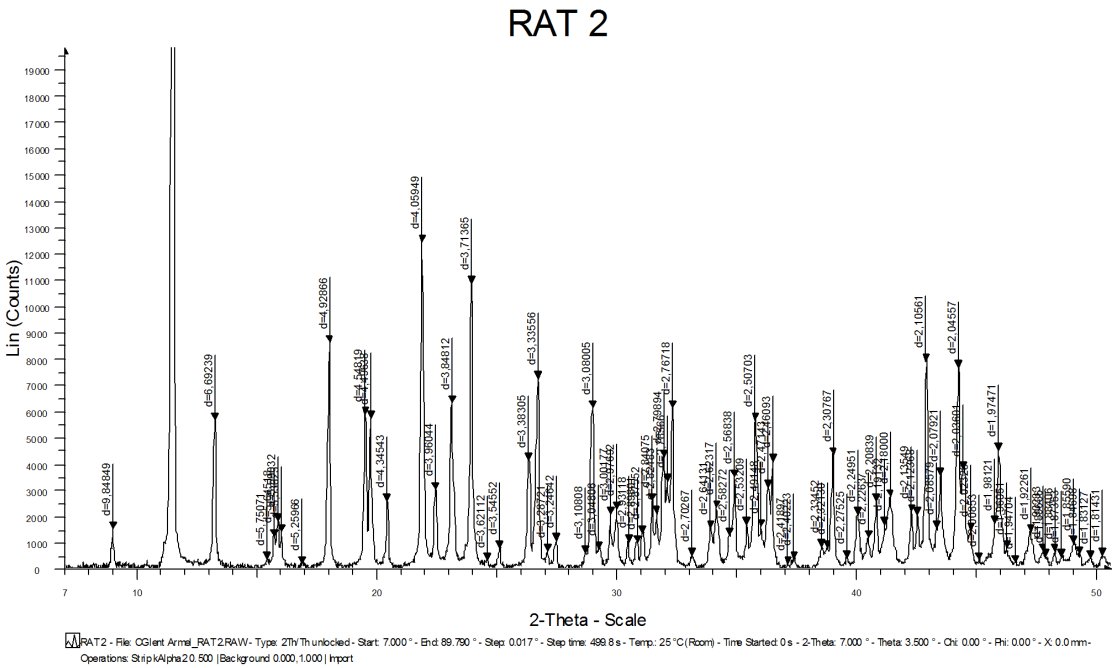
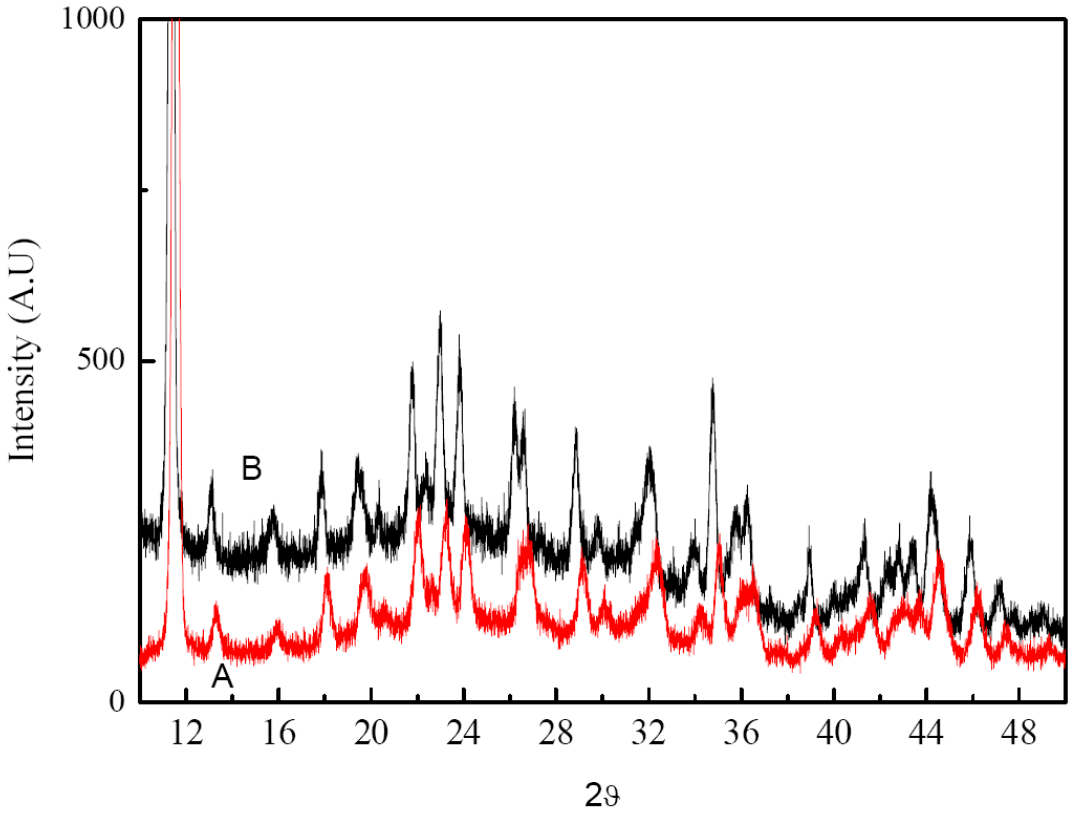
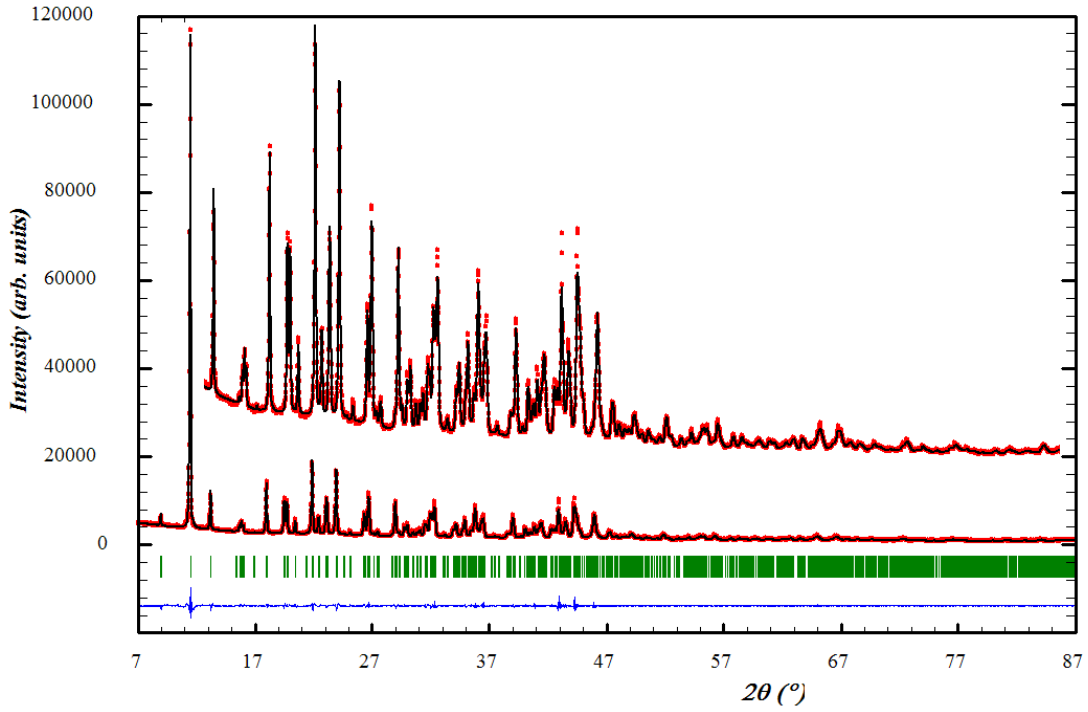


Fig. S2 from *New J. Chem*. **32** (2008) 925-928 : racemic CaT powder patterns from Menahem & Mastai, to be compared to our data above. The fit is obvious in spite of the noisy pattern below.



Powder diffraction pattern, Le Bail fit.



Powder diffraction data, CuKα 1 (after Kα 2 stripping)

2θ obs from peak position extraction by using the EVA - Bruker software

Indexing (McMaille software) :

```
PROGRAM *** CELREF ***  (J.LAUGIER & A.FILHOL 10/78)

OBSERVABLE NUMBER    :    39
ITERATION NUMBER :    10
REFINEMENT CONSTRAINTS : NO
INITIAL VALUES :
   ZERO    LAMBDA      A        B        C      ALPHA     BETA    GAMMA
     1.       0.       1.       1.       1.       1.       1.       1.
  0.000    1.5406   6.2478   8.2204  10.4358   94.908  105.969  107.521
RECIPROCAL CELL :   0.17695  0.12977  0.10140   79.417   71.538   70.193
VOLUME (A**3)  :      483.026

NUMBER OF INDEPENDENT PARAMETERS :     7

FINAL VALUES   : (STANDARD DEVIATIONS : 2nd LINE)

   ZERO    LAMBDA      A        B        C      ALPHA     BETA    GAMMA
 -0.004    1.5406   6.2482   8.2226  10.4385   94.926  105.964  107.508
  0.005    0.0000   0.0014   0.0017   0.0026    0.014    0.013    0.010
RECIPROCAL CELL :   0.17692  0.12974  0.10137   79.404   71.540   70.202
VOLUME (A**3)  :      483.345

   H     K     L  TH(OBS)    TH-ZERO    TH(CALC)     DIFF.

   0     0     1     8.962      8.958      8.957      0.001
   0     1     0    11.474     11.470     11.471      0.000
   0     1    -1    13.209     13.205     13.202      0.004
   1     0    -1    15.386     15.382     15.391     -0.008
   1     0     0    15.675     15.671     15.665      0.006
   0     1     1    15.830     15.826     15.826      0.000
   1    -1     0    15.986     15.982     15.985     -0.003
   0     0     2    17.973     17.969     17.969      0.000
   0     1    -2    19.492     19.488     19.485      0.003
   1    -1     1    19.719     19.715     19.712      0.003
   1     0     1    20.411     20.407     20.416     -0.009
   1    -1    -2    21.867     21.863     21.869     -0.006
   1     1     0    22.421     22.417     22.417      0.000
   1    -2     0    23.084     23.080     23.093     -0.013
   1     1    -2    23.933     23.929     23.923      0.006
   1    -2    -1    24.554     24.550     24.540      0.010
   1    -2     1    25.086     25.082     25.086     -0.004
   0     2     1    26.313     26.309     26.307      0.003
   1     0    -3    26.694     26.690     26.678      0.012
   0     0     3    27.094     27.090     27.095     -0.005
   0     1    -3    27.442     27.438     27.439     -0.001
   2    -1    -1    28.689     28.685     28.673      0.012
   1    -2    -2    28.956     28.952     28.945      0.008
   1     1    -3    29.267     29.263     29.269     -0.006
   2    -1     0    29.729     29.725     29.732     -0.007
   2     0    -1    29.983     29.979     29.982     -0.003
   2    -1    -2    30.462     30.458     30.457      0.001
   1     2    -1    30.819     30.815     30.815      0.000
   2     0    -2    31.066     31.062     31.068     -0.006
   0     1     3    31.457     31.453     31.454     -0.001
   2     0     0    31.639     31.635     31.633      0.002
   2    -2    -1    31.939     31.935     31.938     -0.003
   1     2    -2    32.096     32.092     32.092      0.000
   2    -2     0    32.316     32.312     32.292      0.020
```

```
    1    -3     1    33.902     33.898     33.901     -0.003
    2    -2    -2    34.143     34.139     34.156     -0.017
    2    -1    -3    34.695     34.691     34.689      0.002
    0     3     0    34.895     34.891     34.891      0.000
    2     1    -1    35.412     35.408     35.408      0.000

Figures of Merit :

   M(20) =     61.25
   F(20) =    147.30 (  0.0048,  28)
```

Powder diffraction pattern, CuKα 1 (after Kα 2 stripping)

$2\theta_{obs}$	d_{obs}(Å)	I/Io	h	k	l	$2\theta_{calc}$	d_{calc}(Å)
8.972	9.8485	1.8	0	0	1	8.959	9.8620
11.484	7.6994	100.0	0	1	0	11.474	7.7060
13.219	6.6924	6.8	0	-1	1	13.203	6.7004
15.396	5.75071	0.4	-1	0	1	15.389	5.7529
15.685	5.6452	1.5	1	0	0	15.665	5.6523
15.840	5.5903	2.2	0	1	1	15.833	5.5928
15.996	5.5362	1.7	1	-1	0	15.981	5.5411
16.843	5.2597	0.2	-1	1	1	16.886	5.2463
17.983	4.9287	10.3	0	0	2	17.974	4.9310
19.502	4.5482	7.0	0	-1	2	19.487	4.5515
19.729	4.4964	6.8	1	-1	1	19.710	4.5006
			-1	0	2	19.775	4.4859
20.421	4.3454	3.1	1	0	1	20.419	4.3458
			-1	-1	1	21.340	4.1602
21.877	4.0595	14.8	-1	1	2	21.872	4.0603
22.431	3.9604	3.6	1	1	0	22.422	3.9618
			0	2	0	23.064	3.8530
23.094	3.8481	7.5	1	-2	0	23.092	3.8485
			0	1	2	23.117	3.8444
			0	-2	1	23.166	3.8364
23.943	3.7136	12.9	-1	-1	2	23.925	3.7162
24.564	3.6211	0.4	-1	2	1	24.542	3.6243
25.096	3.5455	1.0	1	-2	1	25.083	3.5472
			1	-1	2	26.224	3.3955
26.323	3.3830	4.9	0	2	1	26.316	3.3838
			0	-2	2	26.585	3.3502
26.704	3.3356	8.6	-1	0	3	26.682	3.3382
			1	1	1	26.753	3.3295
27.104	3.2872	0.8	0	0	3	27.103	3.2873
27.452	3.2464	1.3	0	-1	3	27.443	3.2473
			1	0	2	27.492	3.2417
28.699	3.1081	0.7	-2	1	1	28.667	3.1114
28.966	3.0800	7.3	-1	2	2	28.950	3.0816
			-1	1	3	28.985	3.0780
29.277	3.0481	0.9	-1	-1	3	29.272	3.0485
29.739	3.0018	2.5	2	-1	0	29.727	3.0029
			1	-2	2	29.876	2.9882
29.993	2.9769	2.7	-2	0	1	29.979	2.9781
30.472	2.9312	1.2	-2	1	2	30.453	2.9329
30.829	2.8980	1.2	-1	-2	1	30.822	2.8986
31.076	2.8755	1.6	-2	0	2	31.065	2.8764

31.467	2.8407	3.1	0	1	3	31.466	2.8407
31.649	2.8248	2.5	2	0	0	31.633	2.8262
31.949	2.7989	5.1	-2	2	1	31.932	2.8003
			0	2	2	31.978	2.7964
32.106	2.7857	4.0	-1	-2	2	32.097	2.7864
			1	2	0	32.224	2.7756
32.326	2.7672	7.3	2	-2	0	32.285	2.7705
			0	-2	3	32.352	2.7649
33.119	2.7027	0.6	1	-3	0	33.024	2.7102
			1	1	2	33.164	2.6991
			2	-1	1	33.387	2.6816
33.912	2.6413	1.8	1	-3	1	33.900	2.6421
			1	-1	3	34.072	2.6292
34.153	2.6232	2.8	-2	2	2	34.153	2.6231
			0	-3	1	34.390	2.6056
34.705	2.5827	1.5	-2	0	3	34.659	2.5860
			-1	3	1	34.667	2.5854
			-2	1	3	34.688	2.5839
			-1	0	4	34.755	2.5791
34.905	2.5684	4.2	0	3	0	34.900	2.5687
			2	-2	1	35.142	2.5516
			-1	2	3	35.312	2.5397
35.422	2.5321	2.0	-2	-1	1	35.411	2.5328
			1	0	3	35.651	2.5163
			2	0	1	35.684	2.5140
35.788	2.5070	6.7	-2	-1	2	35.792	2.5067
			-1	-2	3	35.792	2.5067
36.019	2.4915	1.9	1	2	1	36.024	2.4911
			0	-1	4	36.117	2.4848
36.321	2.4714	3.7	-1	-1	4	36.279	2.4741
			0	-3	2	36.306	2.4723
			0	0	4	36.411	2.4655
36.482	2.4609	4.9	1	-2	3	36.475	2.4613
37.137	2.4190	0.2	1	-3	2	37.139	2.4188
			-1	1	4	37.148	2.4182
37.406	2.4022	0.4	2	1	0	37.393	2.4030
			0	3	1	37.750	2.3811
38.533	2.3345	1.0	-2	-1	3	38.476	2.3378
			2	-3	0	38.515	2.3355
			-1	3	2	38.547	2.3336
			-2	2	3	38.555	2.3332
38.761	2.3213	0.9	-2	3	1	38.743	2.3223
38.999	2.3077	5.2	2	-1	2	39.000	2.3076
			0	2	3	39.128	2.3003
39.578	2.2752	0.5	0	-2	4	39.568	2.2757
40.050	2.2495	2.4	2	-2	2	40.035	2.2503
			-2	0	4	40.171	2.2429
			0	-3	3	40.349	2.2335
			0	1	4	40.378	2.2319
40.484	2.2264	1.4	2	-3	1	40.490	2.2260
			-2	1	4	40.705	2.2148
40.828	2.2084	3.1	1	1	3	40.812	2.2092
41.161	2.1913	2.0	-2	3	2	41.143	2.1922
41.385	2.1800	3.3	-1	-2	4	41.346	2.1819
			2	1	1	41.448	2.1768
			2	0	2	41.525	2.1729
			1	2	2	41.653	2.1665
			-1	-3	1	41.744	2.1620
42.288	2.1355	2.6	-1	-3	2	42.246	2.1375
			1	-3	3	42.274	2.1361

42.535	2.1237	2.4	0	3	2	42.538	2.1235
			1	-1	4	42.677	2.1169
42.918	2.1056	9.4	-1	2	4	42.896	2.1066
			-2	-1	4	43.097	2.0972
43.346	2.0858	1.8	1	3	0	43.316	2.0871
43.490	2.0792	4.3	-2	-2	2	43.469	2.0801
			-1	0	5	43.508	2.0783
			-2	-2	1	43.625	2.0730
			-3	1	1	43.641	2.0723
			-3	1	2	43.798	2.0652
44.243	2.0456	9.1	-1	3	3	44.166	2.0489
			1	-4	0	44.190	2.0478
			1	-2	4	44.215	2.0467
			-1	-1	5	44.309	2.0426
44.462	2.0360	4.5	1	-4	1	44.410	2.0382
			2	-3	2	44.422	2.0377
			1	0	4	44.464	2.0358
			-3	2	1	44.488	2.0348
			-2	2	4	44.596	2.0301
44.756	2.0233	1.7	-1	-3	3	44.764	2.0229
45.103	2.0085	0.4	-3	2	2	45.109	2.0082
			0	-1	5	45.271	2.0014
			-2	-2	3	45.314	1.9996
			-2	3	3	45.429	1.9948
			3	-1	0	45.480	1.9927
45.760	1.9812	2.0	-3	0	2	45.746	1.9817
			2	2	0	45.766	1.9809
			3	-2	0	45.842	1.9778
45.919	1.9747	5.4	-3	1	3	45.934	1.9741
			-1	4	1	45.948	1.9735
			-1	1	5	45.972	1.9725
			0	0	5	45.975	1.9724
			2	-1	3	45.979	1.9722
			-3	0	1	46.054	1.9692
			0	-3	4	46.055	1.9691
46.271	1.9605	0.9	0	-4	1	46.285	1.9599
			2	-2	3	46.435	1.9539
46.610	1.9470	0.3	1	-4	2	46.585	1.9480
			1	3	1	46.794	1.9398
			-2	0	5	47.056	1.9296
			0	4	0	47.135	1.9265
			2	1	2	47.139	1.9264
47.238	1.9226	1.6	2	-4	0	47.194	1.9242
			0	2	4	47.248	1.9222