Acta Cryst. (1968). B**24**, 1548

The Crystal and Molecular Structures of Strontium Tartrate Trihydrate and Calcium Tartrate Tetrahydrate*

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(*Received* 15 *May* 1967 *and in revised form* 28 *November* 1967)

Strontium tartrate trihydrate belongs to the monoclinic system with space group $P2_1$. The structure of this compound was solved from a three-dimensional beta synthesis phased on the strontium atom and refined by the full-matrix least-squares method. Calcium tartrate tetrahydrate belongs to the orthorhombic system with the space group $P2_12_12_1$. The structure of this compound was solved by three-dimensional electron density maps and least-squares refinements. The final R indices (for observed structure factors) are 0·109 for strontium tartrate and 0·103 for calcium tartrate. The structures are stabilized by a three-dimensional network of hydrogen bonds. The tartrate ion behaves like a chelating agent towards strontium and calcium. An interesting feature in the structure of calcium tartrate is the large dihedral angle (22°) which the C–O(H) bond makes with the plane of the neighbouring carboxyl group. In both structures the cation exhibits an 8-fold coordination.

Introduction

The determination of the crystal structures of strontium and calcium tartrates forms part of an investigation on the conformation of the tartrate ion in the crystalline state. The first compound to be studied in this series was sodium tartrate dihydrate (Ambady & Kartha, 1968).

Experimental

Strontium tartrate trihydrate

Transparent plate-like crystals of $SrC_4H_4O_6.3H_2O$ were obtained from an aqueous solution of the salt at room temperature. One crystal was chosen and ground into a needle shape with nearly uniform cross section. The crystal data are given below.

$SrC_4H_4O_6.3H_2O$; $M=289·6$

$a=7·55\pm0·02$ Å $b=10·06\pm0·02$ Å

$c=6·47\pm0·02$ Å $\beta=102°0'\pm10'$

$Z=2$ $D_x=2·003$ g.cm^{-3}

D_m (by flotation) 2·028 g.cm^{-3}

μ(Cu $K\alpha$) = 82 cm^{-1}

Space group $P2_1$ (from systematic absences).

Calcium tartrate tetrahydrate

When equal volumes of 0·2N solutions of calcium chloride and Rochelle salt were mixed and kept at room temperature, needle shaped crystals of the tetrahydrate made their appearence (Chattaway, 1916).† The presence of calcium in the crystals was confirmed by flame photometer analysis. The crystal data obtained by the author together with the values reported in a previous determination (Evans, 1936) are given below.

$CaC_4H_4O_6.4H_2O$; $M=260·1$

Present author	Evans
$a=$ 9·24 ± 0·02 Å	9·20 Å
$b=$ 10·63 ± 0·02	10·54
$c=$ 9·66 ± 0·02	9·62
$Z=4$	4
$D_x=1·821$ g.cm^{-3}	
$D_m=1·818$ g.cm^{-3}	1·848 g.cm^{-3}
μ(Cu $K\alpha$) = 67 cm^{-1}	

Space group $P2_12_12_1$ (from systematic absences).

The cell dimensions of both compounds were determined from precession photographs.

Collection of intensity data

Three-dimensional intensity data were collected by the multiple film equi-inclination Weissenberg technique using nickel-filtered copper radiation. Total numbers of reflexions recorded were 887 for strontium tartrate and 903 for calcium tartrate. The intensities were estimated visually, corrected for Lorentz and polarization factors and placed on an absolute scale by Wilson's method. The strontium tartrate data were corrected for absorption assuming the crystal to be a cylinder. Absorption correction was not applied to the calcium tartrate data as μr in this case was less than unity. Initial inter-layer scaling was achieved with the help of the respective cross layer data.

Determination of the structures

Strontium tartrate trihydrate

The x and z coordinates of the strontium atom were readily obtained from the Lp inverse sharpened Patterson function computed with the $h0l$ intensity data.

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* Contribution No. 241 from the Centre of Advanced Study in Physics, University of Madras, Madras–25.

† The author is grateful to Dr J. P. John of the Department of Organic Chemistry, University of Madras for preparing the crystals.

The y coordinate was assumed to be 0·25. The next step was to compute the $h0l$ and $hk0$ beta synthesis (Ramachandran & Raman, 1959). However, both syntheses proved difficult to interpret because of the serious overlap in the $h0l$ map and doubling of peaks due to a spurious mirror in the $hk0$ map. The structure was ultimately solved from a three-dimensional beta synthesis. This type of electron density Fourier synthesis has been successfully applied in the solution of a more complicated structure in this laboratory, namely, that of L-arginine hydrobromide, monohydrate (Mazumdar & Srinivasan, 1966). The beta synthesis uses coefficients of the type

$$(|F_o|^2/|F_{Sr}|)\exp i\alpha_{Sr}$$

where $|F_{Sr}|$ and α_{Sr} are the amplitude and the phase of the structure factor contribution from the heavy atom. Actually the synthesis in its weighted form was computed (Ramachandran & Ramachandra Ayyar, 1963). The weighted coefficients may be expressed as

$$W^2(|F_o|^2/|F_{Sr}|)\exp i\alpha_{Sr}$$

where

$$W=\tanh X \text{ (Woolfson, 1956)}$$

and

$$X=|F_o|\,.\,|F_{Sr}|/\sum_{j=1}^{Q} f_j^2\,.$$

The denominator represents the sum of the scattering factors of all the light atoms. Since there was only one heavy atom in the asymmetric unit, a spurious centre of inversion occurred in the map, resulting in the duplication of peaks. There were also a few strong spurious peaks but practically all of them were located close to the strontium peak. It was possible, however, to locate all but one atom from this map, the average peak heights of oxygen and carbon atoms being 7 e.Å^{-3} and 6 e.Å^{-3} respectively. The remaining atom [in the water molecule O(8)] was located in the second electron density Fourier synthesis computed with phases calculated from twelve out of the thirteen atoms of the asymmetric unit.

In the structure obtained from the beta synthesis, it was observed that the tartrate ion was in the L-configuration. For the sake of uniformity the configuration was changed to the D-form. A solution of the crystals used in this study in dilute hydrochloric acid was found to be dextrorotatory, thereby showing that the compound is the D-tartrate. Examination of the $hk0$ intensity data recorded in a Nonius integrating goniometer revealed a few Bijvoet pairs with measurable intensity differences. In all such cases the observed and calculated values of the ratio $I_H/\bar{I}_H$ were nearly the same, thus agreeing with the classical determination of the absolute configuration of tartaric acid by Bijvoet, Peerdeman & van Bommel (1951).

Calcium tartrate tetrahydrate

The coordinates of the calcium atom were initially obtained from the $h0l$ and $0kl$ Lp inverse sharpened Patterson projections, and later more accurately from a 3-D Patterson synthesis. The new values were

$$x=y=z=0{\cdot}433\,.$$

Minimum functions plotted on $0kl$ and $h0l$ projections did not yield any new information and consequently attempts to solve the structure from projections were abandoned. A 3-D electron density Fourier synthesis ϱ_1 phased on the calcium atom was computed but it was not possible to identify the tartrate ion, as the map contained a large number of peaks of height above 2 e.Å^{-3}. The strategy finally adopted was to sandwich least-squares refinements between successive electron density Fourier syntheses. The thermal parameter of an incorrectly placed atom invariably increased with successive least-squares cycles (Rossmann, Jacobson, Hirshfeld & Lipscomb, 1959). Such atoms are thereafter omitted from succeeding electron density Fourier syntheses. In the present analysis seven of the strongest peaks appearing in ϱ_1 were selected as possible atomic sites and their coordinates were refined through three cycles of least squares. At the end of the third cycle the thermal parameters of two of the atoms had shot up to 6·2 Å^2 and 5·4 Å^2 from the initial value of 2·3 Å^2, while in the case of the rest of the atoms, the thermal parameters were below 3·5 Å^2. These two atoms were removed and a second electron density Fourier synthesis ϱ_2 was computed with the phases from calcium and the remaining five light atoms, the latter being treated as nitrogen atoms. The synthesis revealed the positions of all but two atoms (water molecules) of the asymmetric unit. An electron density difference Fourier synthesis revealed the positions of these two water oxygens also.

Refinement of the structures

The two structures were refined by the full-matrix least-squares method using the *ORFLS* program of Busing, Martin & Levy (1962), the atoms being ascribed individual isotropic thermal parameters. A unit weighting scheme was employed, the unobserved F_o's being given zero weight. Further, a dozen reflexions which showed large discrepancies (due to extinction, misindexing *etc.*) were omitted from the final cycles of refinement. The shifts of the parameters of calcium tartrate were about a tenth of the estimated standard deviations. But in the case of strontium tartrate refinement was stopped when the shifts of the parameters were about half the estimated standard deviations. It was also observed that the thermal parameters of some of the atoms in the structure of strontium tartrate assumed rather low values. This effect could be due to under-correction of the data for absorption (Werner, 1965). Correction based on cylindrical approximation was not satisfactory because of the irregular cross section of the crystal. However, it was better than no correction. Although it is well known that the unit weighting scheme is not suitable for least-squares refinement of photographic data, no further refinements of these two structures were attempted with more appropriate weighting functions, primarily because the two structures appeared to have refined to a reasonable degree of accuracy. The final *R* indices for strontium tartrate and calcium tartrate were 0·109 and 0·103 respectively. The lists of final observed and calculated structure factors for strontium and calcium tartrates are given in Tables 1 and 2 respectively. The final (fractional) coordinates of the atoms with the estimated standard deviations are given in Tables 3 and 4. The intramolecular bond distances are given in Table 5 and the bond angles in Table 6.

The atomic scattering factors for Sr^{2+} given by Thomas & Umeda (1957) were used after including the anomalous dispersion correction for the real part. The atomic scattering factors for O, C and Ca^{2+} were taken from *International Tables for X-ray Crystallography* (1962).

Table 1. *Observed and calculated structure factors for strontium* D-*tartrate*

The columns give *l*, 10|F_o|, 10|F_c| in that order.
The scale factors for layers *k* running from zero to eight are 1·01, 1·03, 1·04, 1·06, 1·03, 1·03, 1·04, 1·01 and 1·02.
Reflexions marked * were omitted from the final refinement.

l	10 F_o	10 F_c
	0 0 l	
1	547	426
2	63	50
3	621	582
4	245	221
5	186	148
	1 0 l	
2	970	1020
3	268	190
4	500	504
5	376	395
6	68	85
7	169	188
	2 0 l	
0	119	148
1	76	66
2	353	377
3	322	354
4	190	177
5	252	293
6	296	340
7	144	196
	3 0 l	
0	159	133
1	521	522
2	179	165
3	61	36
4	333	325
5	161	180
6	97	109
7	170	224
	4 0 l	
0	470	446
1	160	137
2	314	283
3	270	281
4	95	58
5	135	152
6	187	205
	5 0 l	
0	279	255
1	521	502
2	201	209
3	296	276
4	207	226
5	145	138
6	70	79
	6 0 l	
0	266	231
1	40	38
2	355	346
3	154	126
4	0	14
5	229	250
	7 0 l	
0	215	206
1	240	239
2	48	37
3	105	129
4	178	162
	8 0 l	
0	186	195
1	56	48
2	227	203
3	91	103
	9 0 l	
0	357	286
1	202	237
	-1 0 l	
1	555	573
2	126	66
*3	596	464
5	278	282
6	175	184
7	117	130
8	166	204
	-2 0 l	
*1	709	568
2	350	308
3	366	419
4	228	236
5	33	52
6	392	427
7	296	318
	-3 0 l	
1	327	281
*2	791	560
3	364	323
4	461	440
5	318	281
6	332	363
	-3 0 l	
7	84	77
8	88	129
	-4 0 l	
1	700	668
2	104	78
3	259	243
4	428	433
5	153	102
7	203	263
8	38	64
	-5 0 l	
1	105	55
2	565	545
3	195	174
4	150	86
5	222	244
	-6 0 l	
1	301	268
2	228	196
3	169	160
4	193	174
5	102	97
6	173	171
7	198	263
	-7 0 l	
2	293	259
3	290	291
5	296	309
6	201	215
	-8 0 l	
1	405	430
2	196	174
4	215	248
5	205	207
	-9 0 l	
1	159	125
2	167	153
3	193	180
4	164	135
	0 1 l	
1	330	386
2	545	544
3	154	138
4	302	250
5	310	399
6	77	64
7	111	122
8	249	281
	1 1 l	
0	411	490
1	586	668
2	507	458
3	461	483
4	195	215
5	126	143
6	220	248
7	158	169
	2 1 l	
0	236	108
1	410	435
2	678	708
3	103	83
4	323	298
5	358	350
6	52	92
7	229	214
	3 1 l	
0	495	490
1	87	43
2	355	359
3	318	324
4	256	201
5	158	152
6	239	286
7	150	141
	4 1 l	
0	347	394
1	643	610
2	194	146
3	99	82
4	396	421
5	110	139
	5 1 l	
0	481	465
1	145	72
2	215	176
3	456	423
4	54	89
5	171	177
6	225	241
	6 1 l	
0	438	401
1	387	357
2	158	145
3	218	169
4	252	265
5	97	106
	7 1 l	
0	269	226
1	229	220
2	332	305
3	224	237
4	95	73
	8 1 l	
0	271	254
1	196	147
3	243	222
	9 1 l	
0	51	45
1	147	98
	-1 1 l	
1	523	542
2	497	488
3	611	600
4	390	369
5	74	56
6	292	336
7	201	219
8	43	68
	-2 1 l	
1	390	436
2	662	648
3	317	267
4	195	204
5	421	407
6	176	155
7	49	68
8	272	268
	-3 1 l	
1	583	609
2	251	291
3	389	352
5	54	31
6	264	266
7	231	268
8	116	134
	-4 1 l	
1	461	417
2	570	503
3	264	261
4	211	164
5	395	413
6	216	206
8	184	198
	-5 1 l	
1	417	404
2	85	97
3	197	212
4	379	381
5	208	222
6	127	134
	-6 1 l	
2	374	333
3	442	393
5	216	222
6	306	311
	-7 1 l	
1	292	271
2	300	263
3	156	186
4	222	233
5	169	179
	-8 1 l	
2	123	125
3	275	288
5	44	94
	-9 1 l	
1	261	225
2	239	173
4	312	229
	0 2 l	
1	216	208
2	297	286
3	720	754
4	439	467
6	202	259
7	140	185
	1 2 l	
*0	352	632
1	496	495
2	425	428
3	73	72
4	465	456
5	378	436
6	121	150
7	120	154
	2 2 l	
0	530	584
1	166	255
2	431	458
3	441	478
4	153	186
5	122	159
6	209	282
7	111	154
	3 2 l	
0	183	250
1	544	554
2	367	345
3	188	188
4	345	395
5	239	285
6	57	72
7	116	179
	4 2 l	
0	410	288
1	57	65
2	420	407
3	345	367
4	114	125
5	182	203
6	181	230
	5 2 l	
0	247	275
1	377	370
2	224	153
3	220	226
4	244	254
5	160	176
	6 2 l	
0	269	182
1	67	94
2	392	373
3	202	196
4	53	33
5	190	189
	7 2 l	
0	266	216
1	321	285
3	157	149
4	167	201
	8 2 l	
0	136	128
1	178	156
3	323	289
	9 2 l	
0	259	210
1	171	165
	-1 2 l	
1	499	594
2	638	564
3	409	324
4	290	300
5	361	350
6	199	209
7	99	140
8	121	187
	-2 2 l	
1	495	541
2	218	119
3	693	625
4	506	436
5	92	106
6	200	213
7	177	239
	-3 2 l	
1	431	414
2	589	539
3	337	325
4	179	154
5	266	240
6	223	255
8	146	189
	-4 2 l	
1	400	397
2	134	134
3	304	260
4	450	383
5	173	149
6	120	151
7	223	268
	-5 2 l	
1	0	6
2	461	413
3	274	262
4	124	67
5	330	323
6	202	227
	-6 2 l	
1	379	304
2	67	68
3	306	263
4	388	363
5	191	185
6	78	88
7	203	205
	-7 2 l	
2	427	332
3	302	286
4	107	92
5	282	257
6	267	228
	-8 2 l	
1	317	292
2	145	135
3	145	107
4	243	287
5	264	253
	-9 2 l	
1	43	59
2	196	190
3	236	234
4	175	156
	0 3 l	
1	448	204
2	401	395
3	127	58
4	434	344
5	468	414
6	97	106
7	180	202
	1 3 l	
0	396	510
1	336	283
2	252	203
3	332	242
4	255	212
5	133	142
6	251	282
7	123	165
	2 3 l	
0	228	221
1	690	829
2	426	460
3	118	166
4	271	264
5	205	209
7	141	171
	3 3 l	
0	500	545
1	222	126
2	437	442
3	566	620
4	159	188
5	129	120
6	183	217
	4 3 l	
0	237	209
1	454	458
2	263	233
3	209	199
4	386	380
5	249	255
	5 3 l	
0	343	299
1	51	91
2	315	293
3	276	272
4	48	60
5	211	224
	6 3 l	
0	311	298
1	310	318
2	52	82
3	153	170
4	297	295
5	105	107
	7 3 l	
0	206	195
1	198	163
2	286	272
3	176	202
	7 3 l	
4	123	96
	8 3 l	
0	246	250
1	248	217
	9 3 l	
0	98	66
	-1 3 l	
1	548	602
2	583	495
3	730	684
4	431	495
5	159	133
6	271	300
7	226	280
8	39	52
	-2 3 l	
1	569	549
2	787	795
3	184	195
4	343	269
5	401	426
6	160	177
8	142	208
	-3 3 l	
1	396	412
3	396	335
4	347	345
5	137	152
6	184	222
7	181	223
8	71	89
	-4 3 l	
1	177	137
2	428	410
3	278	271
4	134	109
5	373	355
6	259	268
	-5 3 l	
1	267	318
2	137	114
3	409	384
4	448	445
5	212	215
6	136	126
7	195	235
	-6 3 l	
1	177	158
2	451	397
3	457	428
4	123	120
5	153	192
6	255	247
	-7 3 l	
1	406	395
2	260	221
4	226	261
5	164	160
	-8 3 l	
1	138	114
2	159	152
3	220	226
4	39	55
5	141	133
	-9 3 l	
1	208	196
2	191	160
3	61	53
	0 4 l	
0	471	419
1	613	664
2	267	333
3	240	386
4	280	283
6	335	327
7	223	207
	1 4 l	
0	181	302
1	665	779
2	370	327
3	40	40
4	303	300
5	306	330
6	109	99
	2 4 l	
0	617	751
1	134	122
2	228	236
3	472	457
	2 4 l	
4	66	45
5	163	175
6	320	335
7	164	158
	3 4 l	
0	296	279
1	316	321
2	465	409
3	171	153
4	232	270
5	217	236
6	51	79
	4 4 l	
0	453	456
1	140	143
2	298	289
3	235	242
4	113	137
5	190	215
6	222	239
	5 4 l	
0	382	551
1	391	382
2	172	166
3	115	100
4	247	274
5	167	172
	6 4 l	
0	271	255
1	93	70
2	261	270
3	187	197
	7 4 l	
0	242	200
1	286	282
2	81	72
3	193	151
	8 4 l	
0	194	157
1	151	112
2	242	207
	9 4 l	
0	304	228
	-1 4 l	
1	322	293
2	691	673
3	274	217
4	353	341
5	300	287
6	153	152
7	163	170
	-2 4 l	
1	567	514
2	117	105
3	325	299
4	364	339
5	157	152
6	173	206
7	252	296
	-3 4 l	
1	361	353
2	456	426
3	311	201
4	193	143
5	438	408
6	214	210
	-4 4 l	
1	421	473
2	277	224
3	335	284
4	370	318
	-5 4 l	
3	361	340
4	200	186
5	218	230
6	188	219
	-6 1 l	
1	486	425
2	93	77
3	115	80
4	228	302
5	85	95
6	132	126
	-7 4 l	
2	293	315
3	210	210
	-7 4 l	
4	83	54
5	264	199
6	286	252
	-8 4 l	
1	253	250
2	284	239
3	74	86
4	277	216
5	234	177
	-9 4 l	
1	147	95
2	173	141
3	301	237
	0 5 l	
1	511	566
2	483	460
3	188	184
4	318	292
5	227	287
6	117	122
7	125	152
	1 5 l	
*0	425	563
1	269	305
2	302	263
3	492	421
4	330	307
5	173	151
6	219	256
7	150	165
	2 5 l	
0	153	203
1	443	474
2	186	176
4	396	405
5	218	260
7	104	117
	3 5 l	
0	357	460
1	152	130
2	167	170
3	332	360
4	103	95
5	202	224
6	255	261
	4 5 l	
0	255	184
1	223	358
2	298	272
3	127	115
4	177	188
5	215	199
	5 5 l	
0	405	352
2	411	383
3	171	178
4	108	100
5	217	192
	6 5 l	
0	312	261
1	400	368
2	174	135
3	160	167
4	310	237
	7 5 l	
0	96	101
1	89	105
2	324	261
3	206	163
	8 5 l	
0	218	204
1	226	194
	-1 5 l	
1	307	273
2	162	61
3	341	317
4	304	294
5	72	66
6	179	210
7	176	238
	-2 5 l	
1	318	275
2	476	444
3	216	190
4	214	137
5	329	190
6	124	112
7	106	124
	-3 5 l	
1	409	448
3	450	409
4	284	267
5	125	100
6	208	256
7	252	259
8	88	75
	-4 5 l	
1	177	125
2	521	492
3	320	286
4	72	83
5	249	255
6	217	263
	-5 5 l	
1	470	426
2	233	227
3	285	243
4	250	257
5	128	124
6	109	141
7	184	235
	-6 5 l	
1	103	50
2	233	212
3	171	223
4	69	60
5	188	215
6	224	223
	-7 5 l	
1	275	275
2	118	118
3	63	68
4	259	287
5	225	181
	-8 5 l	
1	53	66
2	294	222
3	315	226
4	164	115
	0 6 l	
0	311	309
1	377	390
2	313	260
3	367	381
4	234	283
5	69	40
6	216	252
7	201	191
	1 6 l	
0	133	78
1	491	507
2	482	457
3	131	91
4	263	233
5	254	263
6	111	54
	2 6 l	
0	342	332
1	157	151
2	290	290
3	472	467
4	196	189
5	130	84
6	251	265
	3 6 l	
0	275	257
1	300	300
2	296	241
3	57	91
4	229	239
5	213	234
	4 6 l	
0	393	351
1	198	151
2	311	335
3	312	337
4	75	93
5	118	138
	5 6 l	
0	301	224
1	325	293
2	125	112
3	155	123
4	304	327
	6 6 l	
0	188	181
1	168	138
2	222	223
3	275	239
	7 6 l	
0	208	199
1	243	216
2	76	46
	8 6 l	
0	94	103
1	134	105
	-1 6 l	
1	267	269
2	435	463
3	115	75
4	240	252
5	290	336
6	119	137
7	102	101
	-2 6 l	
1	195	201
2	191	130
3	316	310
4	353	386
5	70	47
6	174	174
7	229	217
	-3 6 l	
1	294	224
2	391	382
3	264	261
4	134	129
5	382	417
6	169	170
7	24	48
	-4 6 l	
1	376	366
2	55	54
3	360	344
4	356	396
5	133	137
6	89	121
	-5 6 l	
1	246	228
2	247	270
3	247	300
5	176	196
6	208	209
	-6 6 l	
1	259	317
2	128	109
3	143	137
4	242	307
5	160	171
6	73	61
	-7 6 l	
2	251	253
3	261	246
4	45	58
5	116	117
	-8 6 l	
1	201	195
2	243	207
3	104	81
4	218	200
	0 7 l	
1	449	469
2	331	310
3	131	160
4	302	256
5	263	285
6	82	87
	1 7 l	
0	376	450
1	140	155
2	161	149
3	417	400
4	232	252
5	124	140
6	197	218
	2 7 l	
0	215	180
1	348	357
2	255	240
3	88	103
4	267	276
5	200	213
	3 7 l	
0	326	343
1	113	111
2	366	343
3	328	329
4	120	139
5	156	159
	4 7 l	
0	193	143
	4 7 l	
1	341	316
2	198	210
3	136	137
4	328	252
5	209	176
	5 7 l	
0	188	165
1	69	78
2	305	313
3	193	186
	6 7 l	
0	122	121
1	251	257
2	94	83
3	186	157
	7 7 l	
0	148	129
1	126	81
2	223	225
	-1 7 l	
1	122	155
2	94	95
3	392	364
4	302	271
5	89	80
6	195	201
	-2 7 l	
1	263	230
2	416	410
3	254	261
4	160	166
5	264	266
6	220	212
7	151	131
	-3 7 l	
1	329	331
2	69	10
3	348	330
4	222	241
5	92	92
6	150	135
	-4 7 l	
1	173	103
2	345	327
3	191	198
4	68	69
5	215	199
6	203	210
	-5 7 l	
1	291	300
2	99	93
3	228	256
4	229	276
5	145	117
6	106	103
	-6 7 l	
1	101	105
2	247	281
3	204	205
4	46	52
	-7 7 l	
1	290	158
2	163	101
3	113	55
4	300	140
	-8 7 l	
2	175	185
	0 8 l	
0	282	266
1	149	147
2	133	132
3	336	299
4	163	185
5	89	98
6	223	217
	1 8 l	
0	66	67
1	183	170
2	331	317
3	99	84
4	140	178
5	230	226
	2 8 l	
0	350	369
1	327	310
2	220	189
	2 8 l	
3	199	226
4	144	140
5	77	101
	3 8 l	
0	203	152
1	418	408
2	187	189
4	290	246
5	171	182
	4 8 l	
0	353	369
1	100	68
2	178	178
3	255	271
	5 8 l	
0	183	203
1	241	281
2	230	163
3	44	67
	6 8 l	
0	245	220
1	117	117
2	191	184
	7 8 l	
1	308	269
2	228	217
	-1 8 l	
1	384	365
2	428	415
3	54	69
4	159	171
5	258	319
6	38	59
	-2 8 l	
1	391	369
2	131	114
3	289	274
4	238	235
6	211	209
	-3 8 l	
1	228	219
2	328	320
3	229	245
4	115	104
5	243	233
6	121	138
	-4 8 l	
1	318	338
3	118	125
4	230	275
6	99	189
	-5 8 l	
1	80	81
2	245	251
3	199	178
5	263	211
	-6 8 l	
1	259	273

Table 2. *Observed and calculated structure factors for calcium tartrate tetrahydrate*

The columns give l, $10|F_o|$, $10|F_c|$ in that order.
The scale factors for the layers k running from zero to eight are 0·95, 0·84, 1·21, 0·92, 0·90, 0·91, 0·93, 0·88 and 0·96.

l	$10\ F_o$	$10\ F_c$
	0 0 1	
2	842	921
4	400	365
6	91	65
8	205	137
0	225	185
2	185	153
	0 1 1	
1	493	584
2	180	164
3	745	809
4	786	753
8	250	187
10	260	265
12	185	166
	0 2 1	
0	598	763
1	167	158
2	169	173
3	42	29
4	428	399
5	426	378
6	345	295
7	103	54
8	134	115
9	170	140
10	52	30
11	205	179
12	75	48
	0 3 1	
1	348	350
2	246	188
3	184	166
4	156	104
5	61	29
6	103	56
7	148	154
8	233	223
9	396	413
10	72	68
12	36	45
	0 4 1	
0	44	26
1	654	678
2	66	55
3	673	663
4	83	63
5	554	473
7	242	213
8	194	177
9	217	136
10	94	94
11	142	135
	0 5 1	
1	479	445
2	319	289
3	101	65
4	361	345
5	185	173
6	128	93
7	134	115
8	191	177
9	314	309
10	170	155
	0 6 1	
0	426	389
2	328	246
3	131	140
4	317	259
5	313	312
6	155	127
8	205	187
	0 7 1	
1	506	490
4	415	453
5	155	158
6	210	193
8	74	110
10	108	125
	0 8 1	
0	518	551
3	171	129
4	174	131
5	130	119
6	174	179
7	130	114
8	175	205
	0 9 1	
1	340	318
2	236	223
4	249	246
5	244	245
6	105	76
7	230	247
	0 10 1	
0	206	104
2	171	171
3	189	208
4	152	150
5	249	228
	0 11 1	
1	250	253
2	105	68
3	168	156
4	113	65
	0 12 1	
0	113	90
3	145	154
5	138	139
	0 13 1	
1	161	148
2	274	217
	1 0 1	
1	470	599
2	21	36
3	1175	986
4	389	339
5	681	675
6	175	187
7	240	226
8	60	100
9	143	142
11	52	64
	1 1 1	
0	105	183
1	201	161
2	311	262
3	110	139
4	208	185
5	207	211
6	240	220
7	201	201
8	110	125
9	272	283
	1 2 1	
0	370	388
1	331	359
2	227	165
3	481	475
4	136	89
5	363	322
6	129	113
7	181	125
8	214	215
9	227	227
10	92	100
11	123	115
12	93	105
	1 3 1	
0	519	500
1	194	210
2	136	116
3	149	119
4	571	550
5	102	66
6	279	268
7	151	167
8	129	131
9	143	153
10	131	138
11	47	98
12	106	148
	1 4 1	
0	1107	1189
1	359	363
2	177	194
3	149	168
4	168	169
5	298	316
6	263	364
7	206	222
8	177	181
9	110	121
10	50	72
	1 5 1	
0	207	250
1	302	353
2	345	381
3	201	192
4	457	440
5	237	202
6	62	80
7	191	187
8	145	155
9	105	103
10	151	163
11	77	69
	1 6 1	
0	425	405
1	34	29
2	175	153
3	259	231
4	246	235
5	146	193
6	65	94
7	145	137
8	89	103
9	56	73
10	68	84
11	91	127
	1 7 1	
0	272	255
1	246	249
2	98	74
3	158	116
4	137	143
5	127	144
6	129	121
7	164	174
8	84	97
9	181	194
	1 8 1	
1	245	233
2	61	70
3	342	294
5	200	167
7	84	101
8	143	152
9	108	103
	1 9 1	
1	250	250
2	286	268
3	92	95
4	215	243
5	153	131
6	147	132
7	108	104
8	138	131
9	98	86
	1 10 1	
0	159	198
1	92	127
2	130	130
6	52	78
8	131	150
	1 11 1	
1	105	122
2	18	68
4	121	143
5	68	79
6	104	96
7	54	65
	1 12 1	
0	111	113
2	135	108
3	126	110
4	106	119
5	108	109
	1 13 1	
0	98	67
1	262	227
2	128	91
	2 0 1	
0	196	213
1	460	468
2	98	84
4	848	947
6	930	1002
7	340	372
8	466	458
9	263	279
10	104	109
	2 1 1	
0	382	451
1	246	238
2	223	200
3	906	953
4	414	388
5	153	136
6	73	61
7	206	184
8	203	207
9	220	271
10	189	228
11	214	234
12	238	225
	2 2 1	
0	496	429
1	377	384
2	255	243
3	293	309
4	428	472
5	165	170
6	95	51
7	343	334
8	310	332
9	165	154
10	185	195
11	213	231
12	210	201
	2 3 1	
0	750	796
1	705	736
2	310	269
3	322	316
4	200	152
5	243	250
6	279	301
7	342	262
8	275	248
9	200	178
10	81	56
	2 4 1	
0	363	353
1	431	429
2	703	604
3	800	743
4	281	273
5	313	275
6	230	231
7	200	186
9	192	207
10	195	223
11	193	193
	2 5 1	
0	435	426
1	343	231
2	438	397
4	423	371
5	411	397
6	267	213
7	235	279
8	298	265
9	103	120
11	153	135
	2 6 1	
0	90	121
1	284	222
2	139	58
3	173	150
4	185	184
5	250	237
6	203	171
7	235	164
8	250	246
9	226	220
10	117	148
	2 7 1	
0	243	244
1	255	238
2	104	122
3	337	286
4	195	180
5	299	273
6	165	154
7	195	205
8	108	98
9	128	112
10	174	183
	2 8 1	
0	132	169
1	157	183
2	292	252
3	162	151
4	235	258
5	203	148
6	195	199
7	215	208
8	104	119
9	269	247
	2 9 1	
0	275	259
1	445	442
2	275	268
3	235	232
4	275	272
5	111	107
6	250	221
7	235	238
8	275	235
9	128	97
	2 10 1	
0	203	194
2	203	232
3	229	246
4	380	354
6	161	158
7	73	83
8	168	153
	2 11 1	
0	215	218
1	154	111
3	174	145
5	148	135
6	267	217
7	215	283
	2 12 1	
1	203	231
2	211	165
3	82	104
4	103	113
5	153	162
	2 13 1	
0	107	78
1	143	106
2	156	179
3	105	92
	3 0 1	
1	346	313
2	338	311
3	584	610
4	449	369
5	93	73
6	306	291
8	188	163
9	101	113
10	106	148
11	121	133
12	231	257
	3 1 1	
0	358	353
1	338	308
2	416	435
3	211	182
4	414	368
5	134	96
6	196	185
7	160	174
8	293	296
10	90	91
11	103	120
	3 2 1	
0	407	378
1	614	633
2	372	339
3	133	111
4	280	245
5	266	205
6	239	254
7	209	214
8	146	138
9	50	41
11	59	63
	3 3 1	
0	350	341
1	84	71
2	161	160
3	664	724
4	93	69
5	392	354
6	133	151
7	82	114
8	146	98
10	81	89
11	109	112
	3 4 1	
0	58	56
1	576	609
2	158	146
3	110	117
4	461	461
5	148	153
6	206	217
7	249	283
8	166	179
9	110	108
	3 5 1	
0	276	289
1	109	147
2	310	333
3	488	485
4	128	107
5	202	166
6	116	87
7	145	149
8	141	181
11	116	141
	3 6 1	
0	220	189
1	388	418
2	174	177
3	106	95
4	280	280
5	116	101
6	169	150
7	144	119
8	193	168
10	136	146
	3 7 1	
0	343	353
1	134	105
2	241	218
3	113	94
4	144	100
6	207	195
7	195	197
8	218	212
9	84	87
10	80	68
	3 8 1	
2	144	143
3	146	161
4	215	215
5	205	224
6	179	171
7	164	157
9	125	126
	3 9 1	
0	254	254
1	223	219
2	254	243
3	167	179
4	141	175
5	210	241
6	73	75
7	64	96
8	127	111
	3 10 1	
1	201	201
2	113	97
3	136	101
7	152	160
	3 11 1	
1	102	86
3	170	154
5	113	119
	3 12 1	
1	122	131
2	131	127
3	109	110
4	124	153
	3 13 1	
0	216	221
1	116	96
2	131	151
	4 0 1	
0	637	611
1	768	850
2	513	519
3	94	93
4	115	107
5	189	132
6	115	88
7	415	439
8	66	93
9	86	71
10	75	96
	4 1 1	
0	122	82
1	436	416
2	98	85
3	617	624
4	65	46
5	329	297
6	81	31
7	86	114
8	154	172
9	86	84
10	127	128
11	173	165
	4 2 1	
0	217	106
1	706	761
2	439	407
3	246	234
4	206	125
5	188	137
6	220	196
7	152	144
8	86	89
10	69	99
11	44	36
	4 3 1	
0	529	510
1	182	134
2	498	482
3	115	97
4	125	118
6	122	85
7	222	222
8	233	251
10	141	143
11	70	64
	4 4 1	
0	107	45
1	111	90
2	242	211
3	159	134
4	441	456
5	114	96
6	270	240
7	115	127
8	213	212
10	63	99
	4 5 1	
0	213	162
1	215	174
2	339	329
3	199	186
4	114	81
6	219	164
8	205	169
10	56	66
	4 6 1	
1	379	359
2	331	309
4	149	158
5	86	51
6	126	157
7	221	211
8	75	84
9	114	129
	4 7 1	
0	245	210
1	81	111
3	361	383
5	213	192
9	93	87
	4 8 1	
1	320	301
3	125	105
4	155	153
7	139	171
	4 9 1	
0	304	356
2	259	270
3	194	206
4	81	104
5	213	204
7	62	77
8	76	121
	4 10 1	
2	164	163
4	228	206
6	199	167
	4 11 1	
0	232	238
2	125	126
3	63	83
4	56	51
6	110	118
	4 12 1	
1	81	88
4	118	170
	5 0 1	
1	79	97
2	365	411
3	96	121
4	551	554
6	219	253
7	103	99
8	59	42
10	79	96
11	129	154
	5 1 1	
0	330	360
1	236	241
2	223	195
3	96	108
4	167	136
5	221	204
6	56	77
7	146	158
8	219	258
10	91	121
11	79	53
	5 2 1	
0	163	145
1	208	172
2	284	292
3	154	141
4	312	272
5	205	214
6	136	166
7	237	239
8	156	169
9	74	60
10	76	77
	5 3 1	
0	275	247
1	58	49
2	256	251
3	337	340
4	218	197
5	258	233
6	77	78
8	99	87
9	68	88
10	133	120
	5 4 1	
0	248	215
1	382	353
2	154	127
3	214	186
4	160	146
5	129	132
6	146	135
7	268	308
8	142	159
9	170	166
10	126	135
	5 5 1	
2	52	40
3	226	238
5	139	175
6	171	172
7	129	164
8	178	170
9	63	70
10	100	105
	5 6 1	
0	52	38
1	298	270
2	304	256
3	275	248
4	313	316
5	159	159
6	213	223
7	137	145
8	48	89
	5 7 1	
0	314	332
1	131	110
2	202	175
3	203	196
4	103	126
5	156	176
6	133	134
7	234	200
8	166	164
	5 8 1	
1	159	162
2	159	172
3	116	108
4	138	172
7	76	78
8	93	89
	5 9 1	
0	131	150
1	81	66
2	99	103
3	150	181
5	131	156
6	186	163
	5 10 1	
0	52	23
1	121	152
2	196	196
3	87	90
4	81	78
6	74	63
	5 11 1	
0	91	90
1	91	70
2	120	103
3	190	174
4	87	70
5	109	121
	5 12 1	
0	32	63
1	144	151
2	116	123
	6 0 1	
0	79	56
1	367	319
2	227	194
3	35	58
4	262	254
5	223	219
6	102	95
7	196	210
8	113	125
9	183	193
10	106	114
	6 1 1	
0	167	179
1	308	292
2	235	206
3	30	39
4	326	370
5	144	108
6	92	103
7	103	97
8	87	82
9	160	164
10	125	139
	6 2 1	
0	274	261
1	82	120
2	127	95
3	326	320
4	255	233
5	349	346
6	141	140
7	175	188
8	130	148
9	152	136
10	151	144
	6 3 1	
0	346	382
1	257	234
2	124	96
3	175	151
4	129	141
5	247	252
6	132	113
7	235	239
8	128	145
9	130	124
10	104	110
	6 4 1	
0	66	72
1	220	215
2	162	166
3	84	109
4	289	231
5	179	181
6	31	80
7	61	67
8	57	67
9	47	65
	6 5 1	
0	237	211
1	155	164
3	122	139
4	44	50
5	177	155
6	125	152
7	102	101
8	147	151
9	123	115
	6 6 1	
0	339	337
1	173	149
2	256	272
3	63	54
4	232	230
5	79	89
6	41	83
7	89	82
8	168	148
9	108	127
	6 7 1	
0	176	190
1	122	106
2	197	226
3	176	171
4	182	181
5	176	186
6	107	105
8	68	67
	6 8 1	
1	46	49
2	77	96
3	169	192
4	60	99
5	187	167
6	156	149
7	193	159
	6 9 1	
0	74	94
1	74	90
2	41	63
3	81	69
4	139	134
5	94	101
6	188	180
	6 10 1	
0	66	68
1	66	63
3	236	216
4	120	141
5	144	126
	6 11 1	
0	60	106
1	166	167
3	63	59
	7 0 1	
1	119	112
3	89	72
4	255	263
5	300	313
7	117	158
	7 1 1	
0	182	127
1	233	223
2	179	180
3	97	98
4	246	209
5	265	271
6	155	176
7	161	189
8	99	92
9	171	166
	7 2 1	
0	350	333
1	166	121
2	141	118
3	195	167
4	209	174
5	176	152
6	124	163
8	186	147
9	114	114
	7 3 1	
0	89	64
1	178	165
2	253	252
3	105	86
4	370	382
5	173	181
6	147	143
	7 4 1	
0	340	358
2	166	143
3	180	165
4	218	220
5	143	138
7	72	79
8	140	136
9	83	85
	7 5 1	
0	102	83
1	121	115
2	174	165
3	57	64
4	238	256
5	67	75
7	117	121
8	96	97
	7 6 1	
0	236	251
1	168	178
2	156	144
3	219	239
4	174	184
5	208	229
	7 7 1	
0	123	139
1	305	323
2	29	40
3	154	165
4	36	38
5	26	73
6	76	83
7	93	106
	7 8 1	
0	100	104
1	65	79
2	75	59
3	122	107
4	115	103
5	157	141
6	89	97
	7 9 1	
0	69	77
1	107	110
2	96	66
3	103	91
4	114	94
5	99	87
	7 10 1	
0	207	196
1	57	70
2	105	122
4	46	49
	8 0 1	
0	473	498
1	62	69
2	62	85
3	81	71
4	155	146
8	222	200
9	66	57
	8 1 1	
0	175	175
1	103	124
2	204	215
3	146	136
4	302	320
5	80	100
7	113	103
8	73	63
	8 2 1	
0	305	257
1	231	210
2	175	183
3	210	195
4	140	131
5	201	192
6	91	90
7	103	126
8	64	76
	8 3 1	
0	169	154
1	408	421
2	98	89
3	207	204
4	138	139
5	144	112
6	48	51
7	140	134
	9 0 1	
1	19	20
2	79	106
3	168	218
4	57	47
5	211	209
6	22	10
	9 1 1	
1	198	240
2	102	115
3	100	113
4	80	67
6	108	77
7	208	176
	9 2 1	
0	176	168
1	99	85
	9 3 1	
0	140	156
1	110	117
2	159	131
4	233	276
5	79	85
6	102	125

Table 3. *Final coordinates (fractional) of atoms in strontium tartrate trihydrate, with mean standard deviations*

	x	*y*	*z*	*B*
Sr	0·2724	0·7500	0·1566	0·91 Å^2
O(1)	0·4813	0·5495	1·0823	3·09
O(2)	0·7381	0·4849	0·9896	1·67
O(3)	0·4928	0·7922	0·9084	2·28
O(4)	0·4220	0·5340	0·5414	2·08
O(5)	0·5358	0·8613	0·4075	2·59
O(6)	0·8199	0·8236	0·5681	1·93
O(7) *W*	0·1073	0·6747	0·7869	3·45
O(8) *W*	1·0017	0·6146	0·2384	6·10
O(9) *W*	0·0620	0·9277	0·2499	5·60
C(1)	0·6131	0·5687	0·9913	0·84
C(2)	0·6257	0·7013	0·8696	1·03
C(3)	0·6075	0·6787	0·6344	1·31
C(4)	0·6544	0·7951	0·5220	0·96

Average e.s.d. for strontium, 0·001 Å; for oxygen and carbon, 0·02 Å; for the water oxygen atoms O(8) and O(9), 0·03 Å.

Table 4. *Final coordinates (fractional) of atoms in calcium tartrate tetrahydrate, with mean standard deviations*

	x	*y*	*z*	*B*
Ca	0·4363	0·4275	0·4328	0·95 Å^2
O(1)	0·2661	0·2588	0·4805	1·94
O(2)	0·2023	0·0593	0·5139	2·15
O(3)	0·5251	0·2051	0·3904	1·65
O(4)	0·4112	−0·0346	0·2778	1·41
O(5)	0·7131	−0·0332	0·5079	1·67
O(6)	0·6939	−0·0780	0·2810	2·00
O(7) *W*	0·1784	0·1762	0·1659	3·30
O(8) *W*	0·9524	0·0805	0·3126	3·74
O(9) *W*	0·8168	0·3099	0·1749	4·37
O(10) *W*	0·5242	0·1576	0·0856	2·05
C(1)	0·2962	0·1422	0·4879	1·38
C(2)	0·4528	0·1094	0·4705	1·08
C(3)	0·4804	−0·0201	0·4091	2·05
C(4)	0·6401	−0·0449	0·4011	1·56

$\sigma(x)=\sigma(y)=\sigma(z)$ for Ca, 0·002 Å; for other atoms, 0·01 Å.

Table 5. *Intramolecular bond distances in strontium and calcium tartrates*

	Sr tartrate	Ca tartrate
C(1)–O(1)	1·27 ± 0·03 Å	1·27 ± 0·014 Å
C(1)–O(2)	1·27	1·26
C(4)–O(5)	1·25	1·24
C(4)–O(6)	1·23	1·31
C(2)–O(3)	1·42	1·44
C(3)–O(4)	1·45	1·43
C(1)–C(2)	1·56	1·50
C(2)–C(3)	1·54	1·52
C(3)–C(4)	1·54	1·50

Distances between non-bonded atoms in the molecule

	Sr tartrate	Ca tartrate
O(1)···O(3)	2·70 Å	2·61 Å
O(4)···O(6)	2·65	2·65
O(1)···O(2)	2·24	2·22
O(5)···O(6)	2·21	2·25

Discussion

The tartrate ion

The intramolecular features of the tartrate ion as found in the two structures are shown in Figs. 1 and 2.

Table 6. *Intramolecular bond angles in strontium and calcium tartrates*

	Sr tartrate	Ca tartrate
O(1)–C(1)–O(2)	124 ± 2°	123 ± 1°
O(1)–C(1)–C(2)	116	116
O(2)–C(1)–C(2)	120	122
C(1)–C(2)–O(3)	110	110
C(1)–C(2)–C(3)	108	115
O(3)–C(2)–C(3)	113	111
C(2)–C(3)–O(4)	110	112
C(2)–C(3)–C(4)	108	110
O(4)–C(3)–C(4)	108	112
C(3)–C(4)–O(5)	113	118
C(3)–C(4)–O(6)	121	118
O(5)–C(4)–O(6)	125	124

The conformation of the tartrate ion is similar to that found in other tartrates (Beevers & Hughes, 1941; Stern & Beevers, 1950; Sadanaga, 1950; Parry, 1951; Sprenkels, 1956; van Bommel & Bijvoet, 1958; Ambady & Kartha, 1968). The two halves of the molecule, each consisting of a carboxyl group, a tetrahedral carbon and a hydroxyl oxygen, are individually planar. The two planes are so oriented that the four carbon atoms assume a zigzag planar configuration. One of the C–O distances in the carboxyl group is as great as 1·31 Å, suggesting that the carboxyl oxygen atom O(6) may be protonated. However, we suspect this distance to be an artifact arising from the inappropriate weighting scheme; for the same reason the standard deviations listed in Tables 4, 5 and 6 may not necessarily be the true values.

Both strontium and calcium are involved in the formation of planar bidentate chelate rings of the type MO(1)C(1)C(2)O(3) where M stands for the cation.

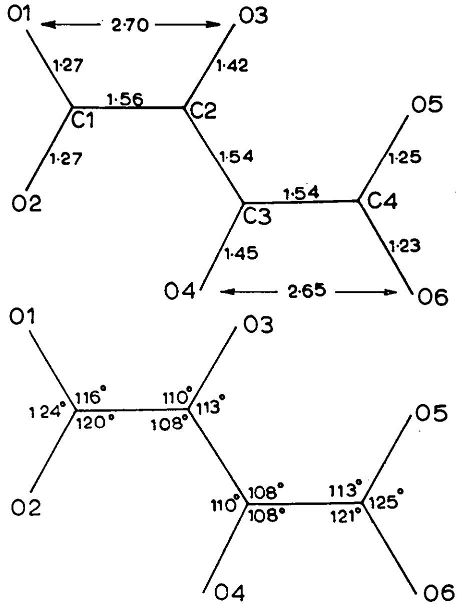

Fig. 1. Intramolecular features of the tartrate ion in strontium tartrate.

Details of the least-squares planes through different groups of atoms in the two structures and the deviations of the atoms from these planes are given in Table 7.

The carboxyl groups

In strontium tartrate neither carboxyl group is found to exhibit any large torsion angle about the C–C bond (Fig. 3). The carboxyl oxygen atoms O(1) and O(2) are involved in strong hydrogen bonds and further O(1) and O(3) take part in the formation of a planar five-membered chelate ring. The planarity of the group C(2)O(3)C(1)O(1)O(2) may be partly dictated by the chelate ring and also by the fact that the hydrogen bond O(9)–H···O(2) lies almost in the plane of C(1)C(2)O(3). The other carboxyl oxygen atoms O(6) and O(5) are hydrogen bonded to O(4*A*) and O(7*A*) respectively, but these bonds are so directed that they do not exert any torque on the carboxyl group. Hence this group remains nearly co-planar with C(4)C(3)O(4).

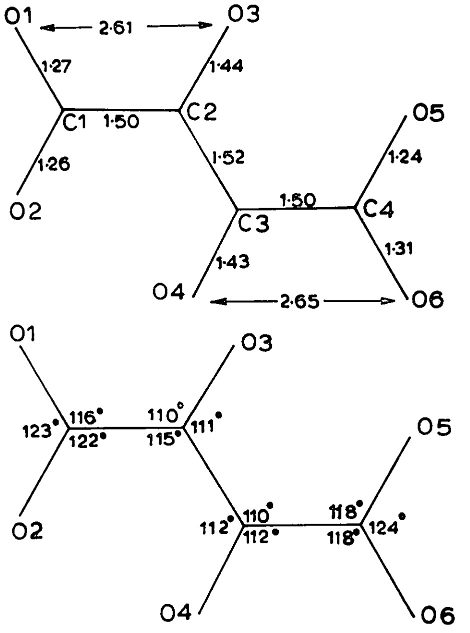

Fig. 2. Intramolecular features of the tartrate ion in calcium tartrate.

In calcium tartrate all four carboxyl oxygen atoms lie in proximity to either water molecules or hydroxyl groups at distances which suggest hydrogen bond formation. The environments of the two carboxyl groups viewed down C(1)–C(2) and C(4)–C(3) are shown in Fig. 4. The angle between the planes defined by C(1)O(1)O(2) and C(1)C(2)O(3) is nearly 22°. As a result the angle between least-squares planes fitted on to the groups C(2)O(3)C(1)O(1)O(2) and C(3)O(4)C(4)-O(5)O(6) is nearly 90° instead of the usual value of about 60° found in tartrates. The large rotation of this carboxyl group about C(1)–C(2) appears to be due to the attractive influence of the cation on O(1) and also due to the hydroxyl group O(3*B*) of another molecule. Even though the distance between O(2) and O(4*A*) is 2·77 Å, it is unlikely that they are linked by a hydrogen bond since the angle C(3*A*)–O(4)–O(3) is nearly 167°. The forces acting on the other carboxyl group are relatively weak and moreover mutually opposing. One should therefore expect this group to be coplanar with C(4)C(3)O(4).

Molecular packing and hydrogen bonding: strontium tartrate trihydrate

The structure projected down the *b* axis is shown in Fig. 5. The backbone carbon atoms lie in sheets parallel to the *bc* plane. As in the structure of D-tartaric acid (Stern & Beevers, 1950) the carboxyl groups of the molecules related by symmetry are turned away from the screw axis.

There are two schemes of hydrogen bonding in the structure. A system of bonds running parallel to the *b* axis links the carboxyl oxygen atoms of one molecule with the hydroxyl groups of another molecule related by symmetry. The hydroxyl oxygen O(3*A*) is situated 2·77 and 2·59 Å away from O(1) and O(2) of the car-

Table 7. *Deviations of atoms from least-squares plane** (Å)

	Plane 1		Plane 2		Plane 3		Plane 4	
	Sr tartrate	Ca tartrate	Sr tartrate	Ca tartrate	Sr tartrate	Ca tartrate	Sr tartrate	Ca tartrate
O(1)			−0·02	−0·14			−0·08	−0·05
O(2)			0·05	0·07				
O(3)			0·06	−0·17			0·05	−0·21
O(4)					0·05	−0·01		
O(5)					−0·09	0·004		
O(6)					0·09	−0·01		
C(1)	0·07	−0·01	−0·01	0·01			0·08	−0·05
C(2)	−0·06	−0·01	−0·07	0·21			0·01	0·22
C(3)	−0·07	0·01			−0·07	0·01		
C(4)	0·06	0·01			0·0	0·001		
Sr							0·05	
Ca								0·12

* Plane 1	C(1)	C(2)	C(3)	C(4)	
Plane 2	O(1)	O(2)	O(3)	C(1)	C(2)
Plane 3	O(4)	O(5)	O(6)	C(3)	C(4)
Plane 4	O(1)	O(3)	C(1)	C(2)	Sr(Ca)

boxyl group of a different molecule. Of these, O(3*A*)–O(2) appears to be a non-bonded short contact in view of the large value (174°) assumed by the angle C(2*A*)–O(3*A*)–O(2).

A second network consists of hydrogen bonds formed through the water molecules. Two carboxyl oxygen atoms O(2*A*) and O(5*A*) belonging to the same molecule are linked by hydrogen bonds formed through the water molecules O(7*A*) and O(9), a pattern similar to that found in the crystal structure of Rochelle salt (Beevers & Hughes, 1941). The environments of the water molecules are shown in Fig. 6. The water molecule O(7*A*) has three neighbours O(9), O(5*A*) and Sr forming a distorted trigonal arrangement. O(9) is similarly surrounded by Sr, O(7*A*) and O(2*A*) at distances 2·54, 2·78 and 2·45 Å respectively. The third water molecule is somewhat isolated. It donates a proton to O(2*B*). Instances of water molecules involved in a single hydrogen bond are not rare in crystal structures (the crystal structure of calcium thymidilate (Trueblood, Horn & Luzzati, 1961) is one such example). The distances and angles involved in hydrogen bonding and the non-bonded intermolecular distances are listed in Tables 8(*a*) and 8(*b*) respectively.

Table 8(*a*). *Distances and angles involved in hydrogen bonding in strontium tartrate, trihydrate*

	Distance	Angle subtended at the water molecule
O(7*A*)···O(9)	2·78 Å	
O(7*A*)···O(5*A*)	2·77	98°
O(8)···O(2*A*)	2·63	
O(9)····O(2*A*)	2·45	
O(9)····O(7*A*)	2·78	94°
O(4)····O(6*A*)	2·77	
O(3*A*)···O(2)	2·78	
O(3*A*)···O(1)	2·60	
	Angle	
C(2*A*)–O(3*A*)···O(2)	174°	
C(2*A*)–O(3)····O(1)	126	
C(3*A*)–O(4*A*)···O(6)	96	

Table 8(*b*). *Non-bonded intermolecular distances less than* 3·5 Å *in the structure of strontium tartrate*

For *A*, *B* refer to Fig. 5

C(1*A*)···O(8)	3·07 Å
C(2*A*)···O(8)	3·42
C(1)····O(3*A*)	3·00
C(4)····O(4*A*)	3·47
O(9)····O(8)	3·18
O(8)····O(4)	3·37
O(1*A*)···O(4)	3·21
O(3)····O(6*A*)	3·25
O(6)····O(2*A*)	3·19
C(1)····O(6*A*)	3·33
C(3)····O(6*A*)	3·27
O(8)····O(5*A*)	3·35

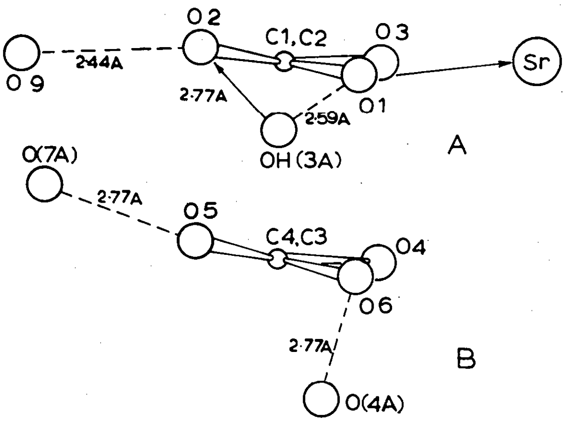

Fig. 3. The environments of the carboxyl groups of strontium tartrate viewed down C(1)–C(2) and C(4)–C(3).

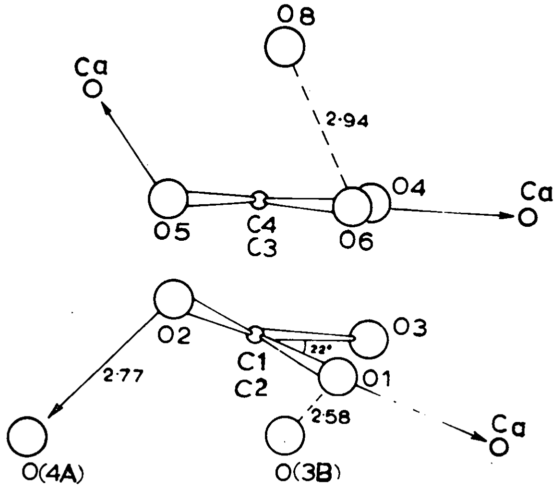

Fig. 4. The environments of the carboxyl groups of calcium tartrate viewed down C(1)–C(2) and C(4)–C(3).

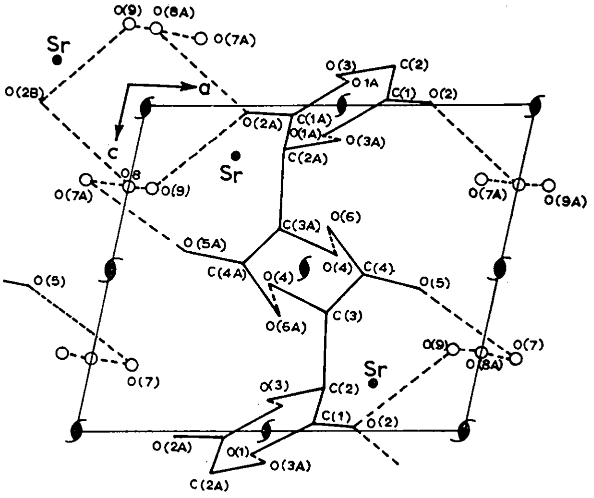

Fig. 5. The crystal structure of strontium tartrate trihydrate viewed down the *b* axis.

Molecular packing and hydrogen bonding: calcium tartrate tetrahydrate

The tartrate molecules lie in channels bonded by the cations, in a direction nearly parallel to the *a* axis, with the carbon atoms forming sheets parallel to the *ab* plane (Fig. 7). The structure is stabilized by a system of hydrogen bonds linking the molecules directly and also through the water molecules. The environments of the water molecules are shown in Fig. 8. The water molecule O(10) has three neighbours O(4), O(3) and O(5*A*) situated at distances less than 3 Å. The angle O(4)–O(10)–O(3) is about 59° and it is likely that one of the protons of this water molecule is involved in the formation of a bifurcated hydrogen bond. The cation is situated close to the bisector of the lone pairs of orbitals of this water. A tentative scheme of proton assignment and also the bond distances and angles involved in hydrogen bonding are given in Table 9(*a*), and non-bonded intermolecular distances are listed in Table 9(*b*).

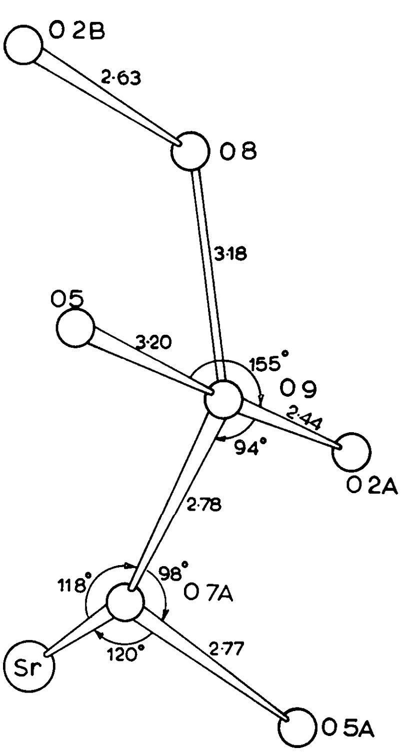

Fig. 6. The environments of the water molecules in the structure of strontium tartrate.

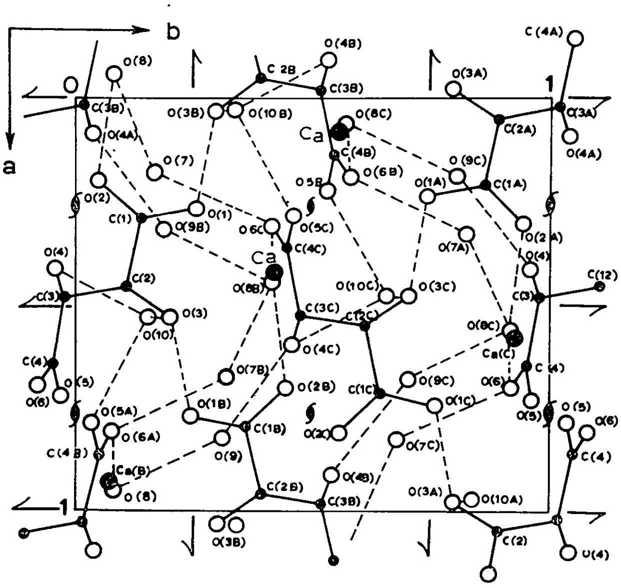

Fig. 7. The crystal structure of calcium tartrate tetrahydrate viewed down the *c* axis.

Table 9(*a*). *Distances and angles involved in hydrogen bonding in calcium tartrate tetrahydrate*

Donor (O*D*)	Acceptor (O*A*)	Distance (O*D*)···(O*A*)	Angle subtended at the water molecule
O(7)	O(8)	2·72 Å	123°
O(7)	O(6*C*)	2·91	
O(8)	O(6*A*)	2·94	130
O(8)	O(2)	3·03	
O(9)	O(8)	3·04	137
O(9)	O(4*C*)	2·72	
O(10)	O(3)	2·99	109
O(10)	O(5*A*)	2·87	
O(4)	O(10)	2·95	
O(3)	O(1*B*)	2·58	

Other angles involved in hydrogen bonding

C(3)–O(4)····O(9)	105°
C(2)–O(3)····O(1*B*)	104
C(6)–O(8)····O(7)	141
O(3)–O(10)···O(4)	60
O(4)–O(10)···O(5)	98

Table 9(*b*). *Non-bonded intermolecular distances less than* 3·5 Å *in the structure of calcium tartrate*

For *A*, *B*, *C* refer to Fig. 7.

O(7) ····C(3*A*)	3·32 Å	O(3) ····O(2*B*)	3·13 Å
O(7) ····O(2*A*)	3·10	O(2*B*)···O(9)	3·48
O(10) ···O(2*A*)	3·19	O(1*B*)···O(8)	3·14
O(6*A*)···O(5)	3·02	O(1*B*)···O(9)	3·44
O(8) ····O(5*A*)	3·35	O(7*B*)···O(10)	3·32
O(9*B*) ··O(5*C*)	3·36	O(9*B*)···O(10)	3·18
C(1*B*)···O(3)	3·21	O(9) ····C(3*C*)	3·39
C(1*B*)···O(9)	3·30	O(10) ···C(3*C*)	3·43
C(2*B*)···O(1)	3·25	O(7) ····C(4*C*)	3·47
C(4) ····O(1*C*)	3·45	O(9) ····O(2*C*)	3·22
O(3*C*)···O(4)	3·26	O(5*A*)···O(1*B*)	3·08
O(3*C*)···O(6)	3·48		

Coordination of strontium and calcium

In both compounds the cations exhibit 8-fold coordination. The coordination polyhedra in both cases are distorted dodecahedra (Figs. 9 and 10). The cation–oxygen distances are given in Table 10. The average Sr–O distance is 2·65 Å which agrees with the sum of the ionic radii of Sr^{2+} and O^{2-} (2·53 Å). The average Ca^{2+}–O distance observed in this crystal is 2·47 Å, which agrees with the values reported in other examples of 8-coordinate calcium (2·49 Å in $CaH(PO_4)$, 2·52 Å in $Ca(H_2PO_4).H_2O$; MacLennan & Beevers, 1955, 1956).

Table 10. *Cation–oxygen distances in the structures of strontium and calcium tartrates*

Sr –O(4)	2·55 Å
O(5*A*)	2·62
O(2*A*)	2·54
O(3*A*)	2·58
O(7*A*)	2·57
O(8*A*)	2·60
O(1*A*)	2·60
O(9)	2·54
Ca–O(1)	2·43 Å
O(3)	2·54
O(2*B*)	2·52
O(5*B*)	2·42
O(8*B*)	2·47
O(4*C*)	2·51
O(10*C*)	2·48
O(6*C*)	2·39

I wish to thank Professor G.N. Ramachandran for his constant encouragement and Dr K. Venkatesan for many valuable suggestions. Thanks are due to Dr S.T. Rao, and Dr M.A. Lonappan for help and to Dr E.

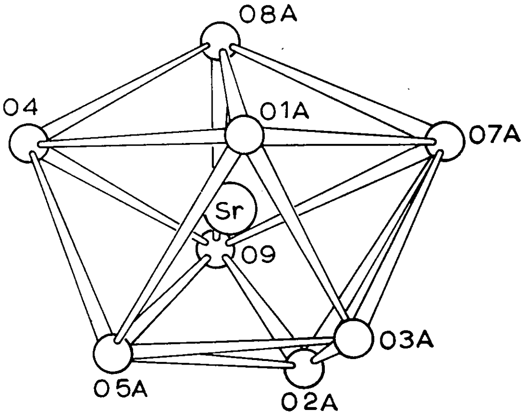

Fig. 9. The coordination polyhedron of strontium.

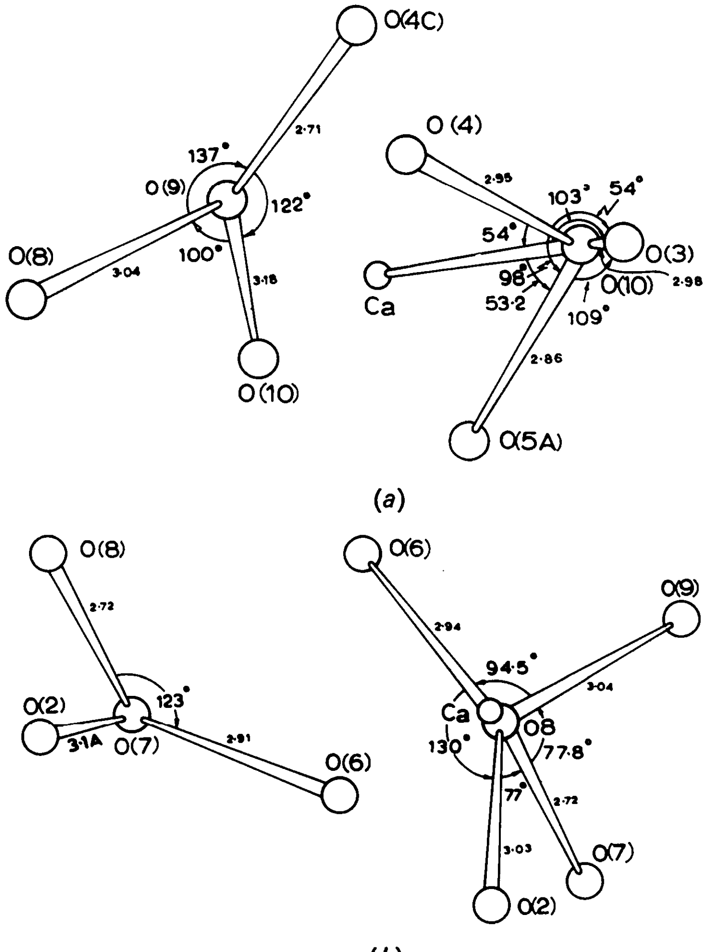

Fig. 8. The environments of the water molecules in the structure of calcium tartrate.

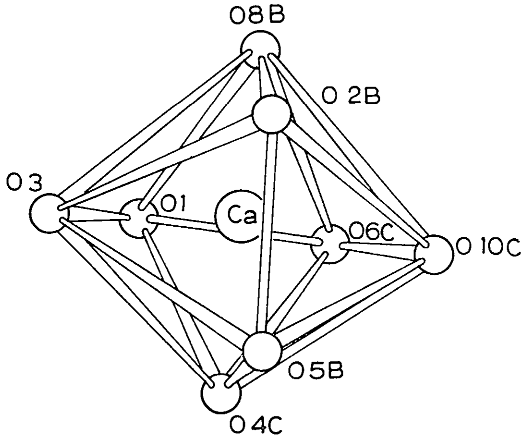

Fig. 10. The coordination polyhedron of calcium.

Subramanian for the Fourier programs. The cooperation extended by the authorities of CDC-3600 computer section of Tata Institute of Fundamental Research, Bombay is gratefully acknowledged. This work was carried out during the tenure of a Research Fellowship awarded by the University Grants Commission, India.

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