peratures are greatly influenced by inhibiting conditions such as the adherence of a metal to the glass tube in which it is cast. The dependence of M_s upon specimen condition also makes it difficult to correlate these experiments in an exact way with the specific heat anomaly found near 0·8° K. by Rayne (1954), or the anomaly in the Knight shift in the nuclear resonance experiments of Knight (1954), although these anomalies are presumably due at least in part to the transformation.

The free energies of the f.c.c. and c.p.h. phases discussed here would not be expected to differ greatly, and in fact must be highly similar if one is to judge by the occurrence of frequent stacking faults. In sodium, however, the c.p.h. form is definitely predominant in the entire range 51–5° K., both after cooling and after cold working. In lithium, on the other hand, cold work seems to convert c.p.h. to f.c.c., and there does not appear to be any temperature range in which c.p.h. lithium is stable against cold work. It is concluded that none of the alkali metals has the same sequence of phases as strontium, which is reported to have the high-temperature phase, b.c.c., replaced by c.p.h. and then at still lower temperatures by f.c.c., each presumably being stable within its temperature range.

Few c.p.h. metals have c/a ratios as near to the ideal ratio 1·633 for the close packing of spheres as do lithium and sodium. Strontium and calcium with c/a ratios of 1·63 and 1·638 are the nearest; cobalt and magnesium are next with 1·623, and all others are more remote. Axial ratios in the Li–Mg system and a discussion of their theoretical significance are being presented in a separate paper.

It should be pointed out that if the recrystallization temperature is near 100° K. for high-purity sodium, as indicated, neither the formation of hexagonal sodium on cooling nor the reverse transformation on heating is likely to involve movement of high-energy boundaries as in recrystallization. This is confirmed by the absence of indications of isothermal transformation or reversion at liquid-nitrogen temperature and lower. These reversion temperatures are also well below the value $T_0 = Q/41{\cdot}4R = 127°$ K. where Q is the activation energy for diffusion (10,450), a temperature which Nowick (1955) points out divides 'low temperature recovery' from 'high temperature recovery' in most cubic metals. The transitions in this range are thus of the martensitic type, as in lithium.

Much credit for the solution of design and construction problems in the low-temperature apparatus is due to Messrs T. J. O'Donnell and J. Getzholtz. The spectrometer has been furnished by the Physics Department of the University of Chicago. Some of the X-ray data were obtained with the assistance of Y. Baskin, and the spectrochemical analyses were made by Mrs Althea Tompkins. This work was supported in part by Contract N6ori-02004 with the Office of Naval Research.

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Short Communications

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The structure of anhydrous scandium phosphate.

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A roughly equimolar mixture of scandium oxide and dilute phosphoric acid, held at 400° C. for periods of a week or more in a hydrothermal bomb, yields anhydrous scandium phosphate in the form of a well crystallized powder. At lower temperatures, a hydrate or mixture of hydrates is produced. For briefer heating periods, the product generally contains unconverted oxide. Powder

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diffraction data of a series of such samples were obtained with Cu $K\alpha$ radiation by means of a Geiger-counter diffractometer.

The diffraction pattern of anhydrous scandium phosphate is easily interpreted. All of the observed reflections can be accounted for by a tetragonal scheme of indexing which leads to the following cell dimensions:

$$a = b = 6{\cdot}578 \pm 0{\cdot}002,\ c = 5{\cdot}796 \pm 0{\cdot}002\ \text{Å}\,.$$

The cell volume is therefore 250·79 Å^3, and the density, calculated on the assumption of four formula weights of $ScPO_4$ per unit cell, is 3·70 g.cm.$^{-3}$. The crystal lattice is body centered, as shown by the suppression of all reflections for which $H+K+L = 2n+1$. The space group is $I4_1/amd$–D_{4h}^{19}, the criteria being the absence of reflections, $HK0$, unless H and K are even; and of reflections HHL unless $2H+L = 4n$. The space group provides two symmetrically equivalent sets of fourfold positions, to which the four scandium and the four phosphorus atoms may be arbitrarily assigned. Only one among the available sixteenfold sets gives suitable oxygen positions if the assumption is made that discrete phosphate groups exist in the structure. Therefore, the distribution of atoms in the cell, with reference to an origin taken at $4m2$ rather than at a center ($2/m$), is as follows:

4 Sc in (a) $\bar{4}2m$: $0, 0, 0;\ 0, \frac{1}{2}, \frac{1}{4};\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2};\ \frac{1}{2}, 0, \frac{3}{4}.$
4 P in (b) $\bar{4}2m$: $0, 0, \frac{1}{2};\ 0, \frac{1}{2}, \frac{3}{4};\ \frac{1}{2}, \frac{1}{2}, 0;\ \frac{1}{2}, 0, \frac{1}{4}.$
16 O in (h) m: $(0, 0, 0;\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$
$0, x, z;\ 0, \bar{x}, z;\ 0, \frac{1}{2}+x, \frac{1}{4}-z;$
$0, \frac{1}{2}-x, \frac{1}{4}-z;\ x, 0, \bar{z};\ \bar{x}, 0, \bar{z};$
$x, \frac{1}{2}, \frac{1}{4}+z;\ \bar{x}, \frac{1}{2}, \frac{1}{4}+z.$

Since the presence of discrete phosphate groups in the structure has already been assumed, the two oxygen parameters were taken so as to give a reasonable P–O distance; that is, 1·56 Å. These parameter values, in fractions of the unit cell, are $x = 0{\cdot}194$, $z = 0{\cdot}345$. In the resulting arrangement, scandium is coordinated to eight oxygens; four (tetrahedron corners) at distances of 2·09 Å and four (two tetrahedron edges) at 2·37 Å. The shortest O–O distances are 2·65 and 2·79 Å.

Intensities were calculated from the expression,

$$I_c \sim \left(\frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}\right) pF^2\,,$$

where the first term is the polarization Lorentz factor, p is the multiplicity, and F is the structure amplitude. Values of the observed intensity, I_o, were taken as estimated areas under the $K\alpha_1\alpha_2$ peaks. Since the scattering powers of Sc^{+3}, P^{+5} and O^{-2} are not very different, and since there are twice as many oxygens as other atoms, the oxygen contribution, in general, strongly affects the intensities. The observed and calculated intensities are in substantial agreement, as shown in Table 1. Therefore, the oxygen parameters used in the calculation cannot be far wrong.

From these data, it follows that anhydrous scandium phosphate crystallizes with the zircon structure (Wyckoff & Hendricks, 1927) ($H3$ type, *Strukturbericht*), in common with a number of rare earth vanadates, $CaCrO_4$, $YAsO_4$, and one other phosphate, YPO_4. The cell size and parameter values found for $ScPO_4$ correspond most closely to those of $ZrSiO_4$, which is not surprising since the ionic radii of scandium and of zirconium are practically identical.

Table 1. *Observed and calculated intensities*

HKL	$\sin^2\theta$	I_o	I_c
101	0·0313	—	22
200	0·0548	850	850
211	0·0861	18	11
112	0·0980	400	471
220	0·1096	37	24
202	0·1254	180	217
301	0·1409	120	114
103	0·1725	53	51
321	0·1957	64	63
312	0·2076	442	432
400	0·2192	165	174
213	0·2273	0	1
411	0·2505	0	0
420	0·2740	64	68
303	0·2821	9	0
004	0·2822		7
402	0·2898	12	8
332	0·3172	145	130
323	0·3369	94	14
204	0·3370		70
422	0·3446	0	12
431	0·3601	18	19
501			2
413	0·3917	85	5
224	0·3923		110
521	0·4149	14	8
314	0·4192		7
512	0·4268	70	76
440	0·4386	14	30
105	0·4547	0	0
530	0·4649	0	0
600	0·4936	55	48
503	0·5017	35	10
433			1
404	0·5020		27
215	0·5101	0	9
611	0·5249	0	0
532	0·5368	74	82
620	0·5484	44	36
523	0·5566	85	3
424	0·5568		104
602	0·5642	0	1
305	0·5650		4
541	0·5798	0	3

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