Table 1. *Crystallographic data for testosterone esters*

Compound	Space group	a(Å)	b(Å)	c(Å)	β	D_m (g.cm^{-3})	D_x (g.cm^{-3})	z
Testosterone formate	$P2_1$	21·7	12·5	12·9	96°	1·22	1·21	8
Testosterone acetate	$P2_12_12_1$	12·6	18·1	7·8	—	1·22	1·22	4
Testosterone propionate	$P2_12_12_1$	12·6	20·3	7·6	—	1·17	1·17	4
Testosterone butyrate	$P2_12_12_1$	12·3	16·3	10·3	—	1·16	1·15	4
Testosterone valerate	$P2_12_12_1$	12·3	16·7	10·3	—	1·18	1·17	4

mum error in the cell dimensions and observed densities is of the order of 1 % and the interaxial angle is accurate to within 1°.

Testosterone formate, $C_{20}H_{28}O_3$

This ester can be recrystallized from n-hexane or ethanol as colourless needles elongated along [001]. The Laue symmetry is $2/m$ and reflexions $0k0$ are systematically absent when k is odd, so that the space group is either $P2_1$ or $P2_1/m$. Since testosterone and its esters are optically active (*British Pharmacopœia*, 1963) the space group is determined as $P2_1$.

Testosterone acetate, propionate, butyrate and valerate, $C_{21}H_{30}O_3$, $C_{22}H_{32}O_3$, $C_{23}H_{34}O_3$ *and* $C_{24}H_{36}O_3$

All four esters can be recrystallized from ethanol as colourless needles elongated along [001]. For each ester, the Laue symmetry is *mmm* and the space group is determined uniquely as $P2_12_12_1$ by the systematic absences.

The authors wish to thank the Department of Applied Physics of this College for the loan of X-ray diffraction equipment.

References

British Pharmacopœia (1963). p. 812.

Acta Cryst. (1965). **19**, 150

Crystallographic data for YCo_3 and Y_2Co_{17}*.

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In the study of the yttrium and cobalt phase diagram YCo_3 and Y_2Co_{17} have been found to exist as single-phase compounds. The samples were prepared by levitation melting from stoichiometric amounts of yttrium and cobalt (both 99·5 % pure). To homogenize the samples, they were wrapped with tantalum foil, sealed in quartz capsules under vacuum and annealed for 200 hours to 800 °C. The compounds were then ground in an agate mortar under carbon

* This work was performed in the Air Force Materials Laboratory, Materials Physics Division (MAYA), under Project No. 7360.

Table 1. *Powder diffraction data for* YCo_3

hkl	d_o	d_c	I_o	I_c	*hkl*	d_o	d_c	I_o	I_c
006	2·710	2·714	*m*	5·0	1,1,10	1·365	1·366	*m*−*s*	4·3
110	2·506	2·508	*s*	12·0	304		1·364		5·4
112	2·400	2·397	*w*	1·5	0,0,12	1·356	1·357	*w*−*m*	2·0
200	2·158	2·171	*m*	3·1	127	1·341	1·341	*vw*	0·8
201		2·153		2·5	2,0,10	1·302	1·303	*w*−*m*	2·9
114	2·134	2·135	*vs*	14·0	218	1·278	1·278	*w*	1·2
202	2·096	2·099	*w*−*m*	3·8	306		1·277		1·0
107	2·051	2·050	*w*	1·3	220	1·251	1·254	*s*	21·0
008	2·038	2·035	*m*−*s*	7·1	221		1·250		1·0
203	2·018	2·016	*w*−*m*	3·1	222	1·241	1·239	*w*	2·4
204	1·916	1·916	*m*−*s*	7·4	2,0,11	1·224	1·223	*w*	1·5
108	1·841	1·843	*s*	11·4	129	1·215	1·216	*m*	3·5
106		1·843		8·4	130	1·204	1·205	*s*	13·2
205	1·804	1·807	*m*−*s*	7·5	131		1·201		1·3
206	1·695	1·695	*w*	2·7	224	1·197	1·198	*s*	21·1
109	1·669	1·670	*w*−*m*	3·5	1,1,12	1·193	1·193	*s*	28·8
210	1·641	1·642	*m*−*s*	8·0	225	1·170	1·170	*m*−*w*	5·4
211		1·635		1·7	0,0,14	1·162	1·163	*m*−*w*	*n.c.*
0,0,10	1·627	1·628	*m*	6·4	1,2,10	1·156	1·156	*m*	n.c.
1,0,10	1·528	1·525	*w*	1·3	2,0,12	1·150	1·151	*m*	n.c.
125	1·466	1·466	*m*	3·6	226	1·139	1·138	*w*	2·5
300	1·446	1·448	*m*	5·1	135	1·130	1·130	*w*−*m*	3·4
209	1·391	1·390	*w*−*m*	2·8	1,0,14	1·122	1·123	*m*	n.c.

n.c. = not calculated

Table 2. *Powder diffraction data for* Y_2Co_{17}

hkl	d_o	d_c	I_o	I_c	*hkl*	d_o	d_c	I_o	I_c
110	4·160	4·167	*vw*	0·4	140	1·570	1·575	*vw*	0·2
202	3·101	3·105	*vw*	0·2	207		1·568		0·5
113	2·906	2·907	*m*–*s*	2·8	404	1·551	1·552	*m*	2·0
104	2·802	2·807	*m*	2·4	306		1·552		2·4
121	2·658	2·661	*vw*	0·1	135		1·547		1·1
122	2·486	2·490	*vw*	0·3	143	1·467	1·468	*w*	0·8
300	2·402	2·406	*s*	12·3	127		1·468		1·0
204	2·315	2·328	*m*	1·8	234	1·453	1·454	*s*	1·8
105		2·306		2·3	226		1·454		10·0
220	2·081	2·083	*vs*	17·9	405		1·450		1·1
303	2·066	2·070	*vs*	19·2	330	1·388	1·389	*m*	5·3
124	2·031	2·032	*s*	2·9	235	1·368	1·369	*w*	2·0
006		2·031		13·7	333	1·314	1·314	*s*	20·0
205	2·024	2·020	*m*–*w*	1·8	137		1·313		0·7
223	1·850	1·853	*vs*	24·3	504	1·303	1·304	*w*	0·7
116	1·824	1·826	*m*–*s*	5·3	119	1·287	1·288	*m*	3·4
125		1·817		3·1	244	1·244	1·245	*m*	1·5
401	1·785	1·784	*vw*	0·1	146		1·244		3·1
402	1·733	1·730	*vw*	0·1	505		1·242		0·9
107	1·692	1·693	*w*–*m*	4·9	600	1·203	1·203	*vs*	30·7
134	1·670	1·672	*w*	2·1	1,0,10		1·202		n.c.
231	1·640	1·640	*vw*	0·1	237	1·193	1·200	*w*–*m*	0·7
232	1·599	1·597	*vw*	0·2	154		1·193		1·5
					245		1·190		1·9

Table 3. *Crystallographic data for* YCo_3 *and* Y_2Co_{17}

Compound	*a*	*c*	α	Space group	D_m	D_x
YCo_3	5·015 Å	16·28 Å		$P6_3/mmc$	7·44	7·46
Y_2Co_{17}	5·722 Å		78° 10′	$R\bar{3}m$	8·00	8·02

tetrachloride which prevents oxidation. The powder was strain relieved in evacuated and sealed quartz capillaries at 300 °C during 2 hours. The composition of both compounds was examined by chemical analysis after the heat treatment.

All crystal data were obtained from the alloy powders. X-ray photographs were taken with a 114·6 mm Norelco camera and Co $K\alpha$ radiation ($\lambda = 1{\cdot}7889$ Å). The YCo_3 and Y_2Co_{17} patterns were both indexed hexagonal (Tables 1 and 2) and there is good agreement between the observed and calculated interplanar spacings. The hexagonal unit cell of the YCo_3 structure has the dimensions $a = 5{\cdot}015$ Å and $c = 16{\cdot}28$ Å and it contains six formula units. The Y_2Co_{17} structure shows one formula unit in the rhombohedral unit cell with $a = 5{\cdot}722$ Å and $\alpha = 78°\ 10'$. The dimensions for the triply primitive hexagonal cell are $a = 8{\cdot}331$ Å and $c = 12{\cdot}186$ Å.

Pycnometric density measurements were carried out for each sample. The measured density and the density calculated from the X-ray data are listed under D_m and D_x in Table 3.

The relative intensities of reflections were computed assuming that YCo_3 and Y_2Co_{17} crystallize isostructural to $CeNi_3$ (Cromer & Olsen, 1959) and Th_2Zn_{17} (Markarov & Vinogradov, 1956). The good agreement between the visually observed intensities and the calculated intensities (Tables 1 and 2) shows that there is little doubt that the most probable structures are those given. Some small discrepancies may be caused by preferred orientation. The space groups for the YCo_3 and Y_2Co_{17} structures are presented in Table 3.

The help of Dr. Karl Strnat who prepared the samples is gratefully acknowledged.

References

CROMER, D. T. & OLSEN, C. E. (1959). *Acta Cryst.* **12**, 689.
MARKAROV, E. J. & VINOGRADOV, J. Z. (1956). *Kristallographia*, **1**, 634.

Acta Cryst. (1965). **19**, 151

Unit cell, space group and refractive indices of $Al(NO_3)_3.9H_2O$ and $Cr(NO_3)_3.9H_2O$.

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The present study has been undertaken to obtain information on the crystal chemistry of hydrated nitrates about which little structural information is available in literature.

According to Groth (1906), $Al(NO_3)_3 . 9H_2O$ is dimorphic existing in both monoclinic and orthorhombic systems with the following axial ratios:

(i) Monoclinic: $a:b:c = 1{\cdot}134:1:1{\cdot}9197$; $\beta = 131°\ 36'$.

(ii) Orthorhombic: $a:b:c = 0{\cdot}8925:1:1{\cdot}0202$.

Repeated crystallization from saturated aqueous solution and also from alcohol under slightly varying rates of evaporation and temperature gave us however only monoclinic