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Crystal data (III) for some estrone-related compounds*. By JEAN M. OHRT, BARBARA A. HANER† and DORITA A. NORTON, *Center for Crystallographic Research, Roswell Park Memorial Institute, Buffalo, New York, U.S.A.*

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Lattice constants for ten estrone-related compounds as determined on a diffractometer with Cu $K\alpha$ radiation are reported.

The lattice constants of ten estrone-related compounds have been determined by the same methods as employed in the preceding papers in this series (Ohrt & Norton, 1963;

Ohrt, Haner & Norton, 1964). The crystal data for the steroids, on which no further work is anticipated, are listed in Table 1.

References

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† Deceased, 11 February 1966.

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OHRT, J., HANER, B. A. & NORTON, D. A. (1964). *Acta Cryst.* **17**, 1611.

Table 1. *Crystal data (III) for some estrone-related compounds*

	1	2	3	4	5
Formula	$C_{19}H_{27}O_2 \cdot \frac{1}{2}C_2H_5OH$	$C_{21}H_{26}O_3$	$C_{22}H_{28}O_4$	$C_{18}H_{21}NO_3$	$C_{24}H_{30}O_6$
Mol. wt.	310.46	326.44	356.47	299.38	414.50
Space group	$P2_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_1$
a (Å)*	7.114	9.105	17.698	12.180	18.704
b (Å)*	36.573	32.300	26.799	16.183	8.678
c (Å)*	6.963	6.115	8.173	7.824	13.746
α (°)	—	—	—	—	—
β (°)	100.60°	—	—	—	91.30°
γ (°)	—	—	—	—	—
Z	4	4	8	4	4
Vol. (Å ³)	1781	1798	3876	1542	2231
ρ_{meas} (g.cm ⁻³)	1.158	1.166	1.199	1.253	1.158
ρ_{calc} (g.cm ⁻³)	1.158	1.205	1.221	1.289	1.234
Solvent	Ethanol	Acetone & methanol	Ethanol	Ethanol	Methanol
	6	7	8	9	10
Formula	$C_{21}H_{30}O_2$	$C_{19}H_{24}O_2$	$C_{19}H_{26}O_3$	$C_{18}H_{24}O_2$	$C_{18}H_{18}O_2$
Mol. wt.	314.47	284.40	302.42	272.39	266.34
Space Group	$P2_12_12_1$	$P2_12_12_1$	$P3_1, P3_2$	$P2_1$	$P2_12_12_1$
a (Å)*	15.296	11.980	7.011	9.288	7.480
b (Å)*	39.316	12.482	—	23.317	25.528
c (Å)*	6.552	10.640	57.076	7.388	7.279
α (°)	—	—	—	—	—
β (°)	—	—	—	109.03°	—
γ (°)	—	—	120.00°	—	—
Z	8	4	6	4	4
Vol. (Å ³)	3940	1591	2430	1513	1390
ρ_{meas} (g.cm ⁻³)	1.091	1.184	1.239	1.156	1.246
ρ_{calc} (g.cm ⁻³)	1.060	1.187	1.240	1.196	1.273
Solvent	Ethanol	Ethanol	Ethanol	Isopropyl alcohol	Ethyl acetate

* Estimated experimental error 0.10%.

- 2,5(10)-Estradien-3,17 β -diol 3-methyl ether $\cdot \frac{1}{2}C_2H_5OH$ (3-Methoxy-2(3),5(10)-19-norandrostadien-17 β -ol).
- 1,3,5(10)-16-Estratetraen-3,17 β -diol 17-acetate 3-methyl ether (Estrone-17-enol acetate 3-methyl ether).
- 1,3,5(10)-Estratrien-3,17 β -diol diacetate (17'' β ''-Estradiol diacetate).
- 1,3,5(10)-Estratrien-3-ol-16,17-dione 16-oxime.
- 1,3,5(10)-Estratrien-3,16 α ,17 β -triol triacetate (Estriol triacetate).
- 1,3,5(10)-Estratrien-17 α -ethyl-3,17 β -diol 3-methyl ether (17 α -Ethylestradiol 3-methyl ether).
- 1,3,5(10)-Estratrien-1-methyl-3-ol-17-one (1-Methylestrone).
- 1,3,5(10)-Estratrien-3,16 α ,17 β -triol 3-methyl ether (Estriol methyl ether).
- 1,3,5(10)-Estratrien-3,16 α -diol (16 α -Estradiol).
- D-1,3,5(10)6,8-Estrapentaen-3-ol-17-one (D-Equilenin).