(Waegell & Ourisson, 1961). In a recent paper (Waegell, Pouzet & Ourisson, 1964), the most likely conformation for these compounds has been calculated by minimizing the angular strain within the ring. It is shown that the 'rocking apart' of the axial methyl groups would result in the formation of a 'reversed' cyclohexanone ring and the values for the ring angles obtained from these calculations are shown to be in good agreement with the angles obtained by the X-ray analysis of the crystal structures described here.

Despite the large distortion in the ring angle at C(1), the atoms C(1), C(6), C(2) and O remain planar, in both compounds, within the accuracy of the determination.

Other bond angles which are significantly different from the accepted values involve the substituents and are strained to reduce the steric hindrance between the methyl groups and the bromine atoms, *e.g.* C(3)–C(2)–Br = 116° in MTC and C(3)–C(2)–Br = 113°, C(5)–C(6)–Br = 113° in DTC.

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Short Communications

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Crystal data (I) for some pregnenes and pregnadienes.*

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Crystal data for seven pregnenes and pregnadienes have been determined from reciprocal lattice measurements on a General Electric XRD 5 X-ray diffraction unit, equipped with goniostat, using Cu $K\alpha$ radiation.

Space groups have been established on the basis of systematic absences and optical activity. Flotation density measurements were made and used to determine the number of molecules per unit cell. Measured and calculated densities agree within the experimental range of error (3%).

The crystal data obtained are given in Table 1.

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Table 1. *Crystal data* (I) *for pregnenes and pregnadienes*

(1) 4-Pregnen-3,20-dione
(2) 5-Pregnen-3β-ol-20-one
(3) 4-Pregnen-11β,17α,21-triol-3,20-dione
(4) 1,4-Pregnadien-17α,21-diol-3,11,20-trione
(5) 5,16-Pregnadien-3β-ol-20-one acetate
(6) 5,16-Pregnadien-3β-ol-20-one
(7) 4-Pregnen-17α,21-diol-3,11,20-trione

	(1)	(2)	(3)	(4)	(5)	(6)	(7)
Formula	$C_{21}H_{30}O_2$	$C_{21}H_{32}O_2$	$C_{21}H_{30}O_5$	$C_{21}H_{26}O_5$	$C_{23}H_{32}O_3$	$C_{21}H_{30}O_2$	$C_{21}H_{28}O_5$
Mol. wt.	314·45	316·47	362·47	358·44	356·49	314·45	360·46
D_m (g.cm^{-3})	$1{\cdot}15_8$	$1{\cdot}15_1$	$1{\cdot}27_8$	$1{\cdot}33_2$	$1{\cdot}13_6$	$1{\cdot}10_1$	$1{\cdot}30_1$
D_x (g.cm^{-3})	1·160	1·188	1·252	1·319	1·166	1·094	1·293
Z (calc.)	4	2	8	4	4	8	4
Space group	$P2_12_12_1$	$P2_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
a (Å)†	12·568	12·054	12·441	9·999	12·494	14·716	10·063
b (Å)†	13·819	11·867	30·496	23·029	27·195	26·764	23·649
c (Å)†	10·363	6·185	10·139	7·839	5·975	9·695	7·780
β	—	91·53°	—	—	—	—	—
Volume (Å^3)	1800	884	3847	1805	2030	3818	1852
Solvent	Heptane–acetone	Methanol	Ethanol	Acetone	Methanol	Acetone–methanol	Acetone

† ±0·008.