The similarity of the behaviour of antimony to that of zinc and cadmium is associated similarly with a markedly higher spacing of the antimony (111) planes which are normal to the trigonal axis, than would correspond to close packing of spheres. For the hexagonal packing of spheres, $c/a = 1·633$, whereas for antimony the equivalent ratio is 1·744, and this is about half way between 1·633 and the c/a of zinc and cadmium, *i.e.* 1·856 and 1·886 at 25 °C (Wyckoff, 1948) respectively.

The pseudo-octahedral twinning (submicroscopic) indicated strongly in the present results is a further expression of the pseudo-cubic form of the antimony structure, and does not appear to have been previously observed. The strong twinning (and secondary twinning) hitherto observed, presumably by optical means, has been identified as of {110} type relative to the f.c. rhombohedral pseudo-cubic axes (Gough & Cox, 1930, 1932; Hall, 1954). Since the deviation from f.c. cubic form is so slight, and since {110} is a plane of symmetry for a cubic lattice, such {110} twinning would only cause a few degrees change in lattice orientation, and this, together with the length of the observed diffraction arcs, may be why we did not observe clearly any twinning of this type, although some might have been present.

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The Crystal Structure of Decammine-μ-peroxodicobalt Tetrathiocyanate

BY NILS-GÖSTA VANNERBERG

Department of Inorganic Chemistry, Chalmers University of Technology and University of Gothenburg, Sweden

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The compound $[(NH_3)_5CoO_2Co(NH_3)_5](SCN)_4$ has been prepared and its structure determined. The space group is *Pnnm* No. 58, with $a = 13·22$, $b = 10·58$, $c = 7·88$ Å. The two cobalt atoms are linked together by a peroxide group, each cobalt atom being bonded to one oxygen atom.

Introduction

Cobalt forms two kinds of μ-peroxo complex ions, *viz.* $[(NH_3)_5CoO_2Co(NH_3)_5]^{5+}$ and $[(NH_3)_5CoO_2Co(NH_3)_5]^{4+}$. The structure of the former was determined and described by Vannerberg & Brosset (1963). In that paper was also given a historical introduction to the subject. In this paper the structure of decammine-μ-peroxodicobalt(III) tetrathiocyanate will be described.

Experimental and crystal data

Very well developed needle-shaped crystals of decammine-μ-peroxodicobalt(III) tetrathiocyanate are formed when a strongly ammoniacal solution of cobalt(II) thiocyanate is allowed to stand in contact with air. (Analysis: Found: Co 20·6, NH_3 30·0, SCN 41·7%. Calculated: Co 21·3, NH_3 30·8, SCN 42·1%.) The crystals have orthorhombic symmetry. The unit cell contains two formula units and has the following lattice constants, as determined from Guinier photographs:

$$a=13{\cdot}22\pm0{\cdot}01,\ b=10{\cdot}58\pm0{\cdot}01,\ c=7{\cdot}88\pm0{\cdot}007\ \text{Å}.$$

The observed density was 1·65 g.cm^{-3}, which is to be compared with the calculated value of 1·66 g.cm^{-3} assuming two formula units in the unit cell.

The crystals were rotated about the needle axis which is parallel to the crystallographic c axis. All zones detectable with Cu $K\alpha$ radiation were registered by the multiple film technique in an integrating Weissenberg camera. The intensities were estimated visually by comparison with a standard scale. The usual corrections for Lorentz and polarization effects were made, but no corrections for absorption.

The systematic extinctions were $h0l$, absent for $h+l=2n+1$, and $0kl$, absent for $k+l=2n+1$, indicating space group $Pnnm$ or $Pnn2$, the former being subsequently proved to be correct by comparison between observed and calculated structure factors.

Structure analysis

The positions of the four cobalt atoms were determined from a Patterson projection on (001). From these positions sufficient structure factor signs were obtained to perform a complete three-dimensional electron-density calculation. At this stage the space group was assumed to be $Pnnm$. From the three-dimensional electron density calculation, the positions of the cobalt ligands and four of the eight thiocyanate ions were found.

The electron-density calculations gave two crystallographically different fourfold positions in which the sulphur atoms of the thiocyanate ions could be placed. Both these positions were located at about 1·5 Å from a twofold axis. It was then thought to be impossible to place the thiocyanate chain in a direction towards the twofold axes.

Both the above mentioned fourfold positions were tried, but after many fruitless attempts to obtain agreement between observed and calculated structure factors, the R index never dropping below 0·29, it was eventually assumed that the missing thiocyanate ions could not be placed in a totally ordered way. Instead the following structural proposal was tried. The above mentioned fourfold positions were occupied by the terminal atoms sulphur and nitrogen in a completely disordered way, while the four carbon atoms were distributed over two fourfold positions close to the twofold axes. Thus the thiocyanate ions passed through the twofold axes, the twofold symmetry being preserved owing to the fact that the orientation of the ions along a definite direction was completely disordered. The R index then obtained was 0·22.

The structure was refined by the least-squares method with a program given by Bränden & Åsbrink (1962), with the use of isotropic temperature factors. It was assumed in the calculation that terminal atoms in the disordered thiocyanate ions occupied the same crystallographic positions. After a few cycles the R index dropped to 0·16. The atomic form factor of cobalt was not corrected for anomalous dispersion and the hydrogen atoms were not included in the calculations. The observed and calculated structure factors are given in Table 3 and the atomic parameters in Table 1.

Table 1. *Parameter values and temperature factors for the atoms in* $[(NH_3)_5CoO_2Co(NH_3)_5](SCN)_4$

Atom	Position	x	y	z	B
Co	g	0·1103	0·1636	0	3·1
O	g	0·491	0·423	0·5	2·8
N(1)	h	0·163	0·047	0·173	1·2
N(2)	h	0·048	0·277	0·171	4·0
N(3)	g	0·232	0·267	0	3·5
N(4)	g	0·370	0·026	0·5	0·8
S(1)	g	0·255	0·251	0·5	3·9
S(2)+N(5)	g	0·405	0·017	0	4·1
S(3)+N(6)	g	0·463	0·387	0	5·6
C(1)	g	0·313	0·123	0·5	4·9
C(2)	g	0·536	0·966	0	2·0
C(3)	g	0·519	0·525	0	4·4

Table 2. *Standard deviations of parameters and temperature factors in* $[(NH_3)_5CoO_2Co(NH_3)_5](SCN)_4$

Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	$\sigma(B)$
Co	0·0005	0·0006	0	0·1
O	0·002	0·003	0	0·7
N(1)	0·001	0·002	0·004	0·4
N(2)	0·002	0·002	0·005	0·6
N(3)	0·003	0·004	0	0·9
N(4)	0·002	0·003	0	0·7
S(1)	0·001	0·001	0	0·3
S(2)+N(5)	0·002	0·002	0	0·5
S(3)+N(6)	0·002	0·002	0	0·6
C(1)	0·004	0·005	0	1·4
C(2)	0·006	0·007	0	2·1
C(3)	0·010	0·011	0	2·8

Description of the structure

Bond lengths and bond angles are tabulated in Tables 5 and 6. The geometry of the cation $[(NH_3)_5Co{-}O_2{-}Co(NH_3)_5]^{4+}$ can be seen in Fig. 1. The five ammonia molecules and an oxygen atom of the peroxide group form a somewhat distorted octahedron about the cobaltic ions. The angles between adjacent ammonia–cobalt bonds are not significantly different from 90°.

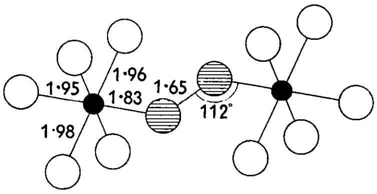

Fig. 1. Configuration of the ion $[(NH_3)_5CoO_2Co(NH_3)_5]^{4+}$. Shaded, O; white, NH_3; black, Co.

Table 3. *Observed and calculated structure factors for* $[(NH_3)_5CoO_2Co(NH_3)_5](SCN)_4$

Unobserved reflexions are omitted

h	k	l	$10F_o$	$10F_c$
4	0	0	119	-167
6	0	0	408	-427
8	0	0	921	633
2	1	0	971	-922
4	1	0	375	-367
5	1	0	230	318
6	1	0	390	429
7	1	0	364	379
8	1	0	321	255
9	1	0	173	13
10	1	0	191	-112
0	2	0	354	-254
1	2	0	910	-857
2	2	0	480	607
3	2	0	404	-447
4	2	0	650	-673
5	2	0	924	834
6	2	0	961	839
7	2	0	718	623
8	2	0	274	-225
9	2	0	169	186
10	2	0	68	157
11	2	0	241	-166
1	3	0	813	-815
2	3	0	256	309
3	3	0	588	261
4	3	0	690	645
5	3	0	1221	1081
9	3	0	643	-622
10	3	0	220	199
0	4	0	899	556
1	4	0	158	-147
2	4	0	433	-493
3	4	0	158	303
4	4	0	205	393
6	4	0	621	-324
7	4	0	357	-454
10	4	0	372	-357
11	4	0	339	370
1	5	0	390	-471
2	5	0	444	397
3	5	0	263	-407
4	5	0	372	384
5	5	0	82	-131
6	5	0	690	-557
8	5	0	639	-461
10	5	0	440	343
2	6	0	292	275
4	6	0	1333	-1025
5	6	0	458	254
6	6	0	292	-170
8	6	0	180	116
10	6	0	567	405
1	7	0	115	114
2	7	0	393	-363
5	7	0	173	-210
6	7	0	151	119
9	7	0	46	91
0	8	0	108	140
1	8	0	675	-546
2	8	0	162	-161
3	8	0	711	-524
4	8	0	314	302
6	8	0	408	-269
7	8	0	354	179
1	9	0	263	-395
2	9	0	194	60
3	9	0	256	303
5	9	0	292	225
0	10	0	375	-358
1	10	0	39	60
2	10	0	227	206
3	10	0	28	86
6	10	0	126	51
8	10	0	82	-142
3	0	1	1211	-1055
5	0	1	181	-211
7	0	1	226	271
9	0	1	533	520
0	1	1	860	639
1	1	1	297	-265
2	1	1	156	216
3	1	1	1243	-1301
4	1	1	405	-497
6	1	1	204	-221
7	1	1	226	146
8	1	1	274	211
10	1	1	380	314
11	1	1	367	-373
1	2	1	722	-685
2	2	1	1042	-1062
4	2	1	127	-122
5	2	1	399	392
6	2	1	389	379
7	2	1	444	436
9	2	1	300	-303
0	3	1	165	-157
1	3	1	259	-324
3	3	1	127	99
4	3	1	645	720
5	3	1	268	-244
6	3	1	249	212
7	3	1	245	156
8	3	1	479	-516
9	3	1	201	-155
10	3	1	329	-248
11	3	1	223	149
1	4	1	213	-231
2	4	1	287	381
3	4	1	217	192
4	4	1	277	328
5	4	1	412	446
6	4	1	377	-379
8	4	1	364	-355
11	4	1	316	-330
0	5	1	383	341
1	5	1	453	419
2	5	1	156	84
3	5	1	252	232
4	5	1	281	-338
7	5	1	575	-621
9	5	1	220	211
1	6	1	169	182
2	6	1	175	132
3	6	1	252	-318
4	6	1	284	265
5	6	1	559	-514
9	6	1	223	166
0	7	1	268	238
1	7	1	505	-460
4	7	1	300	-294
6	7	1	361	-349
7	7	1	405	356
1	8	1	319	-283
2	8	1	351	-408
0	9	1	441	-519
6	0	2	747	-721
8	0	2	862	-861
1	1	2	175	249
2	1	2	202	-289
3	1	2	759	698
6	1	2	862	700
8	1	2	541	469
1	2	2	369	-477
2	2	2	1243	1140
3	2	2	484	-524
4	2	2	152	-164
5	2	2	453	353
6	2	2	404	332
7	2	2	693	633
8	2	2	221	-285
1	3	2	1206	-1130
2	3	2	369	379
3	3	2	369	428
5	3	2	992	847
1	4	2	385	353
2	4	2	663	-601
3	4	2	472	491
4	4	2	507	352
5	4	2	190	-126
1	5	2	178	-178
2	5	2	843	839
3	5	2	194	-186
4	5	2	202	227
5	5	2	213	-121
6	5	2	343	-416
2	6	2	347	326
3	6	2	213	-293
4	6	2	873	-924
1	0	3	253	-110
3	0	3	603	-533
5	0	3	432	-377
7	0	3	196	149
9	0	3	738	809
11	0	3	178	14
0	1	3	82	88
1	1	3	100	41
2	1	3	507	439
3	1	3	678	-632
4	1	3	131	-114
5	1	3	385	349
6	1	3	512	-503
7	1	3	440	386
8	1	3	240	221
9	1	3	157	163
10	1	3	336	379
11	1	3	388	-390
1	2	3	269	-293
2	2	3	709	-645
3	2	3	590	533
4	2	3	411	-393
5	2	3	204	213
6	2	3	204	217
8	2	3	147	213
9	2	3	162	-197
10	2	3	170	-239
11	2	3	178	-125
12	2	3	181	-188
0	3	3	735	-667
1	3	3	90	-59
3	3	3	142	-117
4	3	3	678	665
5	3	3	670	-661
6	3	3	131	20
7	3	3	142	147
8	3	3	279	-320
9	3	3	162	-137
1	4	3	582	-504
2	4	3	727	734
3	4	3	113	137
4	4	3	121	171
5	4	3	240	312
6	4	3	139	-225
0	5	3	523	438
1	5	3	740	688
2	5	3	191	232
3	5	3	307	338
4	5	3	191	-200
5	5	3	144	-96
6	5	3	212	-237
7	5	3	227	-270
9	5	3	248	251
1	6	3	274	297
2	6	3	256	239
3	6	3	209	-259
4	6	3	150	-123
5	6	3	440	-404
7	6	3	168	104
13	6	3	237	-201
0	7	3	235	162
1	7	3	235	-221
4	7	3	300	-350
5	7	3	168	-219
6	7	3	173	-169
7	7	3	328	386
1	8	3	259	-179
2	8	3	170	-152
3	8	3	173	-196
4	8	3	176	-08
6	8	3	279	299
8	8	3	256	211
12	8	3	191	-89
0	9	3	253	-170
1	9	3	181	143
3	9	3	181	-177
6	9	3	181	141
8	9	3	176	-186
10	9	3	155	-162
3	10	3	181	-27
6	10	3	173	-132
9	10	3	147	-190
2	0	4	106	78
4	0	4	142	-118
6	0	4	488	-498
8	0	4	628	631
10	0	4	236	211
14	0	4	134	-216
1	1	4	264	192
2	1	4	311	-293
3	1	4	418	354
6	1	4	493	482
8	1	4	306	325
9	1	4	269	160
10	1	4	168	-102
11	1	4	168	21
0	2	4	293	-158
1	2	4	436	-355
2	2	4	768	655
3	2	4	394	-392
5	2	4	264	269
6	2	4	321	279
7	2	4	514	462
8	2	4	241	-209
9	2	4	163	120
10	2	4	168	102
1	3	4	792	-747
2	3	4	191	218
3	3	4	186	302
4	3	4	119	08
5	3	4	651	628
8	3	4	158	125
9	3	4	165	-286
1	4	4	212	221
2	4	4	371	-404
3	4	4	355	341
4	4	4	363	266
6	4	4	210	-248
11	4	4	163	136
2	5	4	522	585
3	5	4	140	-139
6	5	4	223	-320
7	5	4	163	-27
10	5	4	163	165
2	6	4	272	244
4	6	4	716	-698
7	6	4	168	-04
10	6	4	225	239

Table 4. *System of nomenclature for atoms*

Atom	Fourfold positions	Eightfold positions
A^1	$x, y, 0$	x, y, z
A^2	$\bar{x}, \bar{y}, 0$	$\bar{x}, \bar{y}, z$
A^3	$\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}$	$\frac{1}{2}+x, \frac{1}{2}-y, z$
A^4	$\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}$	$\frac{1}{2}-x, \frac{1}{2}+y, z$
A^{-1}		$x, y, \bar{z}$
A^{-2}		$\bar{x}, \bar{y}, \bar{z}$
A^{-3}		$\frac{1}{2}+x, \frac{1}{2}-y, -z$
A^{-4}		$\frac{1}{2}-x, \frac{1}{2}+y, -z$

Table 5. *Bond lengths and interatomic distances in* $[(NH_3)_5CoO_2Co(NH_3)_5](SCN)_4$

Co^1–O^3	1·83 ± 0·04 Å
Co^1–O^4	2·88 ± 0·04
Co^1–N(1)^1	1·96 ± 0·03
Co^1–N(2)^1	1·98 ± 0·04
Co^1–N(3)^1	1·95 ± 0·05
O^1–O^2	1·65 ± 0·03
O^1–N(1)^3	2·62 ± 0·04
S(1)^1–C(1)^1	1·55 ± 0·06
S(1)^1–N(4)^1	2·82 ± 0·04
C(1)^1–N(4)^1	1·27 ± 0·07
S(2)^1–C(2)^2	1·5 ± 0·1
S(2)^1–N(5)^2	(2·82) assumed
C(2)^2–N(5)^2	1·3 ± 0·1
S(3)^1–C(3)^2	1·6 ± 0·1
S(3)^1–N(6)^2	(2·82) assumed
C(3)^2–N(6)^2	1·2 ± 0·1
N(3)^1–N(4)^4	3·06 ± 0·06
N(2)^1–N(4)^4	3·16 ± 0·06

The distance between the cobalt and the nearest oxygen atom, 1·83 Å, is shorter, and the distance between the oxygen atoms in the peroxide group, 1·65 Å, is significantly longer than the usual distance in peroxides.

The bond lengths in the ordered thiocyanate ions are within the limits of error the same as those found in the ammonium thiocyanate structure reported by Zhdanov & Zvonkova (1949). The ions are almost linear. The bond distances in the disordered groups can be calculated on the assumption that the distance between the terminal atoms (S–N) is 2·82 Å.

The over-all coordination of the complex cation by the anions can be seen in Fig. 2. In the structure the cations are surrounded by twelve thiocyanate ions in a similar way to that in which the oxygen atoms surround the calcium ions in the perovskite structure.

Table 6. *Bond angles in* $[(NH_3)_5CoO_2Co(NH_3)_5](SCN)_4$

O^3–Co^1–$N(1)^1$	$89 \pm 1°$
O^3–Co^1–$N(2)^1$	87 ± 2
O^3–Co^1–$N(3)^1$	176 ± 2
$N(1)^1$–Co^1–$N(1)^{-1}$	88 ± 1
$N(1)^1$–Co^1–$N(2)^1$	93 ± 2
$N(1)^1$–Co^1–$N(3)^1$	93 ± 2
$N(1)^1$–Co^1–$N(2)^{-1}$	176 ± 2
$N(2)^1$–Co^1–$N(2)^{-1}$	86 ± 2
$N(2)^1$–Co^1–$N(3)^1$	90 ± 2
O^4–O^3–Co^1	112 ± 3
O^2–O^1–$N(1)^3$	76 ± 3
Co–$N(1)^1$–O^4	72 ± 3
$S(1)^1$–$C(1)^1$–$N(4)^1$	173 ± 6
Co^1–$N(3)^1$–$N(4)^4$	98 ± 2
$C(1)^4$–$N(4)^4$–$N(3)^1$	117 ± 3

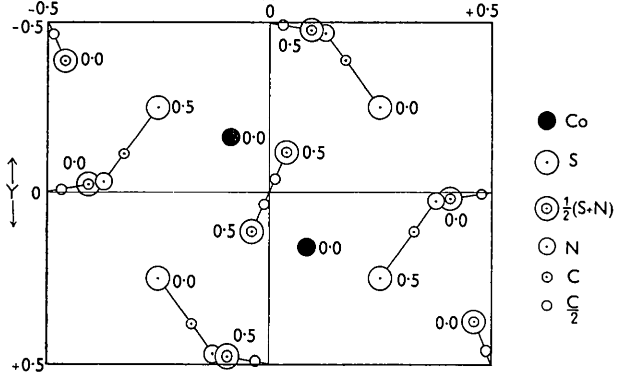

Fig. 2. Projection of the crystal structure of $[(NH_3)_5CoO_2Co(NH_3)_5](SCN)_4$ on (001). All ligands coordinated to the cobalt atoms are omitted.

Discussion of the structure

The structure has certain similarities to the peroxodisulfato ion (Zachariasen, 1934), in which the bridging peroxo group is bonded to the tetrahedral sulphato groups in a typical σ-complex. In the determined structure two octahedral groups are linked together by a peroxo group. The measured bond distances, however show that the peroxocobalt bonds in the present structure can not be pure σ-bonds but that there must also be a weak interaction between the T_{2g} orbitals of the cobalt atoms and the empty anti-bonding p_x–p_x orbitals of the peroxo groups. Back-donation of electrons from the T_{2g} orbitals into the $\sigma^*_{p_x}$ orbital would give the cobalt–oxygen bond some double bond character while diminishing the strength of the oxygen–oxygen bond. This is in accordance with the measured bond lengths.

As mentioned above, the bond distances in the thiocyanate ions agree with the value published for ammonium thiocyanate (Zhdanov & Zvonkova, 1949). The S–C bond, however, is a little shorter, while the C–N bond is a little longer, which may indicate a more pronounced S–C double bond and a less pronounced C–N triple bond. The bond lengths are significantly different from those in compounds such as CH_3–S–C≡N, where the double bond contribution to the S–C bond is unimportant.

The thiocyanate ions is not found to be perfectly linear but the deviation from linearity is not significant. The same phenomenon is found in several investigated thiocyanate groups. (Lindqvist, 1957; Lindqvist & Strandberg, 1957.)

Larsson (1963) has proved that thiocyanate ions or halogens and complex ions like $[Co(en)_2(SCN)_2]^+$ or $[Co(NH_3)_6]^{3+}$ form weak outer sphere complexes, for instance $[Co(NH_3)_6Br]^{2+}$. In the structure determined there are only small indications of such bond formation. This is to be expected as the conditions for the stabilization of an ion pair in the solid state are very unfavourable. There is, however, a weak hydrogen bond between the nitrogen atom of the ordered thiocyanate ion and that ammonia molecule which is opposite to the oxygen atom in the complex ion (Fig. 3). Thus there is a discrete group $[SCN \cdots (NH_3)_5CoO_2Co(NH_3)_5 \cdots NCS]^+$ held together by bonds of very different strengths (Fig. 3).[*]

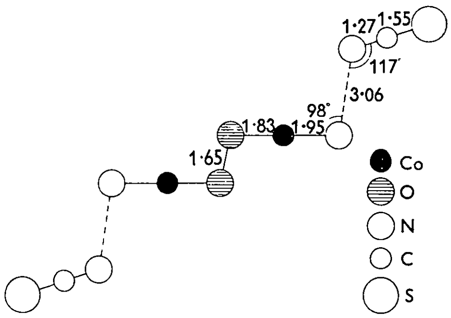

Fig. 3. Hydrogen bonding in the (001) plane.

One of the main products of the oxidation of a solution of ammonia and a cobalt(II) salt by air is $[Co(NH_3)_5H_2O]$. Since the determined structure shows that the oxygen–oxygen bond in $[(NH_3)_5CoO_2Co(NH_3)_5]$ is rather weak and since the decomposition of the ion is favoured by low pH, it is probable that the investigated ion is an intermediate product in the oxidation of cobalt(II) to cobalt(III) by air.

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[*] All other possibilities of hydrogen bond formation can be ruled out because of unfavourable bond distances and bond angles.

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Silicates M_3SiO_5. I. Sr_3SiO_5

BY L. S. DENT GLASSER AND F. P. GLASSER

Chemistry Department, University of Aberdeen, Scotland

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Single crystal X-ray studies show that Sr_3SiO_5 is tetragonal, $P4/ncc$, $a=6{\cdot}934$, $c=10{\cdot}72$ Å, $Z=4$. An approximate structure is deduced from symmetry and packing considerations.

Introduction

Tristrontium silicate, Sr_3SiO_5, was first prepared by Nurse (1952) who published preparative details and optical and X-ray powder data, and very kindly provided us with some single crystals for the present X-ray study. We were especially interested in finding out whether Sr_3SiO_5 belongs to the same class of structure as Ca_3SiO_5 (Jeffery, 1952) and Cd_3SiO_5 (Dent Glasser & Glasser, 1964).

Experimental

Rotation and Weissenberg photographs of single crystals showed that the unit cell is tetragonal, with $a\simeq 6{\cdot}85$, $b\simeq 10{\cdot}62$ Å. Systematic absences were found in $hk0$ for $h+k$ odd, in $0kl$ for l odd, and in hhl for l odd. The space group is therefore No. 130, $P4/ncc$. There is in addition a pronounced systematic weakness among hkl reflexions with $h+k+l$ odd, implying that the structure is approximately body centred.

Powder data

The powder data (Table 1) were indexed by direct comparison of powder photographs and single-crystal rotation photographs taken on the same camera. The observed d-values are mainly taken from Nurse (1952). Three of his lines (3·512, 2·804, 2·737 Å, all very weak) cannot be indexed. These are missing from the pattern recorded by Dear (1957). They evidently do not belong to Sr_3SiO_5. The cell parameters obtained from single-crystal measurements were adjusted slightly to improve the fit of d_c with d_o: the adjusted unit cell has $a=6{\cdot}934$, $c=10{\cdot}72$ Å.

Cell contents

The density of Sr_3SiO_5 was measured by toluene displacement as 4·72, giving $Z=3{\cdot}95$. If it is assumed that $Z=4$, $D_x=4{\cdot}78$. The agreement is satisfactory: furthermore, in the space group $P4/ncc$, all positions have a multiplicity of four or some multiple of four. The calculated cell contents therefore agree with the space group requirements.

Structure

From a knowledge of the space group and density, the structure may be deduced as follows. The unit cell contains 12 strontium, 4 silicon and twenty oxygen atoms. Because there are only four silicon atoms these must be placed in one of the three fourfold positions. One of these $(0, \frac{1}{2}, z)$ lies on the fourfold axis, and can therefore be eliminated because in this position it would be impossible to arrange four oxygen atoms tetrahedrally about it. Both the remaining positions, $0, 0, 0$ ($\bar{4}$) and $0, 0, \frac{1}{4}$ (222), permit a tetrahedral arrangement of oxygen about the silicon, and a possible structure can be deduced starting from either. The structure based on silicon at $0, 0, \frac{1}{4}$ was found, however, to lead to very odd coordination for the strontium atoms, and consideration of the relative intensities of some simple reflexions served to eliminate this possibility. Only the structure based on Si at $0, 0, 0$ ($\bar{4}$) will be discussed.

Sixteen oxygen atoms (O_I) in the general position x, y, z will form tetrahedra about the silicon atoms: these tetrahedra have one twofold axis parallel to c. The remaining four oxygen atoms (O_{II}) must lie on one of the fourfold special positions. $0, 0, 0$ is already occupied by Si; there is not sufficient room to place