SHORT STRUCTURAL PAPER

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Structure of Strontium Hydroxide Phosphate, $Sr_5(PO_4)_3OH$

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Abstract. Hexagonal, $P6_3/m$, $a=9{\cdot}745$ (1) Å, $c=7{\cdot}265$ (1) Å, ideal formula $Sr_5(PO_4)_3OH$, $Z=2$, density not measured. The crystals were prepared hydrothermally by Schnell, Kiesewetter, Kim & Hayek [*Mh. Chem.* (1971) **102**, 1327]. The phosphate tetrahedra are less distorted than in the isostructural hydroxyapatite, $Ca_5(PO_4)_3OH$. Both substances are OH-deficient, with charge balance apparently maintained by Sr and Ca vacancies.

Introduction. Strontium hydroxide phosphate is closely related to hydroxyapatite and, as such, has the possibility of being incorporated into bony tissue and dental enamel. In particular, Sr is known to substitute for Ca in these tissues. Strontium has also been suggested as a caries inhibitor (Curzon, Adkins, Bibby & Losee, 1970). The fact that octastrontium phosphate does not form under conditions suitable for the formation of octacalcium phosphate (Schnell, Kiesewetter, Kim & Hayek, 1971) shows a difference between strontium phosphates and calcium phosphates in crystallization properties. It has, therefore, become increasingly important that the atomic scale structural differences between 'Sr apatites' and 'Ca apatites' be determined.

The general structural features of the isostructural calcium hydroxide phosphate, hydroxyapatite, have been described by Beevers & McIntyre (1946). Kay, Young & Posner (1964), using neutron-diffraction data, located the hydroxyl group. A subsequent, detailed structure refinement with X-ray data was carried out by Sudarsanan & Young (1969). No structural studies have been so far carried out on 'strontium apatites'. Hence, a refinement of the structure of strontium hydroxide phosphate was undertaken in order to elucidate the atomic-scale modifications introduced when Sr is substituted for Ca in hydroxyapatite.

A single-crystal fragment approximating to a cube 0·21 mm on a side was used for measurement of intensities of 1130 independent reflections (out of a possible 1475 in the range $0<\sin\theta/\lambda\leq 0{\cdot}76$) with a computer-controlled four-circle diffractometer. A balanced-filter (Zr and Y) ω-scan technique with Mo K radiation was used for the low-angle reflections for which the absorption edge of Zr fell within the scanning range for peak plus background. Zr-filtered Mo K radiation and the 2θ-scan method were employed for other reflections. Simultaneous diffraction effects were assessed by remeasurement of each reflection intensity after the specimen was rotated about the diffraction vector by one degree (no $hk.0$ reflections were measured because, with the four-circle geometry used, it is not possible to produce rotation about the diffraction vector when the φ and ω axes are parallel). The two measures differed by more than three times the expected standard deviation in 47 cases and those reflections were not used in the refinements. For the stronger reflections, ~40%, the net intensities were measured to 1% statistical precision; the remaining ~60% were measured with statistical error <0·06% of the strongest reflection intensity. The basic experimental conditions are described in detail elsewhere (Mackie, 1972). Absorption corrections were based on the tabular data in *International Tables for X-ray Crystallography* (1959) for a spherical specimen ($\mu R=2{\cdot}5$).

A full-matrix least-squares refinement of all variable positional and temperature parameters was made, starting from the hydroxyapatite parameters (Sudarsanan & Young, 1969). Busing, Martin & Levy's (1962) *ORFLS* program modified by Johnson (1966) and called *XFLS* was used. The sources of the atomic scattering factors used were: for Sr^{2+} and P, Cromer & Waber (1965); for hydroxyl oxygen (O^-), *International Tables for X-ray Crystallography* (1962); and for phosphate oxygens (O^{2-}), Tokonami (1965). Anomalous dispersion corrections were made with values of $\Delta f'$

Table 1. *Comparison of unit cell dimensions of* $Sr_5(PO_4)_3OH$ *and* $Ca_5(PO_4)_3OH$

Crystal	a (Å)	c (Å)
$Sr_5(PO_4)_3OH$	9·745 (1)	7·265 (1)
$Ca_5(PO_4)_3OH$	9·423 (1)*	6·875 (1)*
	9·418 (1)†	6·880 (1)†

* Values redetermined, as part of the present work, by least-squares refinement with the angular readings of 12 independent reflections obtained with crystal X-23-4 described by Sudarsanan & Young (1969).

† Current results with powder specimen of synthetic hydroxyapatite prepared by precipitation according to the method described by Elliott (1964).

and $\Delta f''$ calculated by Cromer (1965). The observed structure factors were corrected for secondary extinction (Zachariasen, 1963). The final cycles of least-squares refinement were done with hydrogen also included in the model at its probable position calculated on the assumption that the O–H distance is 0·992 Å. The final values of the reliability factors are $R_1=0{\cdot}053$, $R_2=0{\cdot}062$, and $wR_2=0{\cdot}073$ where

Table 2. *Positional and thermal parameters of strontium hydroxide phosphate and hydroxyapatite*

All values are multiplied by 10^4, except for fractions; standard deviations are given within parentheses for parameters varied.

A. Strontium hydroxide phosphate

	Multiplier*	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O(1)	5024 (85)	3329 (5)	4812 (5)	$\frac{1}{4}$	35 (5)	35 (5)	54 (6)	28 (4)	0	0
O(2)	4996 (89)	5834 (5)	4628 (5)	$\frac{1}{4}$	21 (4)	33 (5)	81 (7)	11 (3)	0	0
O(3)	10224 (142)	3456 (4)	2611 (4)	786 (4)	86 (5)	44 (4)	41 (4)	43 (4)	−31 (3)	−20 (3)
P	5000 (40)	4002 (1)	3679 (1)	$\frac{1}{4}$	20 (1)	19 (1)	26 (2)	11 (1)	0	0
Sr(1)	3242 (12)	$\frac{1}{3}$	$\frac{2}{3}$	1 (1)	30 (1)	30	25 (1)	15	0	0
Sr(2)	4912 (14)	2442 (1)	9856 (1)	$\frac{1}{4}$	23 (1)	26 (1)	34 (1)	11 (1)	0	0
O(OH)	1476 (69)	0	0	1856 (14)	18 (14)	18	95 (19)	9	0	0

B. Hydroxyapatite (Sudarsanan & Young, 1969)

	Multiplier*	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O(1)	5000	3284 (2)	4848 (2)	$\frac{1}{4}$	39 (2)	30 (1)	54 (2)	27 (1)	0	0
O(2)	5000	5873 (2)	4651 (2)	$\frac{1}{4}$	20 (1)	26 (1)	96 (3)	9 (1)	0	0
O(3)	10000	3437 (2)	2579 (1)	702 (2)	92 (2)	42 (1)	49 (2)	45 (2)	−41 (2)	−27 (1)
P	5000	3987 (2)	3685 (1)	$\frac{1}{4}$	19 (1)	17 (1)	25 (1)	10 (1)	0	0
Ca(1)	3234 (1)	$\frac{1}{3}$	$\frac{2}{3}$	15 (1)	31 (1)	31	18 (2)	16	0	0
Ca(2)	4852 (14)	2468 (2)	9934 (1)	$\frac{1}{4}$	21 (1)	23 (1)	28 (1)	10 (1)	0	0
O(OH)	1525 (20)	0	0	1950 (2)	25 (2)	25	102 (8)	13	13	0

* Multiplier × site multiplicity (arising because one or more symmetry elements act at the site) = site occupancy factor (ideally = 1).

Table 3. *Squares of observed and calculated structure factors for* $Sr_5(PO_4)_3OH$

h	k	$\lvert F_o\rvert^2$	$\lvert F_c\rvert^2$
		$l = 1$	
1	0	120	148
3	0	323	336
4	0	57	64
5	0	550	483
6	0	1705	1598
7	0	163	174
8	0	21	38
9	0	27	36
10	0	2704	2464
11	0	110	47
12	0	445	393
13	0	691	617
14	0	768	704
15	0	119	159
16	0	78	48
17	0	37	19
1	1	1607	1117
4	1	566	543
5	1	14077	15600
6	1	4416	4327
7	1	33	20
8	1	8	9
9	1	2549	2383
10	1	6110	5393
11	1	244	230
12	1	39	57
13	1	1171	1050
14	1	445	339
15	1	29	70
16	1	245	163
1	2	13891	13662
2	2	275	226
3	2	15325	16033
5	2	3352	3500
6	2	399	376
7	2	6572	6006
8	2	1304	1188
9	2	213	171
10	2	1437	1318
11	2	2265	2072
12	2	994	939
13	2	189	160
14	2	290	238
15	2	1638	1403
16	2	164	75
1	3	1301	1069
2	3	9778	9728
4	3	5067	4913
5	3	126	92
6	3	5231	5547
9	3	172	166
10	3	146	86
11	3	132	65
12	3	128	161
13	3	71	108
14	3	70	59
15	3	107	79
1	4	22	1
2	4	3992	3800
5	4	2251	2168
6	4	1228	1296
7	4	1668	1681
8	4	24	6
9	4	366	372
10	4	1779	1663
11	4	763	645
12	4	23	5
13	4	254	159
14	4	502	426
15	4	43	43
1	5	4362	4070
2	5	6976	6548
3	5	32	11
4	5	3079	2973
5	5	2555	2492
6	5	3832	3897
7	5	850	899
8	5	411	331
9	5	310	290
10	5	475	388
11	5	133	90
12	5	757	616
13	5	267	223
1	6	2233	2108
2	6	222	227
3	6	5267	5244
5	6	2041	2024
6	6	46	75
7	6	3599	3598
9	6	25	65
10	6	79	71
11	6	963	828
12	6	319	318
13	6	142	91
1	7	53	15
2	7	439	415
3	7	2179	2036
4	7	58	38
5	7	205	177
6	7	149	241
7	7	729	789
8	7	165	86
9	7	83	19
10	7	139	109
11	7	128	95
12	7	32	1
1	8	422	391
2	8	7	44
3	8	793	774
4	8	566	534
5	8	40	4
6	8	1516	1666
7	8	41	42
8	8	59	94
9	8	30	14
10	8	709	600
11	8	737	528
1	9	354	370
2	9	6797	6671
3	9	739	736
4	9	1168	1114
5	9	1545	1628
6	9	2000	2068
7	9	29	3
8	9	257	223
9	9	112	201
10	9	661	526
11	9	115	14
1	10	664	503
2	10	8	27
3	10	2578	2431
4	10	1567	1538
5	10	42	4
6	10	3	5
7	10	1759	1646
8	10	748	773
9	10	6	6
10	10	67	114
1	11	53	24
2	11	564	487
3	11	164	143
4	11	361	294
5	11	37	2
6	11	51	22
7	11	139	130
8	11	66	2
9	11	25	8
1	12	43	5
2	12	855	807
3	12	758	694
4	12	44	0
5	12	65	10
6	12	624	560
7	12	453	333
1	13	125	75
2	13	900	714
3	13	215	112
4	13	390	351
5	13	74	63
6	13	880	731
1	14	119	142
3	14	150	132
4	14	772	601
5	14	96	62
1	15	58	33
2	15	61	87
3	15	154	129
		$l = 2$	
1	0	6405	7267
2	0	3725	3983
3	0	13972	13322
4	0	26341	26977
6	0	12171	10917
7	0	6983	5996
9	0	2736	2388
10	0	72	8
11	0	741	656
12	0	120	30
13	0	407	355
14	0	267	122
1	1	31759	31739
2	1	554	585
3	1	6046	6027
4	1	4850	4630
7	1	9604	8354
8	1	193	190
9	1	25	14
10	1	7840	6775
11	1	406	499
12	1	70	4
13	1	2722	2237
14	1	72	140
15	1	106	11
1	2	134	217
3	2	2359	1774
4	2	532	509
5	2	5207	4783
6	2	2438	2266
7	2	460	388
8	2	3055	2704
9	2	1911	1638
10	2	143	162
12	2	92	38
13	2	799	769
14	2	501	428
15	2	264	162
1	3	18019	17662
2	3	662	487
3	3	11563	10558
4	3	5157	4722
5	3	15436	14448
6	3	8249	8025
7	3	58	8
8	3	5846	5393
9	3	46	31
10	3	69	40
11	3	13	17
12	3	64	2
13	3	1328	1607
14	3	130	141
15	3	632	573
1	4	140	85
2	4	868	661
3	4	6969	6460
4	4	1244	1182
5	4	3352	3151
6	4	170	145
7	4	1402	1426
8	4	6142	5865
9	4	3630	3328
10	4	4529	3896
11	4	1176	1057
12	4	2302	1908
13	4	447	318
14	4	134	139
15	4	47	42
2	5	24264	24201
3	5	6710	5932
4	5	1044	920
5	5	7002	6779
6	5	18	6
7	5	39	4
8	5	1502	1139
9	5	114	70
10	5	40	62
11	5	1076	1023
12	5	59	35
13	5	116	38
14	5	1195	1100
15	5	14	24
1	6	156	129
2	6	58	7
3	6	14542	13988
4	6	17	5
5	6	152	150
6	6	2804	2878
8	6	55	46
9	6	354	326
10	6	46	14
11	6	98	40
1	7	1252	1114
2	7	878	826
3	7	95	96
4	7	66	22
5	7	5329	5558
6	7	1922	2009
7	7	3229	3433
8	7	3063	4050
9	7	4794	4392
10	7	653	567
1	8	8171	7662
2	8	8427	7699
3	8	659	606
4	8	7095	6926
5	8	300	295
6	8	27	0
7	8	44	8
8	8	53	21
9	8	557	550
1	9	45	83
2	9	536	491
3	9	4407	4336
4	9	767	650
5	9	49	0
6	9	2158	2057
7	9	49	75
8	9	20	10
1	10	349	272
2	10	34	76
4	10	2577	2369
5	10	158	186
6	10	469	479
7	10	2238	2150
1	11	4248	3904
3	11	60	40
4	11	620	595
5	11	524	436
6	11	155	174
1	12	6723	6124
2	12	22	25
3	12	1491	1515
4	12	2799	2675
1	13	1174	1055
2	13	76	79
1	14	67	29
2	14	613	451
		$l = 3$	
0	1	236	254
0	2	2182	2978
0	3	205	245
0	5	642	750
0	6	307	537
0	7	111	152
0	8	119	93
0	9	14	102
0	10	1244	1213
0	11	11	19
0	12	279	284
0	13	835	800
0	14	818	715
1	1	10742	10068
3	1	2439	2250
4	1	872	845
5	1	14306	13214
6	1	2131	1757
7	1	98	102
8	1	19	9
9	1	3560	2911
10	1	7161	5982
11	1	391	251
12	1	60	20
14	1	365	224
1	2	13792	12072
3	2	16704	15570
4	2	34	34
5	2	4096	3733
5	2	3338	3733
6	2	53	33
8	2	1234	1302
9	2	563	562
10	2	1003	1002
11	2	2763	2850
12	2	997	1021
13	2	161	163
1	3	873	859
2	3	2509	2608
3	3	2040	2393
4	3	5791	6201
5	3	302	276
6	3	2645	2948
7	3	2653	2964
8	3	37	14
9	3	168	119
10	3	171	104
11	3	120	114
12	3	161	181
13	3	151	174
1	4	339	325
2	4	6728	7190
3	4	422	465
5	4	1612	1702
6	4	1020	1167
7	4	1191	1305
8	4	39	15
9	4	367	368
10	4	2097	2255
11	4	747	761
12	4	49	35
1	5	1948	1977
2	5	5350	5728
3	5	25	17
4	5	1961	2142
5	5	1752	1930
6	5	3820	4425
7	5	136	211
8	5	414	463
9	5	179	156
1	6	1668	1798
3	6	1756	1977
4	6	2396	2398
5	6	771	830
6	6	20	15
7	6	2497	2828
8	6	139	141
9	6	34	11
10	6	169	87
1	7	448	476
3	7	1111	1100
4	7	249	212
5	7	31	5
6	7	127	223
7	7	465	560
8	7	50	35
9	7	19	36
10	7	91	80
1	8	47	6
2	8	31	33
3	8	677	729
4	8	177	221
5	8	43	12
6	8	1020	1201
7	8	79	137
8	8	177	216
9	8	19	13
1	9	769	855
2	9	4654	5237
3	9	627	675
4	9	300	397
5	9	1304	1184
6	9	1100	1227
7	9	27	19
8	9	146	174
1	10	600	638
2	10	60	84
3	10	2092	2282
4	10	1006	1153
5	10	107	13
7	10	1332	1491
1	11	96	47
2	11	477	535
3	11	123	158
4	11	173	215
5	11	55	59
1	12	28	75
2	12	1320	1029
3	12	369	363
4	12	19	3
1	13	204	216
2	13	612	584
3	13	63	17
1	14	213	156
		$l = 4$	
1	0	721	830
2	0	2123	3423
5	0	379	367
6	0	1673	1628
7	0	16	3
8	0	3400	3884
9	0	3057	2893
10	0	2454	2357
12	0	3707	3811
14	0	1235	1286
1	1	1316	1247
2	1	7273	7521
3	1	1033	971
4	1	8007	8953
5	1	10514	11328
6	1	6102	6205
7	1	1409	1409
8	1	1665	1646
9	1	3057	2940
10	1	98	42
11	1	318	312
12	1	1006	1027
13	1	129	75
14	1	220	228
1	2	6554	8528
2	2	402	439
4	2	7410	7970
5	2	4865	4407
6	2	557	566
7	2	5779	5737
8	2	2208	2363
9	2	128	94
10	2	891	840
11	2	446	463
12	2	550	538
1	3	356	408
2	3	4862	4617
3	3	3063	2880
4	3	203	174
5	3	1538	1591
7	3	2575	2669
8	3	446	437
9	3	5638	5802
10	3	910	1013
11	3	774	749
12	3	2921	2801
1	4	18721	20180
3	4	74	20
4	4	21747	23457
5	4	49	40
5	4	65	40
7	4	2759	3094
8	4	808	830
9	4	212	225
10	4	54	15
11	4	51	11
12	4	175	227
1	5	1914	1900
2	5	23	12
3	5	59	39
4	5	1524	1022
5	5	708	851
6	5	2163	2470
7	5	1838	1972
8	5	1631	1701
9	5	1619	1755
10	5	1261	1358
11	5	326	327
1	6	5611	5769
2	6	4477	4556
3	6	21	16
4	6	2501	2809
5	6	1423	1546
6	6	1039	1215
7	6	2147	2536
8	6	1532	1679
9	6	1516	1769
10	6	514	551
2	7	1906	1035
3	7	1653	1731
5	7	504	630
6	7	32	32
7	7	115	124
8	7	691	737
9	7	1365	1189
1	8	468	536
2	8	349	341
4	8	903	968
5	8	2411	3286
6	8	1069	1311
7	8	970	1009
8	8	1930	2129
1	9	1602	1712
2	9	4260	4391
4	9	119	200
6	9	107	233
7	9	270	319
1	10	4343	4664
2	10	1051	1110
3	10	642	697
4	10	316	344
5	10	259	326
6	10	5	34
1	11	307	375
2	11	474	1017
3	11	1229	1361
4	11	70	55
5	11	4107	4424
1	12	1512	1439
2	12	606	660
3	12	162	208
4	12	540	519
1	13	650	613
2	13	1151	1166
1	14	305	348
		$l = 5$	
1	0	24	30
2	0	2	5
3	0	7	12
4	0	192	185
5	0	164	126
6	0	979	902
7	0	96	84
8	0	26	13
9	0	13	16
10	0	1403	1750
12	0	311	296
13	0	449	413
14	0	562	512
1	1	1118	1016
2	1	12201	12577
3	1	14	43
4	1	287	293
6	1	2718	2680
7	1	38	5
8	1	15	8
9	1	1568	1492
10	1	3603	3585
11	1	102	141
12	1	64	57
13	1	752	743
1	2	6747	6466
2	2	231	210
3	2	8440	8030
4	2	69	37
5	2	1954	2000
6	2	245	325
7	2	3856	3954
8	2	792	742
9	2	45	96
10	2	768	792
11	2	1427	1376
12	2	732	692
13	2	194	113
2	3	5593	5088
3	3	4329	4108
4	3	2441	2446
5	3	46	40
6	3	3173	3413
7	3	1022	1013
8	3	142	178
9	3	146	127
10	3	23	56
11	3	66	50
12	3	134	118
1	4	25	1
2	4	2558	2437
4	4	665	679
5	4	1373	1443
6	4	823	891
7	4	1059	1069
8	4	17	2
9	4	259	233
10	4	1040	1086
11	4	464	472
1	5	2503	2492
2	5	4125	4101
3	5	7	11
4	5	1916	1965
5	5	1597	1619
7	5	616	689
8	5	157	181
9	5	254	214
10	5	339	264
1	6	1032	1016
2	6	150	127
3	6	3418	3653
4	6	1648	1999
5	6	1423	1516
6	6	29	58
7	6	2149	2353
8	6	47	35
9	6	29	42
10	6	30	45
3	7	1320	1354
4	7	46	19
6	7	190	174
7	7	557	593
8	7	67	77
9	7	10	10
1	8	60	160
2	8	69	36
3	8	309	536
4	8	510	456
5	8	50	3
6	8	1359	1215
7	8	21	27
8	8	62	68
2	9	4457	4671
3	9	470	506
4	9	813	826
5	9	1223	1236
6	9	1445	1521
7	9	67	2
1	10	431	375
2	10	42	34
3	10	1638	1689
4	10	1037	1062
1	11	30	17
2	11	470	401
3	11	137	97
4	11	259	229
2	12	615	565
3	12	490	555
1	13	46	50
2	13	501	557
		$l = 6$	
0	0	17848	17612
1	0	3166	3458
2	0	190	134
3	0	168	176
4	0	11260	11675
5	0	4307	4165
6	0	10397	9146
8	0	10963	10309
10	0	68	89
11	0	848	754
13	0	147	133
1	1	20107	20625
2	1	245	240
3	1	609	578
4	1	3506	3494
5	1	307	330
6	1	370	359
7	1	4952	4699
8	1	722	768
9	1	96	19
10	1	5363	5235
11	1	265	335
13	1	2108	2050
1	2	522	507
2	2	14631	14241
3	2	301	278
4	2	130	105
5	2	2016	1911
6	2	442	501
7	2	367	361
8	2	1921	1868
9	2	590	572
10	2	20	6
11	2	2243	2144
12	2	27	29
1	3	11373	11690
2	3	19	8
3	3	8737	8402
4	3	2506	2381
5	3	6214	6297
7	3	150	98
8	3	2909	2806
9	3	12	4
10	3	31	11
11	3	21	3
1	4	600	570
2	4	747	754
3	4	2105	2025
4	4	63	94
5	4	2606	2611
6	4	270	278
7	4	1627	1613
8	4	4154	4060
9	4	2808	2881
10	4	3147	3065
11	4	301	408
1	5	572	562
2	5	8404	8753
3	5	2648	2668
4	5	307	341
6	5	43	2
7	5	93	108
8	5	973	1111
9	5	153	88
10	5	30	80
1	6	28	10
2	6	31	11
3	6	10209	10877
4	6	77	62
5	6	40	26
6	6	2122	2147
7	6	192	160
8	6	177	176
1	7	198	186
2	7	108	185
3	7	115	98
4	7	19	44
5	7	2706	2825
7	7	2019	2137
8	7	1826	1928
1	8	3149	3092
3	8	306	909
5	8	310	312
6	8	13	7
7	8	27	22
1	9	24	6
2	9	263	207
3	9	2698	3041
4	9	149	197
5	9	113	54
6	9	1513	1717
1	10	378	378
2	10	28	10
3	10	55	65
4	10	1224	1319
5	10	71	36
1	11	2403	2329
2	11	1342	1368
4	11	467	490
2	12	46	3
1	13	701	810
		$l = 7$	
1	0	14	4
2	0	28	37
3	0	22	7
5	0	10	10
6	0	347	324
10	0	1219	1134
11	0	47	35
12	0	228	181
1	1	1019	938
2	1	7639	7412
3	1	45	17
4	1	151	167
5	1	6048	5979
6	1	1601	1674
7	1	22	4
8	1	19	7
9	1	1324	1261
10	1	2710	2543
11	1	165	133
12	1	13	20
1	2	4494	4139
2	2	193	121
3	2	5064	4929
4	2	20	28
5	2	1556	1513
6	2	161	124
7	2	2959	2913
8	2	548	493
9	2	46	100
10	2	748	689
11	2	1234	1129
1	3	512	469
2	3	2939	2922
3	3	2704	2534
4	3	1925	1876
5	3	35	58
6	3	2214	2330
7	3	1070	1001
8	3	155	131
9	3	42	86
10	3	70	45
11	3	54	28
1	4	21	14
2	4	1808	1814
3	4	334	356
4	4	329	310
5	4	963	963
6	4	597	636
7	4	805	850
8	4	10	1
9	4	228	197
10	4	1014	934
1	5	1752	1697
2	5	2736	2740
4	5	1078	1063
5	5	904	1026
6	5	1950	1949
7	5	409	427
8	5	219	213
9	5	155	150
1	6	629	595
2	6	96	85
3	6	2097	2127
4	6	1570	1606
5	6	949	908
6	6	38	29
7	6	1761	1830
8	6	29	29
1	7	15	14
2	7	202	200
3	7	962	954
4	7	25	26
5	7	127	79
6	7	179	117
7	7	413	364
1	8	201	125
2	8	41	32
3	8	422	373
4	8	168	187
5	8	29	3
6	8	776	774
1	9	253	265
3	9	476	355
4	9	575	561
5	9	630	736
1	10	276	215
2	10	50	7
3	10	1212	1176
4	10	814	793
1	11	37	6
2	11	261	218
3	11	90	86
		$l = 8$	
0	0	31339	32931
1	0	214	249
2	0	1355	1626
3	0	7903	8542
4	0	1160	1214
5	0	106	178
6	0	828	775
7	0	18	2
8	0	1653	1432
9	0	1493	1429
10	0	1316	1273
11	0	224	251
12	0	1969	1980
1	1	495	419
2	1	3741	3589
3	1	539	481
4	1	3045	3118
5	1	5222	5352
6	1	2476	2803
7	1	652	573
8	1	1107	1060
9	1	1476	1385
10	1	40	27
11	1	261	231
1	2	3520	3292
2	2	317	257
3	2	1177	1113
4	2	4177	4061
5	2	2218	2243
6	2	204	280
7	2	3192	3031
8	2	1416	1280
9	2	54	60
10	2	464	434
11	2	259	255
1	3	22	11
2	3	1830	1767
3	3	1271	1188
4	3	73	70
5	3	682	641
6	3	521	486
7	3	1295	1273
8	3	126	123
9	3	2655	2627
10	3	538	536
1	4	8206	8659
2	4	4402	4420
3	4	29	35
4	4	10513	10892
5	4	171	133
6	4	1020	1026
7	4	1559	1581
8	4	287	271
9	4	24	79
1	5	1265	1216
2	5	22	19
3	5	11	24
4	5	631	571
5	5	397	361
6	5	1002	1173
7	5	990	978
8	5	945	892
1	6	2802	2785
2	6	2074	2171
3	6	49	28
4	6	1340	1456
5	6	704	729
6	6	548	539
7	6	1349	1418
1	7	10243	10105
2	7	569	592
3	7	1148	1102
4	7	4276	4378
5	7	232	237
6	7	48	12
7	7	71	81
1	8	239	237
2	8	67	94
3	8	368	387
4	8	452	448
5	8	1505	1691
1	9	942	851
2	9	2276	2200
3	9	163	205
4	9	130	133
1	10	2428	2258
2	10	561	552
3	10	466	507
1	11	209	153
2	11	604	572
		$l = 9$	
1	0	28	14
2	0	147	230
3	0	53	3
4	0	55	39
5	0	165	182
6	0	102	135
7	0	27	46
8	0	28	22
9	0	105	33
10	0	490	427
11	0	49	9
1	1	1373	1331
2	1	5151	5085
3	1	395	390
4	1	221	175
5	1	3796	3837
6	1	612	590
7	1	40	14
8	1	10	5
9	1	1065	954
10	1	2138	2059
1	2	2811	2624
2	2	33	6
3	2	3503	3412
4	2	49	32
5	2	1311	1019
6	2	12	5
7	2	1703	1597
8	2	432	404
9	2	149	203
10	2	357	310
1	3	345	253
2	3	1001	1075
3	3	904	860
4	3	1455	1400
5	3	95	62
6	3	804	857
7	3	1065	971
8	3	32	2
9	3	46	45
1	4	135	59
2	4	1825	1693
4	4	12	0
5	4	532	547
6	4	393	383
7	4	503	433
8	4	19	1
1	5	737	679
2	5	1806	1754
3	5	22	4
4	5	574	620
5	5	624	599
6	5	1544	1490
7	5	92	81
1	6	475	412
2	6	48	45
3	6	700	709
4	6	744	740
5	6	247	300
6	6	35	4
1	7	97	94
2	7	195	188
3	7	423	385
4	7	78	77
2	8	29	20
3	8	313	261
4	8	76	88
1	9	397	327
2	9	1806	1782
3	9	234	238
1	10	256	231
2	10	57	33
		$l = 10$	
0	0	2433	2427
1	0	1165	1263
2	0	255	191
3	0	227	202
4	0	4458	4457
5	0	2422	2298
6	0	2903	2967
7	0	1082	1070
9	0	826	852
1	1	6068	5915
2	1	24	5
3	1	543	557
4	1	1266	1299
5	1	216	214
6	1	109	43
7	1	1863	1823
8	1	59	75
9	1	27	19
1	2	110	58
2	2	5365	5285
3	2	355	299
4	2	38	10
5	2	1394	1405
6	2	430	394
7	2	123	119
8	2	1007	902
1	3	2304	2263
2	3	69	49
3	3	2945	2810
4	3	931	931
5	3	2754	2778
6	3	2160	2106
8	3	1562	1412
2	4	73	95
3	4	1060	1025
4	4	112	108
5	4	836	870
6	4	47	38
7	4	510	570
1	5	277	227
2	5	4600	4646
3	5	1097	1083
4	5	275	235
5	5	1675	1808
6	5	24	3
2	6	41	16
3	6	3579	3722
5	6	65	27
1	7	74	84
2	7	139	162
3	7	37	62
4	7	49	11
1	8	1791	1706
2	8	2040	2041
3	8	207	163
1	9	35	14
		$l = 11$	
1	0	38	3
2	0	25	3
3	0	64	2
4	0	167	81
5	0	13	15
6	0	246	192
7	0	46	18
8	0	57	1
1	1	242	223
2	1	2361	2349
3	1	23	4
4	1	63	58
5	1	2045	2086
6	1	606	670
7	1	16	2
1	2	1329	1343
2	2	77	58
3	2	1653	1620
4	2	45	16
5	2	451	434
6	2	130	115
7	2	1001	939
1	3	132	150
2	3	1233	1225
3	3	838	737
4	3	434	[illegible]
5	3	16	[illegible]
6	3	771	772
2	4	564	523
3	4	233	201
4	4	170	148
5	4	351	314
1	5	549	606
2	5	1008	978
3	5	29	4
4	5	416	434
1	6	140	173
2	6	67	31
3	6	1030	982
1	7	8	0
2	7	16	58
		$l = 12$	
0	0	13306	13546
1	0	62	43
3	0	3500	3665
4	0	209	328
5	0	19	1
6	0	190	188
1	1	61	72
2	1	1440	1464
3	1	461	386
4	1	1151	1144
5	1	1174	1220
1	2	491	474
2	2	153	186
3	2	474	487
4	2	620	554
5	2	1229	1229
1	3	159	160
2	3	702	735
3	3	350	316
4	3	29	17
1	4	2570	2584
2	4	1473	1532
3	4	301	351
1	5	190	179
		$l = 13$	
1	1	174	196

$$R_1=\sum(|F_o|-|F_c|)/\sum|F_o|\,,$$
$$R_2=\sum(|F_o|^2-|F_c|^2)/\sum|F_o|^2,$$
$$wR_2=\{\sum w(|F_o|^2-|F_c|^2)^2/\sum w|F_o|^4\}^{1/2},$$

and w is the reciprocal of the variance estimated from counting statistics.

Results and discussion. Table 1 gives the lattice parameters obtained for strontium hydroxide phosphate by least-squares refinement with the angular readings of twelve independent reflections obtained from the diffractometer. As the ionic radius of Ca^{2+} is 1·00 Å and that of Sr^{2+} is 1·16 Å (Shannon & Prewitt, 1969), a larger cell in the Sr case is to be expected. As expected, strontium hydroxide phosphate is isostructural with hydroxyapatite (space group $P6_3/m$). The positional and temperature factors, with their standard deviations, are given in Table 2. Structure factors are given in Table 3. The site-occupancy factors (multipliers) indicate obvious OH deficiencies in both the strontium and the calcium hydroxide phosphates (Table 2). Compared with the PO_4 present, Sr and Ca appear to be deficient in approximately the amounts required to explain the OH deficiences in terms of loss of $Sr(OH)_2$ and $Ca(OH)_2$ respectively.

A comparison of the bond angles and interatomic distances with those of hydroxyapatite is presented in Table 4. Some small differences are noted. The phosphate tetrahedron is similarly but less distorted in this strontium analog than it is in hydroxyapatite itself (±1·4° *vs.* ±2·0°, respectively, departure from the tetrahedral angle). The hydroxyl oxygen is farther away from the mirror planes at $z=\frac{1}{4}$ and $\frac{3}{4}$ (0·46 Å *vs.* 0·37 Å in hydroxyapatite), increasing the Sr(2)–O distance to 2·50 Å (*vs.* 2·39 Å for hydroxyapatite). No significant differences appear in the thermal parameters (Table 2). Thus, the differences in crystal-chemical properties mentioned in the introduction can only be correlated with the seemingly subtle differences in PO_4-tetrahedron distortion and in OH displacement from the mirror plane.

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Table 4. *A comparison of bond angles and interatomic distances with those of hydroxyapatite*†

Standard deviation, in units of the last significant figure, is given in parentheses.

	$Sr_5(PO_4)_3OH$	$Ca_5(PO_4)_3OH$
1. PO_4 Tetrahedra		
(*a*) Bond angles (°)		
O(1)–P–O(2)	110·5 (3)	111·13 (1)
O(1)–P–O(3)	110·9 (2)	111·41 (4)
O(2)–P–O(3)	108·1 (2)	107·47 (5)
O(3)–P–O′(3)	108·2 (2)	107·76 (8)
(*b*) Interatomic distances (Å)		
O(1)–P	1·539 (4)	1·539 (1)
O(2)–P	1·546 (4)	1·539 (1)
O(3)–P	1·537 (4)*	1·532 (1)*
O(1)–O(2)	2·535 (5)	2·538 (2)
O(2)–O(3)	2·495 (5)*	2·476 (1)*
O(1)–O(3)	2·535 (5)*	2·537 (1)
O(3)–O′(3)	2·489 (5)	2·475 (2)
2. Environment of metallic atoms		
Interatomic distances (Å)		
M(1)–O(1)	2·561 (3)**	2·405 (1)**
M(1)–O(2)	2·565 (3)**	2·454 (1)**
M(1)–O(3)	2·901 (4)**	2·802 (1)**
M(2)–O(1)	2·757 (5)	2·710 (1)
M(2)–O(2)	2·476 (4)	2·357 (1)
M(2)–O(3)	2·661 (3)*	2·511 (1)*
M(2)–O″(3)	2·512 (3)*	2·345 (2)*
M(2)–O(OH)	2·498 (2)	2·389 (1)
M(2)–M_2''(2)	4·248 (2)	4·084 (1)

† The Function and Error Program of Busing, Martin & Levy (1964) was used for the calculations. The values for hydroxyapatite were calculated from the results for the crystal X-23-4 of Sudarsanan & Young (1969). M represents Sr or Ca, as appropriate. O′(3) is related to O(3) by reflection in m at $z=\frac{1}{4}$. A doubly primed symbol O″(3) designates an atom with coordinates y, $y-x$, $z+\frac{1}{2}$ where x, y, z are those of the atom designated by O(3).

* The number of asterisks indicates the number of times the distance is repeated for symmetry-related sites of the second atom.

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