Unit cell and space group of L-serine dimorph

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Although Shoemaker *et al* (1953) reported the crystal structure of DL-serine, no work has yet been reported on the crystal structure of L-serine. Crystals of L-serine $CH_2(OH)CH(NH_2)COOH$ were grown by slow evaporation of aqueous solution of pure sample obtained from British Drug House Ltd., U.K., at room temperature. Rhombic needle shaped single crystals and microcrystals were obtained. Dimorphism was detected from powder photography. The needle axis of the single crystals, which are uniaxial, are parallel to c-axis. Normal beam Weissenberg technique was used to record intensities on layers $kh0$ and $hk1$. A good powder pattern of the microcrystals was recorded on a powder camera of radius 57.4 mm. using CuK_α radiation. This has been indexed. Both crystal forms have orthorhombic symmetry.

Cell dimensions as revealed by Weissenberg and rotation photographs were refined from powder data (Table 1). Constants of analysis for α-L serine were $\sin^2\theta_{100} = 68 \times 10^{-4}$, $\sin^2\theta_{010} = 80.1 \times 10^{-4}$ and $\sin^2\theta_{001} = 190.6 \times 10^{-4}$. $\sin^2\theta$ values were observed within an accuracy of 4×10^{-4} near $2\theta = 62°$, and the axial lengths so obtained are $a = 9.349 \pm 0.006$Å, $b = 8.614 \pm 0.006$Å and $c = 5.59 \pm 0.004$Å. Density of these crystals $\rho = 1.54$ g cm^{-3}, measured by flotation method agrees with the calculated density $\rho = 1.552$ g cm^{-3} for $Z = 4$. The conditions limiting possible reflections are : $h00$, $h = 2n+1$ and $l00$, $l = 2n+1$. The probable space group is therefore $P2_122_1$ for an optically active molecule.

Powder data of β-L serine (Table 1) has been analysed by Lipson's (1949) method. Constants of analysis were found the same as for α-L serine except $\sin^2\theta_{100} = 17 \times 10^{-4}$. The unit cell has $a = 18.689 \pm 0.012$Å, $b = 8.614 \pm 0.006$Å, and $c = 5.59 \pm 0.004$Å. Crystalline density as determined by a small specific gravity bottle is 1.54(5) g cm^{-3} and $Z = 8$. Indices for each line were given within a discrepancy of $\sin^2\theta_{obs} \sim \sin^2\theta_{calc} = 5 \times 10^{-4}$ and the conditions limiting possible reflections are nil. The probable space group for an optically active molecule is therefore $P222$. Determination of the crystal structure is in progress.

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Table 1

Indices	α — L serine $10^4 \times \sin^2 \theta$ Observed	α — L serine $10^4 \times \sin^2 \theta$ Calculated	Indices	β — L serine $10^4 \times \sin^2 \theta$ Observed	β — L serine $10^4 \times \sin^2 \theta$ Calculated
			300	157	153
			001	190	191
			310	230	233
101	254	259	201	254	259
011	272	271 ⎫	011	272	271 ⎫
200		272 ⎭	400		272 ⎭
			111	293	288
020	323	320	020	323	320
120	389	388	220	389	388
			311	425	424 ⎫
			500		425 ⎭
201	463	463	401	463	463
021	506	511	510	506	505 ⎫
			021		511 ⎭
211	543	543	411	543	543
121	574	579			
220	593	592	420	593	592
310	694	692	610	694	692
002	762	762	002	762	762
102	826	830	202	826	830
			330		870 · 874
031	909	911	031, 212	909	911
131	983	980			
202	1030	1034	402	1030	1034
			331	1003	1005
400	1090	1088	800	1090	1088
122	1147	1151	222	1147	1151
			431	1184	1184
401	1282	1279 ⎫	801	1282	1279 ⎫
040		1282 ⎭	040		1282 ⎭
140	1350	1350 ⎫	240	1350	1350 ⎫
222		1355 ⎭	422		1355 ⎭
420	1403	1408	820	1403	1408
011	1471	1472			
141	1543	1540	241	1543	1540
421	1602	1599	821	1602	1599
322	1691	1695			
232	1752	1755	432	1752	1755
013	1796	1796			
340	1899	1894	640	1899	1894 ⎫
			541		1897 ⎭
511	1970	1971	10, 11	1970	1971
			10, 20, 150	2018	2020
332	2093	2095	632	2093	2095
422	2168	2171	822	2168	2171
			912	2217	2220 ⎫
			513		2221 ⎭
223	2310	2308	423	2310	2308
530	2421	2421	10, 30	2421	2421
512	2546	2543	10, 12	2546	2543
233	2705	2708	433	2705	2708
620	2770	2768	12, 20	2770	2768
060, 413	2885	2884	060, 813	2885	2884
540	2985	2982	10, 40	2985	2982
333	3053	3048 ⎫	633	3053	3048 ⎫
004		3050 ⎭	004		3050 ⎭
630	3167	3169	12, 30	3167	3169

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Thermoluminescence and isothermal annealing kinetics of the F-centres in X irradiated KCl and KCl:KNO₃

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In recent years several papers (Jain & Mahendra 1965, Partridge & May 1969) have been published for and against the view that direct correlation exists between F-centre bleaching and thermoluminescence in alkali halides, especially KCl, pure and doped This note. which reports the annealing characteristics of F centre in KCl and KCl : KNO₃ single crystals and the accompanying thermal glow, strikingly supports the view that no connection exists between the F-centre decay and thermoluminescence (Partridge & May 1969).

Single crystals of KCl and KCl doped with KNO₃ ($1 8 \times 10^{-2}$ mole; determined by infrared absorption technique (Wardzynski 1958)) were grown in our laboratory from analar BDH salts and then cleaved to proper size for optical absorption measurements with a Beckman DU spectrophotometer. Thermoluminescence of these samples were measured with the help of a photomultiplier and a quick response optical recorder described elsewhere (Mukherjee 1968). For the production of F-centres a Philips sealed X-ray tube (Cu-target) was employed.

The concentration of F-centres with the same dose of X-ray irradiation at 28°C (room temperature) are found to be higher for KCl : KNO₃ than that for pure KCl (Mukherjee & Bose 1966). When the doped crystal is irradiated and stored in the dark at room temperature the F-centre concentration decreases with time over a long period (~200 minutes). For the pure crystal there is very little decay of the centres with time and the concentration seems to attain a stable value within a few minutes. It has been further observed that room temperature bleaching of F-centres in pure KCl is accompanied by a detectable afterglow; in the case