(*a*) The density is less than that of c.c.p. and the possibility of a transition to the latter structure is thus likely as the simplicity of the transition mechanism has been demonstrated above. Each sphere (in a face) makes only 6 contacts with the 12 neighbours in its first coordination sphere and the spread of a displacement is facilitated.

(*b*) As n increases the ratio of pentagonal pyramidal prism to cuboctahedron coordination decreases. The chemical properties of the assembly would thus also have to change with n.

(*c*) The layers parallel to icosahedron faces are in a cubic stacking sequence. The energy for hexagonally stacked additions might be almost identical and any such stacking fault would prevent the icosahedral packing from continuing. It is possible that the inclusion of a small atom with a decided preference for icosahedral coordination might stabilize a nucleus from which a normally cubic material might grow.

J. D. Bernal (private communication, 1960) has pointed to the existence of a class of hierarchic structures, indefinitely extended in three dimensions, which are non-lattice packings. The unit of packing is the arrangement of 13 spheres as an icosahedron making a quasi-spherical unit, 13 of which are packed together to make a quasi-sphere of the next order. Tetrahedral units are used to pack the interstices and as all smaller units are available for packing the interstices between larger units it is difficult to give simple rules for this packing. However, there is a clear relationship between the early stages of such a hierarchy and the packing described above. Counting the central sphere as the zeroth layer, the first three layers of Bernal's structure are the same as in the i.s.p. described above. Looking at the packing of the layers parallel to the faces of the core icosahedron the stacking sequence is *ABCA* (that is, c.c.p.). If the fourth layer were *B* as in i.s.p. then the coordination about the spheres on the five-fold axes in the layer below (third layer) would be pentagonal pyramidal prisms, but if the fourth layer were C (stacking fault in hexagonal sequence) and spheres were also placed on the five-fold axis as before then 12 icosahedra (each of 13 spheres) would appear round the first icosahedron with a tetrahedron of 4 spheres filling each cavity between 4 icosahedra. The resulting solid of 279 spheres is thus the second-order icosahedral unit described by Bernal. The outside shell is not close packed (i.s.p. would have 309 spheres instead of 279) and, on attempting to pack these large units together, description of the exact position of each atom becomes very difficult. It is improbable that the density can be kept up even to the value of 0·68818.

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Crystal data for some 5α-pregnane »ol-ones«.

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Crystal data for seven 5α-pregnane 'ol-ones' have been determined from goniostat-collected reciprocal lattice measurements using Cu $K\alpha$ radiation. Space groups were deduced from systematic absences and the fact that these compounds are optically active.

The number of molecules per unit cell was calculated in the usual way using floatation density measurements, assuming no solvent of crystallization. That solvent of crystallization (probably alcohol) is sometimes present in crystals of 5α-pregnane compounds, however, is indicated by the discrepancies between the calculated and measured densities.

The crystal data obtained are given in Table 1.

Table 1. *Crystal data*

	1.	2.	3.	4.	5.	6.	7.
Formula	$C_{21}H_{34}O_2$	$C_{21}H_{32}O_3$	$C_{21}H_{32}O_3$	$C_{21}H_{30}O_5$	$C_{21}H_{32}O_5$	$C_{21}H_{34}O_5$	$C_{21}H_{34}O_5$
Molecular wt.	318·48	332·5	332·5	362·45	364·47	366·48	366·48
(g.cm.$^{-3}$, meas.)	1·100	1·208	1·171	1·185	1·154	1·205	1·198
(g.cm.$^{-3}$, calc.)	1·061	1·206	1·173	0·991	1·041	1·278	1·214
Z	4	4	4	2	4	4	8
Space group	$P2_1$	$P2_122$	$P2_1$	$P2_1$	$P2_1$	$P2_12_12_1$	$P2_12_12_1$
a (Å)*	13·485	10·667	17·546	16·525	11·545	12·539	14·061
b (Å)*	12·385	23·447	7·502	7·504	25·523	12·830	23·468
c (Å)*	12·114	7·320	14·637	9·820	8·447	11·686	11·995
β	99·88°	—	102·63°	94·50°	110·96°	—	—
V (Å^3)	1993	1831	1880	1214	2324	1880	3958
Solvent	ethanol	ethanol	ethanol	ethanol	ethanol	ethanol	toluene

1. 5α—pregnane—3β—ol—20—one
2. 5α—pregnane—11α—ol—3, 20—dione
3. 5α—pregnane—3β—ol—11, 20—dione
4. 5α—pregnane—17α, 21—diol—3, 11, 20—trione
5. 5α—pregnane—3β, 17α, 21—triol—11, 20—dione
6. 5α—pregnane—3α, 11β, 17α, 21—tetrol—20—one
7. 5α—pregnane—3β, 11β, 17α, 21—tetrol—20—one

* ±0·004 Å.