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Crystallographic data for three trimethylsteroids.

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During other work we have recently determined X-ray single-crystal and powder diffraction data for the three trimethylsteroids dihydrolanosteryl acetate, euphyl acetate, and tirucallyl acetate (Tables 1 and 2). The single-crystal X-ray data were obtained with a Weissenberg camera, and the powder data with a Philips 90° diffractometer, the traces being taken up to $2\theta = 60°$. The intensities were estimated from the traces but should be used with caution as powder samples free from preferred orientation were not obtained. Iron radiation (filtered through Mn) was used throughout. The crystal densities were measured by the gradient-tube method (Low & Richards, 1952).

Table 2. *Powder data for three trimethylsteroids*

Dihydrolanosteryl acetate		Euphyl acetate		Tirucallyl acetate	
d (Å)	*I*	*d* (Å)	*I*	*d* (Å)	*I*
17·34	14	12·28	32	8·31	71
10·89	20	9·88	27	7·50	23
8·23	12	9·73	17	7·30	49
7·38	25	6·87	37	7·04	14
6·94	50	6·69	50	6·13	28
6·51	8	6·22	100	5·57	100
6·19	33	6·02	72	5·26	28
5·93	100	5·41	41	5·05	7
5·56	78	5·12	86	4·73	6
5·12	63	4·93	36	4·33	67
4·77	58	4·83	17	4·27	26
4·51	22	4·64	8	3·72	13
4·41	30	4·49	8	3·54	9
4·29	7	4·37	77	3·51	5
3·91	5	4·29	5	3·38	22
3·58	83	4·15	5	3·34	14
3·52	100	3·97	5	3·19	5
3·47	5	3·83	20	3·08	7
3·43	5	3·66	14	2·48	5
3·33	5	3·51	9	2·38	3
3·18	17	3·44	28	2·33	3
3·07	25	3·41	25	—	—
3·04	14	3·35	23	—	—
2·94	12	3·25	16	—	—
2·20	22	—	—	—	—
1·96	17	—	—	—	—

Apart from the absence of a double bond in the side chain of dihydrolanosteryl acetate, these three compounds are stereoisomeric; chemical evidence for their structures has been summarised by Gascoigne & Simes (1955) and Klyne (1955). The cell dimensions of tirucallyl acetate indicate that its crystal structure is of the 'normal' sterol type and has the classification *a*211 (Bernal, Crowfoot & Fankuchen, 1940). The cell dimensions of dihydrolanosteryl acetate are similar to those of dihydrolanosteryl iodoacetate (namely, $a = 7{\cdot}6$, $b = 10{\cdot}9$, $c = 38{\cdot}6$ Å; $P2_12_12_1$; Fridrichsons & Mathieson, 1953, and the crystal structures of the two compounds appear to be closely related. A somewhat similar molecular arrangement is probable in the crystals of euphyl acetate, but with a greater inclination of the molecules to (100).

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Table 1. *Single-crystal data for three trimethylsteroids*

Compound	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	Density (g.cm.^{3}) Meas.	Calc.	*Z*	Space group	Crystal form
Dihydrolanosteryl acetate, $C_{32}H_{54}O_2$	7·51 ±0·01	11·32 ±0·04	34·92 ±0·06	—	1·044 ±0·005	1·053	4	$P2_12_12_1$	Colourless needles elongated along [100] showing {001} and {011}
Euphyl acetate, $C_{32}H_{52}O_2$	7·55 ±0·01	13·78 ±0·04	27·77 ±0·06	—	1·071 ±0·005	1·077	4	$P2_12_12_1$	Colourless needles elongated along [100] showing {010} and {014}
Tirucallyl acetate, $C_{32}H_{52}O_2$	8·66 ±0·01	7·47 ±0·01	22·83 ±0·05	99 ±1	1·075 ±0·005	1·070	2	$P2_1$	Colourless needles elongated along [010] showing {001} and {102}