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The Crystal Structure of Strontium 3-Deoxy-2-*C*-hydroxymethyl-D-*erythro*-pentoate

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The crystal structure of a strontium 3-D-glucoisosaccharate, $Sr(C_6H_{11}O_6)_2$, has been determined by X-ray diffraction methods in order to elucidate the molecular structures of the two glucoisosaccharinic acids. A crystal structure analysis has previously established that α-D-glucoisosaccharinic acid is 3-deoxy-2-*C*-hydroxymethyl-D-*erythro*-pentoic acid. The crystals are orthorhombic, space group $P2_12_12$, $a=20{\cdot}040$, $b=6{\cdot}909$, $c=5{\cdot}738$ Å. The unit cell contains 2 stoichiometric units. Only four of the six carbon atoms in each anion form a planar zigzag chain. Each strontium atom has eight oxygen neighbours at the corners of a distorted Archimedean antiprism.

Introduction

In order to establish the stereochemistry of the D-glucoisosaccharinic acids (Feast, Lindberg & Theander, 1965), an X-ray study of a strontium D-glucoisosaccharate has been performed. The salt is formed by treatment of a 4-*O*-substituted D-glucose with strontium hydroxide.

The possible Fischer diagrams of the corresponding acid are shown in Fig. 1.

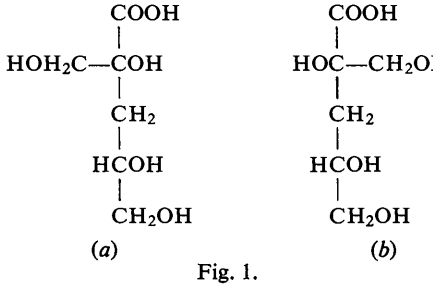

Fig. 1.

Experimental

A powder specimen of strontium D-glucoisosaccharate was kindly supplied by A. Ishizu (*Swedish Forest Products Research Laboratory*). Single crystals suitable for X-ray analysis were obtained by slow cooling of a saturated aqueous solution. A crystal which measured $0{\cdot}03\times0{\cdot}07\times0{\cdot}10$ mm³ was used for the collection of X-ray diffraction data. The axis parallel to the long dimension of the crystal was chosen as the *c* axis.

Powder photographs were taken in a Guinier focusing camera with Cu $K\alpha_1$ radiation ($\lambda=1{\cdot}54056$ Å) and potassium chloride ($a=6{\cdot}2930$ Å) as an internal standard. The least-squares refined unit-cell dimensions obtained from the X-ray powder pattern are shown in Table 1.

The single crystal was mounted on a General Electric XRD-5 orienter equipped with a scintillation detector and a pulse-height analyser. Ni-filtered Cu *K* radiation was used and the pulse-height analyser was set to collect about 90% of the $K\alpha$ radiation. The θ–2θ scanning technique was used to measure 789 reflexions with $2\theta\leq125°$, 775 of which were significant. A 2θ range of 2° for $2\theta\leq80°$ and of 4° for $80°<2\theta\leq125°$ was scanned at a rate of 2° per minute. A 20 second background count for $2\theta\leq80°$ and a 40 second background count for $2\theta>80°$ were collected at each end of the scan range. Lp and absorption correction ($\mu=58$ cm^{-1}) were applied on the net intensity counts. No extinction effects were observed and thus no correction for extinction was deemed necessary.

Table 1. *Crystallographic data for strontium-α-D-glucoisosaccharate*

Lattice constants	$a=20{\cdot}040\pm5$ Å
	$b=6{\cdot}909\pm2$ Å
	$c=5{\cdot}738\pm2$ Å
Cell volume	794·5 Å³
Density (X-ray)	1·864 g.cm^{-3}
Molecules per unit cell	2
Space group	$P2_12_12$ (No. 18)

Structure determination and refinement

The general position in $P2_12_12$ is fourfold; therefore the strontium atoms must occupy a twofold special position. They were placed in the positions of type (*a*) and the *z* parameter was determined from the Patterson function. The strontium atoms do not affect the $F(hk0)$'s with $h+k=2n+1$. However, the signs of most of the remaining $F(hk0)$'s were determined by the heavy atom method. The strontium contribution was subtracted from these structure factors and the signs of differences were used in the method described by Woolfson (1957) for applying the Sayre sign relationship. Thus, the signs of the 15 strongest $F(hk0)$'s with $h+k=2n+1$ were determined.

A two-dimensional electron density synthesis was calculated using the signs obtained for the $F(hk0)$'s and yielded trial positions for all the carbon and oxygen

atoms in this projection. The z parameters were derived from the three-dimensional Patterson function. The trial structure with anisotropic temperature factors was refined by a full-matrix least-squares treatment. The scattering factor curves used for carbon and oxygen were those given by Freeman (1959) and for strontium that by Cromer & Waber (1965), corrected by the real part of the anomalous dispersion coefficient. In the refinement the 700 strongest reflexions were used (see Table 2) and Hughes's (1941) weighting procedure with $|F_{o,\min}| = 6$ was applied. The final reliability index $R = \Sigma \, ||kF_o| - |F_c|| / \Sigma \, |kF_o|$ was 0·058.* At this stage the shifts in all atomic parameters were less than 3% of their standard deviations.

The coordinates and temperature factors obtained are given in Table 3. These parameters were used for the calculation of a three-dimensional difference elec-

* When all the 775 observed reflexions were included R became 0·063.

Table 2. *Observed and calculated structure factors*

H K L	10|F_o|	10|F_c|
2 0 0	673	752
4 0 0	173	192
6 0 0	235	274
8 0 0	547	535
10 0 0	648	680
12 0 0	554	539
14 0 0	363	345
16 0 0	54	55
18 0 0	518	534
20 0 0	268	267
22 0 0	123	124
0 0 1	47	55
2 0 1	340	308
3 0 1	72	13
4 0 1	143	177
5 0 1	499	458
6 0 1	90	92
7 0 1	196	217
8 0 1	268	250
9 0 1	1018	1032
10 0 1	274	250
11 0 1	475	490
12 0 1	37	40
13 0 1	400	475
14 0 1	230	212
15 0 1	216	195
16 0 1	137	144
17 0 1	233	226
18 0 1	59	49
19 0 1	509	468
20 0 1	81	84
21 0 1	260	274
22 0 1	31	37
0 0 2	1030	913
1 0 2	64	97
2 0 2	148	141
3 0 2	206	195
4 0 2	527	494
5 0 2	104	112
6 0 2	776	797
7 0 2	257	277
8 0 2	426	447
9 0 2	25	54
10 0 2	440	435
11 0 2	125	126
12 0 2	565	555
13 0 2	62	62
14 0 2	423	407
15 0 2	59	63
16 0 2	77	52
17 0 2	274	248
18 0 2	451	410
19 0 2	149	153
20 0 2	348	326
21 0 2	37	2
22 0 2	229	230
0 0 3	56	45
1 0 3	832	810
2 0 3	422	358
3 0 3	458	433
4 0 3	36	37
5 0 3	605	631
6 0 3	40	27
7 0 3	256	256
8 0 3	169	167
9 0 3	283	305
10 0 3	94	74
11 0 3	198	202
12 0 3	47	34
13 0 3	435	453
14 0 3	71	35
15 0 3	290	256
16 0 3	281	271
17 0 3	164	156
18 0 3	120	91
20 0 3	47	36
0 0 4	479	451
1 0 4	166	177
2 0 4	192	178
3 0 4	142	153
4 0 4	388	373
5 0 4	207	219
6 0 4	436	437
7 0 4	299	293
8 0 4	250	255
9 0 4	24	19
10 0 4	130	104
11 0 4	208	221
12 0 4	263	247
13 0 4	137	120
14 0 4	460	429
15 0 4	104	92
16 0 4	247	243
17 0 4	42	10
18 0 4	284	259
0 0 5	243	231
1 0 5	42	69
2 0 5	122	116
3 0 5	137	132
4 0 5	215	223
5 0 5	503	484
6 0 5	136	115
7 0 5	367	357
8 0 5	89	71
9 0 5	153	141
10 0 5	112	121
11 0 5	126	119
12 0 5	177	157
13 0 5	51	271
14 0 5	130	114
15 0 5	139	140
0 0 6	240	222
1 0 6	9	160
2 0 6	200	196
3 0 6	111	110
4 0 6	288	271
5 0 6	94	124
6 0 6	205	207
7 0 6	127	121
8 0 6	173	183
9 0 6	55	11
1 1 0	599	654
2 1 0	481	542
3 1 0	709	692
4 1 0	614	560
5 1 0	815	882
6 1 0	252	268
7 1 0	254	215
8 1 0	276	283
9 1 0	808	793
10 1 0	107	89
11 1 0	150	191
12 1 0	403	404
13 1 0	356	344
14 1 0	127	124
15 1 0	482	491
16 1 0	143	146
17 1 0	364	361
18 1 0	98	121
19 1 0	301	294
20 1 0	243	254
21 1 0	172	158
0 1 1	787	765
1 1 1	149	140
2 1 1	541	522
3 1 1	208	183
4 1 1	966	925
5 1 1	141	120
6 1 1	453	474
7 1 1	249	237
8 1 1	703	647
9 1 1	275	251
10 1 1	611	605
11 1 1	117	126
12 1 1	235	248
13 1 1	96	96
14 1 1	496	497
16 1 1	301	296
17 1 1	70	50
18 1 1	304	343
19 1 1	69	38
20 1 1	210	207
21 1 1	53	34
22 1 1	240	234
0 1 2	41	18
1 1 2	641	614
2 1 2	291	275
3 1 2	789	765
4 1 2	415	387
5 1 2	737	718
6 1 2	122	117
7 1 2	306	291
8 1 2	356	338
9 1 2	658	659
10 1 2	95	91
11 1 2	306	310
12 1 2	109	108
13 1 2	375	401
14 1 2	260	265
15 1 2	365	360
16 1 2	141	144
17 1 2	249	248
18 1 2	106	122
19 1 2	224	232
21 1 2	223	208
0 1 3	441	407
1 1 3	125	128
2 1 3	392	411
3 1 3	270	292
4 1 3	711	720
5 1 3	58	46
6 1 3	390	379
7 1 3	160	161
8 1 3	444	443
9 1 3	39	30
10 1 3	326	321
11 1 3	210	225
12 1 3	203	214
13 1 3	199	208
14 1 3	425	423
15 1 3	136	140
16 1 3	286	276
17 1 3	123	128
18 1 3	213	233
19 1 3	63	62
20 1 3	159	159
0 1 4	164	147
1 1 4	317	334
2 1 4	252	252
3 1 4	418	407
4 1 4	192	204
5 1 4	414	405
6 1 4	203	206
7 1 4	213	227
8 1 4	151	157
9 1 4	324	327
10 1 4	86	61
11 1 4	226	218
12 1 4	133	153
13 1 4	282	284
14 1 4	78	79
15 1 4	280	276
16 1 4	166	161
17 1 4	213	208
0 1 5	251	249
1 1 5	122	150
2 1 5	321	297
3 1 5	207	202
4 1 5	289	280
5 1 5	151	130
6 1 5	240	240
7 1 5	161	149
8 1 5	255	261
9 1 5	72	67
10 1 5	260	270
11 1 5	102	108
12 1 5	189	196
13 1 5	164	152
14 1 5	190	192
0 1 6	71	64
1 1 6	41	195
2 1 6	180	169
3 1 6	181	187
4 1 6	139	137
5 1 6	168	175
6 1 6	97	89
7 1 6	158	177
8 1 6	131	136
9 1 6	195	197
0 2 0	392	368
1 2 0	330	303
2 2 0	146	131
3 2 0	585	577
4 2 0	952	1023
5 2 0	217	218
6 2 0	563	582
7 2 0	435	422
8 2 0	294	375
9 2 0	218	205
10 2 0	560	542
11 2 0	74	66
12 2 0	320	326
13 2 0	61	60
14 2 0	476	485
15 2 0	28	33
16 2 0	370	371
17 2 0	54	20
18 2 0	296	271
19 2 0	59	53
20 2 0	245	250
21 2 0	33	15
22 2 0	258	260
0 2 1	229	245
1 2 1	736	706
2 2 1	130	133
3 2 1	423	432
4 2 1	301	321
5 2 1	965	930
6 2 1	98	118
7 2 1	568	566
8 2 1	134	117
9 2 1	291	290
10 2 1	122	112
11 2 1	362	382
12 9 1	171	159
13 2 1	396	418
14 2 1	122	122
15 2 1	298	295
16 2 1	156	156
17 2 1	338	320
18 2 1	82	95
19 2 1	293	282
20 2 1	48	21
21 2 1	104	99
22 2 1	58	40
0 2 2	706	737
1 2 2	292	273
2 2 2	704	662
3 2 2	345	353
4 2 2	565	579
5 2 2	41	28
6 2 2	305	330
7 2 2	120	115
8 2 2	468	436
9 2 2	102	119
10 2 2	449	473
11 2 2	171	182
12 2 2	176	191
13 2 2	40	61
14 2 2	330	307
15 2 2	47	54
16 2 2	387	388
17 2 2	94	93
18 2 2	273	265
19 2 2	42	29
20 2 2	152	146
21 2 2	126	127
0 2 3	270	241
1 2 3	319	332
2 2 3	122	114
3 2 3	271	254
4 2 3	104	93
5 2 3	346	352
6 2 3	226	244
7 2 3	347	341
8 2 3	97	111
9 2 3	396	387
10 2 3	83	95
11 2 3	405	429
12 2 3	357	359
13 2 3	305	286
14 2 3	48	50
15 2 3	220	216
16 2 3	130	132
17 2 3	286	273
18 2 3	60	69
19 2 3	278	281
0 2 4	364	345
1 2 4	157	168
2 2 4	369	368
3 2 4	108	102
4 2 4	307	326
5 2 4	150	152
6 2 4	256	256
7 2 4	116	109
8 2 4	301	283
9 2 4	126	130
10 2 4	347	376
11 2 4	147	145
12 2 4	294	300
13 2 4	132	137
14 2 4	129	122
15 2 4	115	120
16 2 4	131	134
17 2 4	112	115
0 2 5	423	415
1 2 5	381	360
2 2 5	210	209
3 2 5	315	312
4 2 5	124	119
5 2 5	132	132
6 2 5	194	196
7 2 5	164	180
8 2 5	137	149
9 2 5	255	252
10 2 5	104	106
11 2 5	234	240
12 2 5	152	159
13 2 5	122	127
14 2 5	19	11
0 2 6	185	174
1 2 6	123	111
2 2 6	156	160
3 2 6	94	100
4 2 6	116	97
5 2 6	112	100
6 2 6	166	165
7 2 6	145	157
1 3 0	178	211
2 3 0	314	285
3 3 0	618	545
4 3 0	309	296
5 3 0	610	639
6 3 0	114	111
7 3 0	486	467
8 3 0	29	27
9 3 0	434	414
10 3 0	44	45
11 3 0	436	442
12 3 0	159	178
13 3 0	393	400
14 3 0	41	31
15 3 0	322	343
16 3 0	41	18
17 3 0	121	110
19 3 0	206	196
20 3 0	104	87
21 3 0	273	267
0 3 1	223	272
1 3 1	105	118
2 3 1	560	562
3 3 1	190	176
4 3 1	658	650
5 3 1	153	143
6 3 1	423	440
7 3 1	62	80
8 3 1	401	398
9 3 1	117	99
10 3 1	380	395
11 3 1	145	140
12 3 1	273	262
13 3 1	159	150
14 3 1	307	293
15 3 1	149	160
16 3 1	334	354
17 3 1	41	50
18 3 1	174	155
19 3 1	83	73
20 3 1	234	223
21 3 1	47	23
0 3 2	225	199
1 3 2	520	543
2 3 2	86	75
3 3 2	589	555
4 3 2	267	268
5 3 2	350	342
6 3 2	260	262
7 3 2	351	342
8 3 2	122	115
9 3 2	320	310
10 3 2	59	66
11 3 2	283	276
12 3 2	99	65
13 3 2	313	306
14 3 2	162	136
15 3 2	363	385
16 3 2	67	59
17 3 2	275	265
18 3 2	106	113
19 3 2	213	219
20 3 2	29	26
0 3 3	346	340
1 3 3	115	101
2 3 3	386	397
3 3 3	191	204
4 3 3	399	354
5 3 3	162	152
6 3 3	283	288
7 3 3	185	192
8 3 3	434	446
9 3 3	116	122
10 3 3	452	457
11 3 3	97	100
12 3 3	304	298
13 3 3	88	90
14 3 3	162	171
15 3 3	75	69
16 3 3	204	215
18 3 3	177	173
0 3 4	189	201
1 3 4	266	285
2 3 4	234	243
3 3 4	222	217
4 3 4	83	52
5 3 4	209	207
6 3 4	106	51
7 3 4	310	327
8 3 4	100	95
9 3 4	326	331
10 3 4	102	107
11 3 4	274	289
12 3 4	130	127
13 3 4	179	175
14 3 4	73	86
15 3 4	157	159
16 3 4	113	114
0 3 5	230	216
1 3 5	144	151
2 3 5	286	300
3 3 5	140	152
4 3 5	208	223
5 3 5	48	38
6 3 5	221	215
7 3 5	104	106
8 3 5	195	190
9 3 5	137	143
10 3 5	158	145
11 3 5	61	75
12 3 5	188	191
0 3 6	67	44
1 3 6	143	157
2 3 6	88	91
3 3 6	190	189
4 3 6	85	87
0 4 0	905	789
1 4 0	328	300
2 4 0	415	420
3 4 0	41	24
4 4 0	306	284
5 4 0	104	84
6 4 0	679	652
7 4 0	100	99
8 4 0	377	376
9 4 0	80	39
10 4 0	199	219
11 4 0	98	50
12 4 0	352	350
13 4 0	56	122
14 4 0	245	227
15 4 0	58	14
16 4 0	163	161
17 4 0	27	35
18 4 0	231	232
19 4 0	125	127
0 4 1	149	152
1 4 1	444	452
2 4 1	167	155
3 4 1	320	323
4 4 1	338	346
5 4 1	337	337
6 4 1	205	191
7 4 1	340	356
8 4 1	51	43
9 4 1	262	302
10 4 1	104	121
11 4 1	359	365
12 4 1	48	69
13 4 1	267	356
14 4 1	54	63
15 4 1	269	265
16 4 1	42	44
17 4 1	162	186
18 4 1	75	50
19 4 1	228	232
0 4 2	516	493
1 4 2	105	91
2 4 2	311	296
3 4 2	269	252
4 4 2	246	257
5 4 2	165	156
6 4 2	406	414
7 4 2	177	148
8 4 2	223	223
9 4 2	85	80
10 4 2	234	237
11 4 2	68	47
12 4 2	453	442
13 4 2	76	112
14 4 2	281	270
15 4 2	101	101
16 4 2	142	146
17 4 2	124	119
18 4 2	223	226
0 4 3	78	73
1 4 3	304	305
2 4 3	107	96
3 4 3	246	304
4 4 3	155	161
5 4 3	315	340
6 4 3	142	153
7 4 3	424	415
8 4 3	115	116
9 4 3	250	239
10 4 3	28	32
11 4 3	219	219
12 4 3	118	126
13 4 3	135	165
14 4 3	68	80
15 4 3	195	183
16 4 3	139	168
17 4 3	171	179
0 4 4	321	291
1 4 4	102	96
2 4 4	245	241
3 4 4	129	127
4 4 4	134	131
5 4 4	207	221
6 4 4	309	315
7 4 4	173	178
8 4 4	260	272
9 4 4	35	30
10 4 4	141	162
11 4 4	59	64
12 4 4	200	192
13 4 4	92	93
14 4 4	139	164
0 4 5	25	18
1 4 5	193	199

Table 2 (*cont.*)

H K L	$10\|F_o\|$	$10\|F_c\|$	H K L	$10\|F_o\|$	$10\|F_c\|$	H K L	$10\|F_o\|$	$10\|F_c\|$	H K L	$10\|F_o\|$	$10\|F_c\|$
2 4 5	102	107	4 5 2	49	16	3 6 0	70	75	4 6 3	61	51
3 4 5	149	156	5 5 2	285	286	4 6 0	340	312	5 6 3	227	234
4 4 5	134	130	6 5 2	11	48	5 6 0	24	6	6 6 3	92	79
5 4 5	158	185	7 5 2	233	250	6 6 0	209	186	7 6 3	112	116
6 4 5	46	48	8 5 2	258	273	7 6 0	86	70	9 6 3	165	142
7 4 5	227	232	9 5 2	335	344	8 6 0	202	199	10 6 3	62	40
8 4 5	67	72	10 5 2	169	183	9 6 0	25	28	11 6 3	166	170
9 4 5	82	92	11 5 2	267	272	10 6 0	183	212			
			12 5 2	72	49	12 6 0	167	180	0 6 4	182	162
1 5 0	471	481	13 5 2	104	206	13 6 0	25	13	1 6 4	72	52
2 5 0	63	72	14 5 2	121	58	14 6 0	220	215	2 6 4	182	170
3 5 0	373	362	15 5 2	168	182	15 6 0	113	95	3 6 4	77	50
4 5 0	158	156	16 5 2	85	56				4 6 4	225	240
5 5 0	195	176				0 6 1	104	102	5 6 4	74	50
6 5 0	169	165	0 5 3	255	270	1 6 1	241	229	6 6 4	121	139
7 5 0	183	197	1 5 3	159	162	2 6 1	61	55			
8 5 0	289	322	2 5 3	271	285	3 6 1	270	250			
9 5 0	374	393	3 5 3	120	123	4 6 1	142	142	1 7 0	209	196
10 5 0	154	166	4 5 3	275	290	5 6 1	360	345	2 7 0	87	76
11 5 0	224	234	5 5 3	134	140	6 6 1	54	56	3 7 0	195	189
12 5 0	101	90	6 5 3	210	204	7 6 1	255	267	4 7 0	110	109
13 5 0	152	164	7 5 3	63	84	8 6 1	105	100	5 7 0	107	177
14 5 0	23	1	8 5 3	202	215	9 6 1	220	215	6 7 0	39	17
15 5 0	229	234	9 5 3	67	80	10 6 1	92	90	7 7 0	246	178
16 5 0	68	4	10 5 3	194	193	11 6 1	152	149	8 7 0	29	29
17 5 0	234	222	11 5 3	73	77	12 6 1	45	44	9 7 0	213	200
18 5 0	69	47	12 5 3	164	166	13 6 1	173	176	10 7 0	39	41
			13 5 3	80	76	14 6 1	40	34	11 7 0	191	195
0 5 1	376	373	14 5 3	205	217						
1 5 1	182	191				0 6 2	194	174	0 7 1	242	236
2 5 1	309	317	1 5 4	198	226	1 6 2	173	183	1 7 1	51	62
3 5 1	31	34	2 5 4	155	169	2 6 2	213	195	2 7 1	229	226
4 5 1	261	267	3 5 4	192	218	3 6 2	39	52	3 7 1	98	84
5 5 1	97	64	4 5 4	111	110	4 6 2	325	317	4 7 1	194	182
6 5 1	228	241	5 5 4	192	192	5 6 2	43	48	6 7 1	143	132
7 5 1	162	192	6 5 4	134	123	6 6 2	261	263	7 7 1	80	58
8 5 1	362	359	7 5 4	173	173	7 6 2	37	37	8 7 1	210	204
9 5 1	158	159	8 5 4	89	88	8 6 2	262	259	9 7 1	67	73
10 5 1	368	362	9 5 4	202	206	9 6 2	78	77	10 7 1	206	205
11 5 1	153	162	10 5 4	102	114	10 6 2	181	191			
12 5 1	252	259	11 5 4	147	141	11 6 2	41	48	0 7 2	129	109
13 5 1	44	7				12 6 2	137	112	1 7 2	247	235
14 5 1	186	200	0 5 5	68	87	13 6 2	40	51	2 7 2	54	46
15 5 1	72	65	1 5 5	57	56				3 7 2	159	157
16 5 1	170	174	2 5 5	130	146	0 6 3	150	141	5 7 2	139	141
17 5 1	112	108	3 5 5	96	111	1 6 3	167	176	6 7 2	89	52
			4 5 5	190	200	2 6 3	97	75	7 7 2	176	170
0 5 2	95	88				3 6 3	212	199	0 7 2	57	39
1 5 2	218	220	0 6 0	214	193						
2 5 2	85	90	1 6 0	136	131				0 7 3	116	130
3 5 2	320	341	2 6 0	240	230				1 7 3	38	48
									2 7 3	136	140
									3 7 3	68	56

Table 3. *Parameters of non-hydrogen atoms and their estimated standard deviations*

The thermal parameters are of the form $T=\exp[-(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{12}hk+b_{13}hl+b_{23}kl)]$.

				Thermal parameter $\times 10^4$					
	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Sr	0	0	0·2648±2	10	130	142	3	0	0
O(0)	0·0643±4	0·180±2	−0·037±2	11	272	136	−35	−7	46
O(1)	0·1627±4	0·267±2	−0·188±2	13	282	88	−34	23	45
O(2)	0·1078±4	0·168±1	0·390±2	10	138	149	−10	16	2
O(2′)	0·2141±4	−0·047±1	0·197±2	16	121	305	7	−5	13
O(4)	0·0953±4	0·751±1	0·161±2	16	151	161	19	14	−12
O(5)	0·0289±4	0·763±2	0·581±2	21	280	166	60	28	77
C(1)	0·1240±5	0·229±2	−0·019±2	10	128	130	−18	−26	−20
C(2)	0·1535±5	0·254±2	0·227±2	12	206	53	12	4	83
C(2′)	0·2222±5	0·155±2	0·247±2	9	171	152	19	−18	−26
C(3)	0·1636±5	0·471±2	0·282±2	14	88	210	16	−33	−2
C(4)	0·0975±6	0·582±2	0·315±3	11	158	238	−23	5	6
C(5)	0·0897±8	0·649±3	0·566±3	29	287	113	57	14	70

tron density synthesis. It was possible to pick out likely hydrogen atom positions from 7 peaks in the synthesis. These 7 hydrogen atoms are those bonded to carbon and the C–H distances found were about 0·9 Å. Refinement of the structure including the obtained hydrogen positions reduced the R value to 0·043. However, since no convergence was achieved it was concluded that these positions could not be refined from the available data. The hydrogen atoms bonded to carbon were therefore located by geometrical considerations assuming a C–H distance of 1·1 Å (Table 4).

The remaining four hydrogen atoms are all bonded to oxygen. Attempts to locate them from the difference synthesis were not successful. This may be related to the different nature of the C–H and O–H bonds resulting in different electron densities at the hydrogen atoms.

Table 4. *Estimated coordinates for hydrogen atoms bonded to carbon*

	x	y	z
H(2′, 1)	0·241	0·172	0·425
H(2′, 2)	0·256	0·220	0·121
H(3, 1)	0·195	0·486	0·439
H(3, 2)	0·193	0·539	0·141
H(4, 1)	0·055	0·486	0·270
H(5, 1)	0.086	0.522	0.681
H(5, 2)	0.133	0.740	0·613

Description and discussion of the structure

The configuration of the α-D-glucoisosaccharate ion (Fig. 2) (Johnson, 1965) is in agreement with the Fisher representation in Fig. 1(*a*).

In the field of monosaccharinic acids of open-chain type few crystal structures have been determined. The

arabonic acid (Furberg & Helland, 1962) and gluconic acid (Littleton, 1953) determined in the forms of their strontium and potassium salts respectively show some structural similarities to the D-glucoisosaccharinic acids.

Least-squares planes were calculated for O(2′)C(2′)-C(2)C(3)C(4) and O(0)O(1)C(1)C(2) respectively. The perpendicular distances of the atoms from the planes are shown in Table 5.

Table 5. *Least-squares planes*

The coefficients q_i are direction cosines relative to a, b, and c; D is the origin-to-plane distance. The atom indicated with an asterisk was omitted from the calculation of the least-squares plane II.

Plane I	Atom	Deviation
$q_1 = -0.071$	O(2′)	0·02 Å
$q_2 = -0.179$	C(2′)	0·05
$q_3 = 0.981$	C(2)	−0·09
$D = 0.836$ Å	C(3)	−0·06
	C(4)	0·08

The root mean square deviation of the atoms in this plane is 0·065 Å.

Plane I	Atom	Deviation
$q_1 = -0.285$	O(0)	0·00 Å
$q_2 = 0.958$	O(1)	0·00
$q_3 = 0.013$	C(1)	−0·01
$D = 0.820$ Å	C(2)	0·00
	*O(2)	−0·30

The r.m.s. deviation of the atoms in this plane [O(2) omitted] is 0·007 Å.

The atoms O(2′)C(2′)C(2)C(3)C(4) form an almost planar zigzag chain. The twist of the carbon chain at C(4) can be regarded as a rotation around the C(3)–C(4) bond. In the arabonate ion (Furberg & Helland, 1962) and the gluconate ion (Littleton, 1953) all the carbon atoms are bonded to oxygen and form planar zigzag chains. It should be noted that C(3) is the only carbon atom without any oxygen bonded to it (see Fig. 2).

The O(0)···O(2) distance is as short as 2·60 Å and the O(2) atom is only 0·30 Å removed from the O(0)O(1)C(1)C(2) plane. This structural feature which seems to be common to all α-hydroxycarboxylic ions and acids (Jeffrey Parry, 1952; Kroon, Peerdeman & Bijvoet, 1965) will be discussed elsewhere (Norrestam, Werner & Glehn, 1968).

Table 6. *Interatomic distances and angles for non-hydrogen atoms in the* α-D-*glucoisosaccharinic ion and their standard deviations*

O–O distances within the coordination polyhedron around strontium are marked with asterisks in the table.

C(1) –C(2)	1·54 ± 2 Å
C(2) –C(2′)	1·54 ± 2
C(2) –C(3)	1·54 ± 2
C(3) –C(4)	1·55 ± 2
C(4) –C(5)	1·52 ± 2

Table 6 (*cont.*)

C(1) –O(0)	1·25 ± 2
C(1) –O(1)	1·27 ± 2
C(2) –O(2)	1·44 ± 2
C(2′)–O(2′)	1·43 ± 2
C(4) –O(4)	1·46 ± 2
C(5) –O(5)	1·45 ± 2
O(0) –O(1)	2·24 ± 1
*O(0) –O(2)	2·60 ± 1
O(2) –O(2′)	2·82 ± 1
*O(4) –O(5)	2·76 ± 1
O(0) –C(1) –C(2)	118·4 ± 0·9°
O(1) –C(1) –C(2)	116·4 ± 0·9
O(0) –C(1) –O(1)	125·2 ± 1·0
C(1) –C(2) –C(3)	110·3 ± 0·9
C(1) –C(2) –C(2′)	111·2 ± 0·9
C(1) –C(2) –O(2)	107·7 ± 0·8
C(2′)–C(2) –C(3)	107·4 ± 0·9
C(2′)–C(2) –O(2)	109·6 ± 0·9
O(2) –C(2) –C(3)	110·7 ± 0·9
C(2) –C(2′)–O(2′)	108·4 ± 0·9
C(2) –C(3) –C(4)	113·4 ± 0·9
C(3) –C(4) –C(5)	110·8 ± 1·1
C(3) –C(4) –O(4)	110·5 ± 0·9
O(4) –C(4) –C(5)	109·2 ± 1·1
C(4) –C(5) –O(5)	108·1 ± 1·1

Distances and angles for non-hydrogen atoms within the anion are given in Table 6 and Sr–O distances and intermolecular O···O distances shorter than 3·2 Å, in Table 7(*a*). The average C–C bond length in the anion is 1·54 Å and no significant deviation from this value is observed. The two C–O bonds in the carboxyl group and the four other C–O bonds within the anion do not deviate significantly from their average values, 1·26 Å and 1·45 Å respectively. Only one bond angle C(2)–C(3)–C(4) formed by sp^3–sp^3 bonds deviates from the tetrahedral value of 109·47° by more than 3σ.

Table 7(*a*). Sr–O *distances and intermolecular* O···O *distances shorter than* 3·2 Å

O···O distances within the coordination polyhedron around strontium are marked with asterisks in the table.

Code for symmetry-related atoms

(i) $\bar{x}, \bar{y}, z$
(ii) $\frac{1}{2}+x, \frac{1}{2}-y, \bar{z}$
(iii) $\frac{1}{2}-x, \frac{1}{2}+y, \bar{z}$
(iv) $x, y, z+1$
(v) $x, y-1, z$

Sr–O(0)	2·493 ± 8 Å
Sr–O(2)	2·555 ± 7
Sr–O(4)	2·639 ± 8
Sr–O(5)	2·514 ± 9
O(0) ···O(5) (i)	2·90 ± 1 Å
O(1) ···O(2) (iv)	2·75 ± 1
O(1) ···O(2′) (iii)	2·79 ± 1
O(2′)···O(4) (v)	2·77 ± 1
*O(2) ···O(5) (i)	2·99 ± 1
*O(2) ···O(4) (v)	3·18 ± 1

Table 7(*b*) *Proposed hydrogen bonding scheme*

O(1) ···H–O(2) (iv)	2·75 Å
O(1) ···H–O(2′) (iii)	2·79
O(2′)···H–O(4) (v)	2·77
O(0) ···H–O(5) (i)	2·90

Eight oxygen atoms related by a twofold axis form a distorted Archimedean antiprism around each strontium ion (Fig. 3). This coordination polyhedron consists of oxygen atoms from four different anions. Each anion is thus coordinated to two cations.

The distances O(0)···O(2) (2·60 Å), O(4)···O(5) (2·76 Å) and O(2)···O(2′) (2·82 Å) are the shortest intramolecular O···O distances except for the O(0)···O(1) (2·24 Å) distance within the carboxylic group. The atoms O(0), O(2) and O(4), O(5) respectively are coordinated to two strontium ions. It might be suggested that these short O···O distances are a result of the influence of the strontium ions. However, the short O(0)···O(2) distance is common to all α-hydroxycarboxylic groups (see above).

On each anion there are four hydrogen atoms available for hydrogen bonding and there are four intermolecular O···O distances less than or equal to 2·90 Å outside the coordination polyhedron. This gives a plausible intermolecular hydrogen bonding scheme involving all the oxygen atoms [Table 7(*b*)]. The assumed hydrogen bonds link the molecule in all directions and form a three-dimensional network (Fig. 4).

This investigation has been carried out within a research programme directed by Dr. Peder Kierkegaard

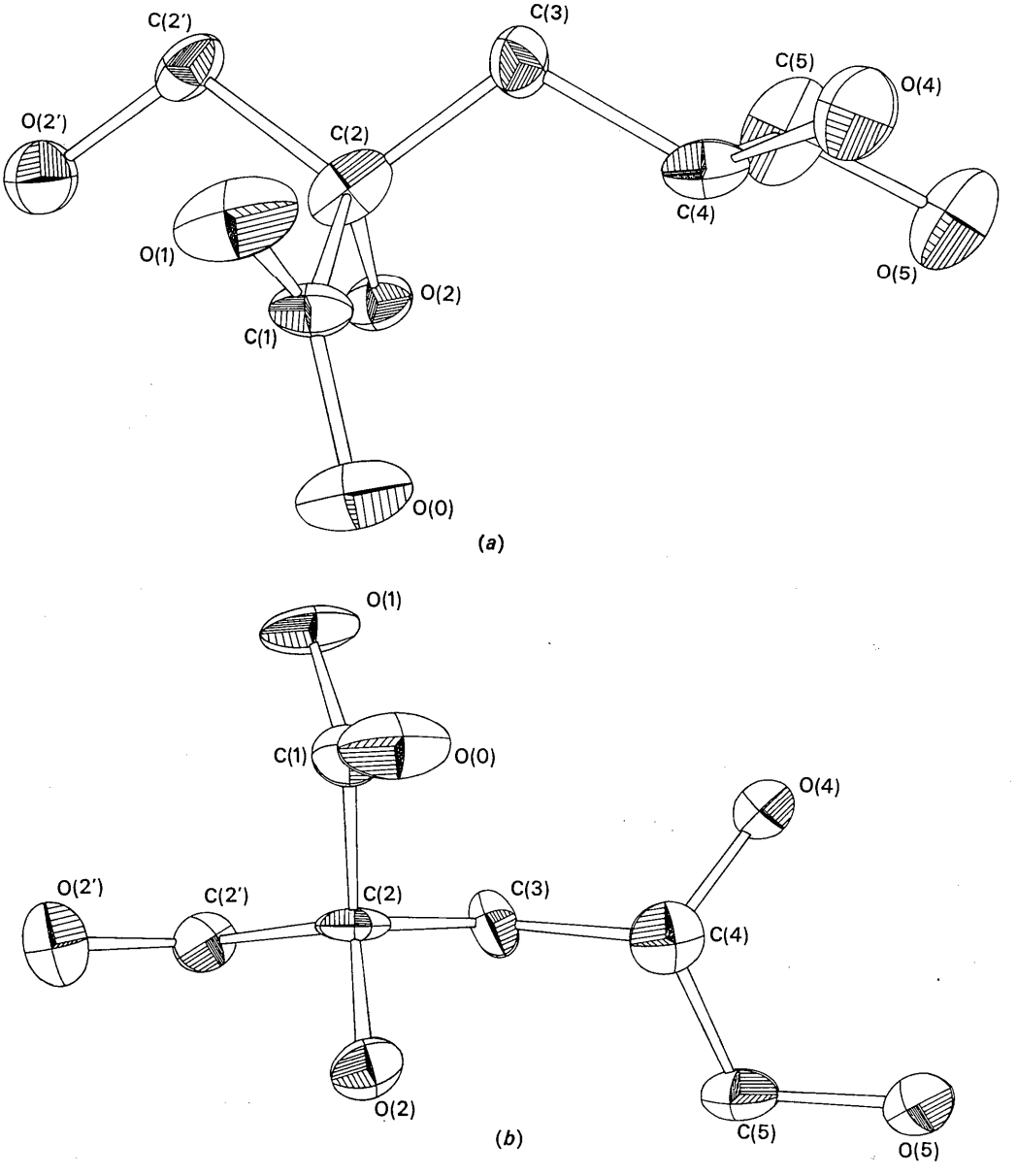

Fig. 2. Structure of the α-D-glucoisosaccharate ion. (*a*) O(2′), C(2′), C(2), C(3) and C(4) approximately in the plane of the paper. (*b*) Rotated 90° from (*a*).

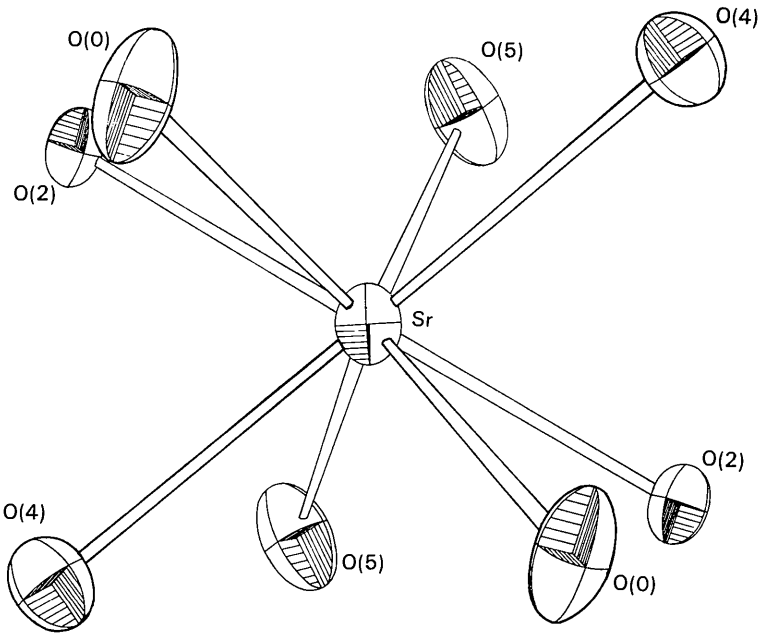

Fig. 3. The coordination polyhedron around strontium.

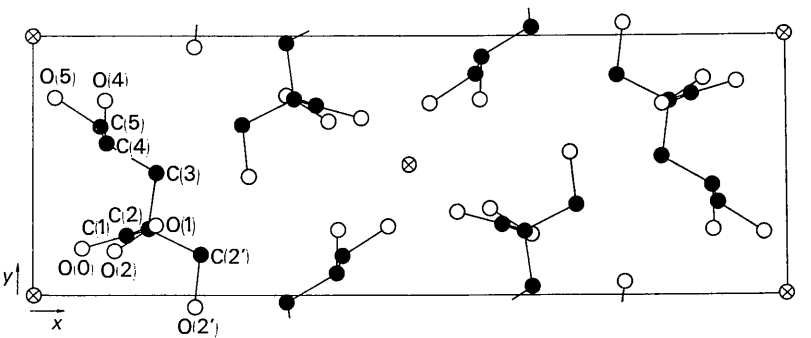

Fig. 4. The unit cell projected along the *c* axis. ⊗ strontium, ○ oxygen, ● carbon.

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