Acta Cryst. (1965). **19**, 479

Crystal data (II) for some androstanes*.

By JEAN M. OHRT, BARBARA A. HANER and DORITA A. NORTON, *Biophysics Department, Roswell Park Memorial Institute, Buffalo, New York* 14203, *U.S.A.*

(*Received* 2 *February* 1965)

Norton, Lu & Campbell (1962) reported the single-crystal data for a series of androstanes. This paper reports the same data for a second set of androstanes (Table 1) using the same techniques described in the earlier paper. No further work on these compounds is contemplated.

* This investigation was supported in part by Public Health Service Research Grant CA-06183 from the National Cancer Institute.

Reference

NORTON, D. A., LU, C. T. & CAMPBELL, A. E. (1962). *Acta Cryst.* **15**, 1189.

Table 1. *Crystal data* (II) *for some androstanes*

	1	2	3	4	5	6	7	8	9
Formula	$C_{19}H_{26}O_2$	$C_{19}H_{26}O_2$	$C_{19}H_{28}O_2$	$C_{19}H_{28}O_2$	$C_{19}H_{30}O_2$	$C_{19}H_{30}O_2$	$C_{19}H_{24}O_3$	$C_{21}H_{30}O_3$	$C_{26}H_{34}O_3$
Mol. Wt.	286·40	286·40	288·41	288·41	290·43	290·43	300·38	330·45	394·53
D_m (g.cm^{-3})	1·178	1·164	1·147	1·186	1·132	1·147	1·264	1·162	1·148
D_x (g.cm^{-3})	1·175	1·174	1·143	1·177	1·103	1·084	1·253	1·201	1·207
Space group	$P2_12_12_1$	$P2_12_12$	$A2$	$P2_1$	$P2_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_1$
Z	4	4	4	4	2	4	4	4	2
a (Å)*	12·963	12·302	21·337	14·691	11·614	12·146	9·263	12·800	10·860
b (Å)*	16·929	18·644	6·186	11·093	8·096	23·434	26·531	18·169	16·241
c (Å)*	7·366	7·065	12·704	10·872	9·422	6·248	6·477	7·856	6·236
β (°)	—	—	91·27	113·23	99·23	—	—	—	99·17
V (Å^3)	1619	1620	1676	1628	874	1779	1592	1827	1086
Solvent	Ethanol	Methanol	Unknown	Methanol	Ethanol	Ethanol	Methanol—acetone	Methanol	Ethanol

* ± 0·009 Å

1. 4-Androsten-3,17-dione (androstenedione)
2. 1,4-Androstadien-17β-ol-3-one (1-dehydrotestosterone)
3. 5α-Androstan-3,17-dione (androstanedione)
4. 4-Androsten-17β-ol-3-one (testosterone)
5. 5α-Androstan-17β-ol-3-one (allodihydrotestosterone)
6. 5-Androsten-3β, 17β-diol (adrenostenediol)
7. 4-Androsten-3,11,17-trione (adrenosterone)
8. 4-Androsten-17β-ol-3-one 17-acetate (testosterone acetate)
9. 5α-Androstan-17β-ol-3-one 17-benzoate (dihydrotestosterone benzoate)

Acta Cryst. (1965). **19**, 479

An X-ray investigation of the stereochemistry of $Zn(NCS)_2(C_6H_5NH_2)_2$.

By T. M. SHEPHERD and IDA WOODWARD, *Chemistry Department, Queen's University of Belfast, Belfast, Northern Ireland.*

(*Received* 22 *June* 1964)

The stereochemistry of the complex $Zn^{II}(NCS)_2(C_6H_5NH_2)_2$ is of interest in connection with studies in these laboratories on the factors governing the configuration of metal complexes. Nelson & Shepherd (unpublished work) have established, from magnetic and spectral data, that the corresponding Co(II) and Ni(II) complexes have octahedral (or tetragonal) structures with bridging NCS groups. X-ray powder patterns show that these and the corresponding Cd(II) complex are isomorphous, but that $Zn(NCS)_2(C_6H_5NH_2)_2$ has a different crystal structure. An attempt to determine this structure sufficiently to establish the coordination number of the zinc atom is described here.

Single crystals obtained by recrystallization from ethanol were used. These were needle-shaped, approx 1·5 mm long, and 0·3 mm in cross section. The needle axis being taken as the c axis, rotation photographs with Cu $K\alpha$ radiation about the [001] and [1$\bar{1}$0] axes and Laue photographs showed the unit cell to be orthorhombic with the cell dimensions:

$$a = 14{\cdot}56 \pm 0{\cdot}05 \text{ Å}$$
$$b = 9{\cdot}10 \pm 0{\cdot}05$$
$$c = 12{\cdot}7 \pm 0{\cdot}1$$

The values of a and b were derived from the observed spacings of 39 $h0l$ reflexions, and their uncertainties are an estimate based on the standard deviations of the observed and calculated values. c was obtained from layer line measurements of a rotation photograph.