



X-Ray Crystal Structure of Four Inclusion Complexes of the Novel Host Gossindane: An Oxidation Product of Gossypol

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Abstract. Gossindane, the oxidation product of gossypol, demonstrates inclusion properties towards four solvents chosen accidentally. The crystal data of these complexes with ethanol (**I**), ethylacetate (**II**), dichloromethane (**III**) and water (**IV**) are: (**I**): $C_{26}H_{30}O_6 \cdot 2C_2H_5OH$, monoclinic, $P2_1/c$, $a = 8.687(2) \text{ \AA}$, $b = 10.986(3) \text{ \AA}$, $c = 14.778(3) \text{ \AA}$; $\beta = 110.94^\circ$, $V = 1317 \text{ \AA}^3$, $Z = 2$, $R = 0.069$, $N = 1368$; (**II**): $C_{26}H_{30}O_6 \cdot 0.5C_4H_8O_2$, monoclinic, $P2_1/c$, $a = 8.960(2) \text{ \AA}$, $b = 21.937(5) \text{ \AA}$, $c = 14.712(3) \text{ \AA}$, $\beta = 111.98(2)^\circ$, $V = 2681 \text{ \AA}^3$, $Z = 4$, $R = 0.083$, $N = 2653$; (**III**): $C_{26}H_{30}O_6 \cdot CH_2Cl_2$, monoclinic, $P2_1/c$, $a = 8.886(2) \text{ \AA}$, $b = 21.778(6) \text{ \AA}$, $c = 14.996(4) \text{ \AA}$, $\beta = 111.31(3)^\circ$, $V = 2704 \text{ \AA}^3$, $Z = 4$, $R = 0.131$, $N = 1580$; (**IV**): $C_{26}H_{30}O_6 \cdot 2H_2O$, monoclinic, $C2/c$, $a = 29.422(9) \text{ \AA}$, $b = 6.720(2) \text{ \AA}$, $c = 27.525(9) \text{ \AA}$, $\beta = 117.43(2)^\circ$, $V = 4830 \text{ \AA}^3$, $Z = 8$, $R = 0.096$, $N = 2240$.

In the solvates H-bonded host molecules form bilayers with very similar structures and a nearly hydrophobic surface. Guest molecules are placed in channels formed between these bilayers and may be H-bonded to host molecules (ethanol). In the hydrate two water molecules using their H-bonding capacity incorporate gossindane molecules into bilayers.

Key words: X-ray crystallography, gossindane, inclusion complexes, H-bond, crystal structure

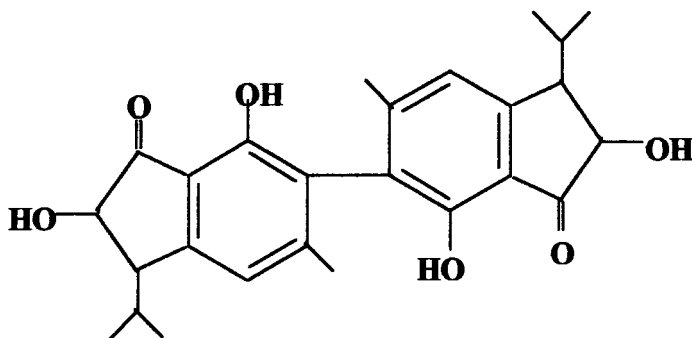
Supplementary Data relating to this article are deposited with the British Library as supplementary publication No. 82241 (12 pages).

1. Introduction

Gossypol [1–3] and 1,1'-binaphthyl-2,2'-dicarboxylic acid (BNDA) [4,5], having a binaphthyl skeleton, are versatile host molecules. Gossypol is a 2,2'-binaphthyl which has hydroxyl, aldehyde, methyl and isopropyl groups at the different positions of the molecule whereas BNDA is a 1,1'-binaphthyl having only carboxylic groups at positions 2 and 2'. Chemical modifications of these hosts, for example, moving of the substituents along the BNDA molecule [4] or changing certain substituents by other in the case of gossypol [6,7] give rise to molecules which are still versatile hosts. Therefore one may conclude that inclusion tendency is an intrinsic ability of the naphthyl systems when two halves are joined by an ordinary

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bond. In order to verify this suggestion the two naphthyl moieties of gossypol molecules should be destroyed and the inclusion ability of the obtained compound tested. Previously the preparation of such a substance by an oxidation of gossypol with pure oxygen in alkaline medium [8] has been reported. It contains an indane nucleus instead of the gossypol naphthalene nucleus and was named



gossindane [8]. We have crystallized gossindane from its solutions in ethanol, ethylacetate, dichloromethane and aqueous acetone. We have obtained clathrates in the first three cases and a hydrate in the case of aqueous acetone. The present paper is devoted to the X-ray crystal structures of gossindane with ethanol (**I**), ethylacetate (**II**), dichloromethane (**III**) and water (**IV**).

2. Experimental

Single crystals of the gossindane host-guest complexes with ethanol, ethylacetate and dichloromethane were obtained from solutions in the respective solvents by slow evaporation at room temperature. Single crystals of gossindane dihydrate were grown from solutions in aqueous acetone, under the same conditions.

Crystallographic experiments were carried out on a "Syntex-P2₁" diffractometer. Unit cell dimensions of the crystals were measured by a least-squares fit of the setting angles of 15 reflections with 2θ in the range 25–30° (Table I). Intensities of the reflections were measured with graphite-monochromatized CuK $_{\alpha}$ -radiation. No significant intensity variation was observed for two standard reflections monitored after each group of 100 reflections. The intensities were corrected for Lorentz and polarization factors but not for absorption. The structures have been solved by direct methods using the program SHELXS 86 [9]. Solvent molecules and hydrogen atoms were located from difference Fourier syntheses with the exception of the gossindane complex with dichloromethane where hydrogen atoms were placed in idealized positions assuming C—H and O—H distances of 0.96 and 0.85 Å, respectively. Structures were refined anisotropically by the full-matrix least-squares method using SHELX-76 programs [10]. Final atomic coordinates are given in Table II.

Table I. Crystal data for gossindane inclusion complexes

Formula	C ₂₆ H ₃₀ O ₆ · 2C ₂ H ₅ OH	C ₂₆ H ₃₀ O ₆ · 0.5C ₄ H ₈ O ₂	C ₂₆ H ₃₀ O ₆ · CH ₂ Cl ₂	C ₂₆ H ₃₀ O ₆ · 2H ₂ O
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P2/c	P2 ₁ /c	P2 ₁ /c	C2/c
<i>a</i> (Å)	8.687(2)	8.960(2)	8.886(4)	29.422(9)
<i>b</i> (Å)	10.986(3)	21.937(5)	21.778(12)	6.720(2)
<i>c</i> (Å)	14.778(3)	14.712(3)	14.996(7)	27.525(9)
β (°)	110.94(2)	111.98(2)	111.31(4)	117.43(2)
<i>V</i> (Å ³)	1317	2681	2704	4830
<i>D_x</i> (g/cm ³)	1.20	1.19	1.31	1.27
<i>Z</i>	2	4	4	8
Radiation	CuK α	CuK α	CuK α	CuK α
Absorption coefficient (mm ⁻¹)	67.3	66.1	250.2	68.5
2 θ _{max} (°)	116	116	110	116
Unique data collected	1821	3658	3390	3360
No. of reflections with <i>I</i> > 2 σ (<i>I</i>)	1343	2650	1582	2240
Final R indices [<i>I</i> > 2(<i>I</i>)]	0.067	0.083	0.132	0.096
R indices (all data)	0.092	0.113	0.243	0.182
Weighting scheme	1	1	1	1
Goodness-of-fit on F ²	1.104	1.890	4.576*	5.150**

* Control reflections were still unstable and crystals were very small.

** Control reflections were still unstable.

3. Discussion

3.1. MOLECULAR STRUCTURE

The gossindane molecule consists of two identical halves joined by a single C(2)—C(2') bond. Each indane nucleus has hydroxyl groups at positions 1(1') and 6(6'), carbonyl oxygens at positions 7(7'), and isopropyl and methyl groups at positions 5(5') and 3(3'), respectively (Figure 1).

Because of the repulsion of the —OH and —CH₃ substituents *ortho*-situated relatively to the C(2)—C(2') bond the gossindane molecule does not have a planar conformation but at the same time it cannot freely rotate around this bond (the dihedral angle between the aromatic fragments is about 69.5° in complexes **I**, **II**, **III** and 75.2° in the hydrate). This situation gives rise to the existence of the two gossindane atropoisomers. As gossindane is obtained from racemic gossypol it is also racemic.

However, an atropoisomerism is not the only source of the optical activity. Another source of the activity is asymmetric carbon atoms. There are asymmetric atoms, C(5)(C(5')) and C(6)(C(6')), in each half of the gossindane molecule and

Table II. Atom coordinates ($\times 10^4$) and temperature factors ($\text{\AA}^2 \times 10^3$) of gossindane complexes with ethanol (**I**), ethylacetate (**II**), dichloromethane (**III**) and water (**IV**)

Atoms	x/a	y/b	z/c	U_{iso}^*
(I)				
O1	2574(4)	4663(3)	2419(2)	60(2)
O2	883(4)	4876(4)	3774(3)	65(2)
O3	1144(5)	3667(4)	5577(3)	67(2)
C(1)	4944(5)	3400(4)	2993(3)	42(2)
C(2)	3642(5)	3994(4)	3140(3)	44(2)
C(3)	6097(5)	2771(4)	3769(3)	46(2)
C(4)	5924(6)	2705(5)	4673(4)	49(2)
C(5)	3952(6)	3106(5)	5642(4)	51(2)
C(6)	2534(6)	4053(5)	5375(4)	52(2)
C(7)	2122(6)	4339(5)	4304(4)	50(2)
C(8)	3448(5)	3879(4)	4040(3)	43(2)
C(9)	4553(5)	3215(4)	4797(3)	45(2)
C(10)	7553(7)	2145(7)	3650(5)	64(3)
C(11)	3411(7)	1806(5)	5770(4)	59(2)
C(12)	2224(8)	1266(6)	4840(5)	73(3)
C(13)	4883(9)	957(7)	6218(6)	80(3)
C(1s)	0	7922(16)	2500	159(10)
C(2s)	65(27)	9104(15)	2088(13)	138(12)
O(1s)	274(23)	8165(18)	3542(11)	119(12)
O(1s')	1355(22)	7190(17)	2578(16)	122(11)
(II)				
C(1)	5423(6)	6700(3)	9668(4)	42(2)
C(2)	4143(6)	6987(3)	9834(4)	43(2)
C(3)	6458(7)	6324(3)	10407(4)	50(3)
C(4)	6225(7)	6228(3)	11287(4)	52(3)
C(5)	4269(7)	6378(3)	12217(4)	51(3)
C(6)	3049(7)	6907(3)	12057(4)	50(3)
C(7)	2643(7)	7102(3)	10999(4)	49(3)
C(8)	3920(6)	6871(3)	10705(4)	41(2)
C(9)	4914(7)	6483(3)	11410(4)	43(2)
C(10)	7856(8)	6007(3)	10290(5)	70(3)
C(11)	3511(9)	5736(3)	12141(6)	71(4)
C(12)	2232(10)	5608(4)	11122(7)	91(4)
C(13)	4774(10)	5237(4)	12438(7)	98(5)
O(1)	3175(5)	7363(2)	9137(3)	60(2)
O(2)	1489(5)	7408(2)	10494(3)	63(2)
O(3)	1669(5)	6749(2)	12254(3)	65(2)
C(1')	6943(7)	7074(3)	8652(4)	47(2)
C(2')	5609(6)	6767(3)	8708(4)	42(2)
C(3')	4549(6)	6491(3)	7859(4)	45(2)

Table II. Continued

Atoms	x/a	y/b	z/c	U_{iso}^*
(II) Continued.				
C(4')	4828(6)	6511(3)	6986(4)	46(2)
C(5')	6888(7)	6772(3)	6165(4)	49(2)
C(6')	8337(7)	7220(3)	6565(4)	47(2)
C(7')	8595(7)	7327(3)	7625(4)	47(2)
C(8')	7210(6)	7069(3)	7787(4)	42(2)
C(9')	6205(6)	6772(3)	6964(4)	42(2)
C(10')	3101(7)	6147(3)	7862(5)	63(3)
C(11')	7379(9)	6136(4)	5942(6)	79(4)
C(12')	8400(11)	5794(4)	6866(8)	100(5)
C(13')	5933(14)	5763(5)	5328(9)	161(8)
O(1')	7982(5)	7365(2)	9457(3)	64(2)
O(2')	9745(5)	7583(2)	8232(3)	65(2)
O(3')	9771(5)	7012(2)	6475(3)	64(2)
O(1s)	712	5940	4462	260
O(2s)	0	5000	5000	127
C(1s)	-1557	5316	3573	174
C(2s)	-172	5480	4437	123
C(3s)	-1007	4500	4841	142
C(4s)	-114	4121	5824	219
(III)				
C(1)	4027(21)	7054(8)	8066(11)	39(8)
C(2)	2682(20)	6710(8)	8078(11)	38(7)
C(3)	1665(20)	6465(8)	7210(11)	42(8)
C(4)	1978(21)	6542(8)	6382(10)	47(8)
C(5)	4040(19)	6890(8)	5590(10)	38(7)
C(6)	5551(21)	7337(8)	6048(12)	44(8)
C(7)	5746(22)	7369(9)	7131(13)	50(9)
C(8)	4373(20)	7079(8)	7239(12)	40(8)
C(9)	3371(20)	6828(8)	6395(12)	39(8)
C(10)	197(19)	6095(9)	7185(12)	56(8)
C(11)	4456(24)	6281(9)	5255(14)	56(9)
C(12)	5358(27)	5850(9)	6006(16)	81(12)
C(13)	2990(32)	5986(12)	4562(17)	122(16)
O(1)	5089(14)	7308(6)	8900(7)	57(6)
O(2)	6893(15)	7627(7)	7727(9)	65(6)
O(3)	6979(15)	7103(6)	5983(9)	66(7)

Table II. Continued

Atoms	x/a	y/b	z/c	U_{iso}^*
(III) Continued.				
C(1')	1271(20)	6881(8)	9221(10)	41(7)
C(2')	2510(18)	6596(8)	9022(11)	34(7)
C(3')	3582(19)	6214(8)	9722(12)	42(8)
C(4')	3384(20)	6112(8)	10577(12)	45(8)
C(5')	1658(20)	6304(8)	11661(11)	39(7)
C(6')	483(21)	6870(9)	11511(11)	50(8)
C(7')	-121(24)	7016(8)	10436(12)	45(8)
C(8')	1085(20)	6768(8)	10100(11)	39(8)
C(9')	2127(23)	6391(8)	10771(11)	46(8)
C(10')	4900(21)	5889(9)	9505(12)	60(9)
C(11')	904(22)	5705(8)	11698(11)	50(8)
C(12')	2124(23)	5171(9)	11923(12)	67(10)
C(13')	-560(22)	5539(9)	10821(14)	74(10)
O(1')	245(14)	7269(5)	8558(7)	53(6)
O(2')	-1311(16)	7320(6)	9987(9)	65(6)
O(3')	-786(15)	6750(6)	11857(8)	60(6)
C(1s)	-2676(59)	9094(12)	8187(23)	272(41)
Cl(1)	-2885(13)	9760(5)	7632(7)	181(7)
Cl(2)	-2055(19)	9084(10)	9294(9)	345(14)
(IV)				
C(1)	1674(3)	-4147(12)	2595(3)	41(4)
C(2)	1385(3)	-2581(11)	2226(3)	37(3)
C(3)	1086(3)	-1330(12)	2357(3)	40(3)
C(4)	1041(3)	-1567(12)	2837(3)	44(4)
C(5)	1309(3)	-3632(12)	3723(3)	41(3)
C(6)	1814(3)	-4830(13)	4009(3)	42(3)
C(7)	1894(3)	-5676(13)	3542(3)	46(4)
C(8)	1628(3)	-4353(11)	3075(3)	37(3)
C(9)	1312(3)	-3122(12)	3197(3)	41(4)
C(10)	788(4)	303(15)	1983(4)	78(6)
C(11)	831(4)	-4879(15)	3658(3)	57(4)
C(12)	763(4)	-6787(16)	3345(4)	79(6)
C13	351(4)	-3613(18)	3402(4)	74(5)
O(1)	1953(2)	-5461(9)	2497(2)	52(3)
O(2)	2144(2)	-7183(9)	3585(2)	55(3)
O(3)	1842(2)	-6326(9)	4385(2)	57(3)

Table II. Continued

Atoms	x/a	y/b	z/c	U_{iso}^*
(IV) Continued.				
C(1')	1647(3)	-758(11)	1582(3)	35(3)
C(2')	1399(3)	-2373(11)	1683(3)	35(3)
C(3')	1115(3)	-3683(11)	1252(3)	47(4)
C(4')	1073(3)	-3439(12)	740(3)	40(4)
C(5')	1331(3)	-1301(12)	108(3)	38(3)
C(6')	1821(3)	-80(12)	320(3)	43(3)
C(7')	1888(3)	789(12)	859(3)	42(4)
C(8')	1618(3)	-557(11)	1061(2)	35(3)
C(9')	1316(3)	-1858(12)	642(3)	39(3)
C(10')	847(4)	-5453(14)	1345(3)	65(5)
C(11')	851(3)	-134(13)	-294(3)	47(4)
C(12')	373(3)	-1470(17)	-500(3)	69(4)
C(13')	777(4)	1803(15)	-65(4)	67(5)
O(1')	1924(2)	589(8)	1964(2)	50(2)
O(2')	2133(2)	2310(9)	1064(2)	54(3)
O(3')	1850(2)	1389(8)	-29(2)	53(3)
O(1w)	2496(2)	16(9)	4539(2)	56(3)
O(2w)	2504(2)	5081(9)	1945(2)	53(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalised $U(i, j)$ tensor.

having the same configuration (R or S). Therefore the gossindane molecule has a twofold symmetry axis which is directed perpendicularly to the C(2)—C(2') bond.

The aromatic rings are planar in all complexes (0.04 Å) whereas the conformation of the five membered rings varies from the half-chair to the envelope. It is half-chair in both halves in the case of the hydrate, half-chair and envelope in the different halves in complex **I** and envelope in both halves in complexes **II** and **III**.

Intramolecular H-bonds O(1)—H...O (O(1')—H...O(2')) close six-membered rings consisting of atoms O(2)—C(7)—C(8)—C(1)—O(1)—H (O(2')—C(7')—C(8')—C(1')—O(1')—H') except for the hydrate of gossindane. In this case the hydrogen atom of the O(1)—H group is directed away from the O(2) atom in order to form a H-bond with water molecules (Table III).

In all four structures hydrogen atoms H(11) (H(11')) of the isopropyl group are directed towards the O(3) (O(3')) oxygen atom although there are alternating opposite positions for each of these two atoms. The orientation and interatomic distances (Table III) show that the atoms are hydrogen bonded.

The bond lengths and angles are in good agreement with those observed in the analogous fragments of the gossypol molecule [11–13] and different derivatives of

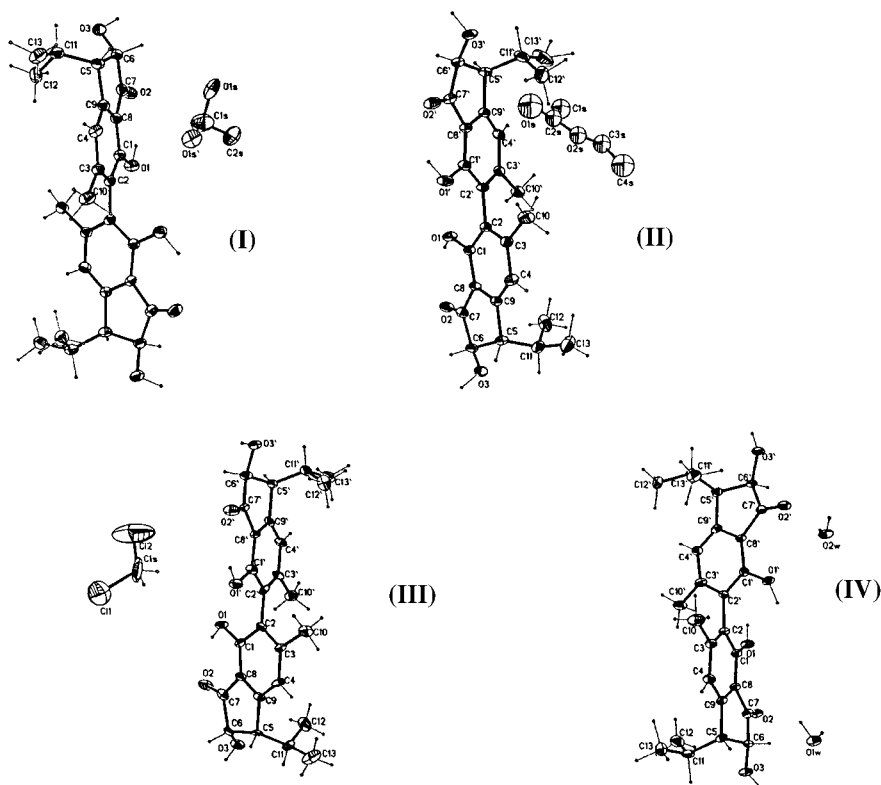


Figure 1. Conformation of the gossindane molecule in the complexes of gossindane with ethanol (I), ethylacetate (II), dichloromethane (III) and water (IV).

indane [14–16]. It is worthy of note that some endocyclic angles of the pentacycle deviate from tetrahedral standard values which is usual for such strained systems (Table IV, V, Supplementary Data).

3.2. CRYSTAL STRUCTURE

Gossindane forms with ethanol, dichloromethane, ethylacetate and water different clathrates with host : guest ratios respectively of 1 : 2, 1 : 1, 1 : 0.5 and 1 : 2. These complexes may be divided into solvates consisting of the first three clathrates with gradually decreasing guest content and the hydrate. The solvates are host-guest complexes in which guest molecules are located in channels formed between bilayers. The structure of the bilayers is changed significantly in the ethylacetate solvate compared to the ethanol complex but only slightly relative to the dichloromethane solvate.

In the ethanol solvate crystallizing in the $P2_1/c$ space group a crystal twofold axis is coincident with the gossindane molecule intrinsic twofold axis and the asymmetric part of the unit cell contains a half of the host molecule. This half

Table III. H-bonds of gossindane complexes with ethanol (I), ethylacetate (II), dichloromethane (III) and water (IV)

	Symmetry	D···A (Å)	D—H (Å)	H···A (Å)	∠D—H···A (deg.)
(I)					
O(1)—H···O(2)	$-x, y, 0.5 - z$	2.898	1.14	2.22	116
O(3)—H···O(2)	$-x, 1 - y, 1 - z$	2.791	0.96	1.96	144
(II)					
O(1)—H···O(2')	$x - 1, y, z$	2.896	0.66	2.39	138
O(3')—H···O(2)	$1 + x, 1.5 - y, -0.5 + z$	2.781	0.98	1.86	141
O(1')—H···O(2)	$1 + x, y, z,$	2.937	1.08	2.32	115
O(3)—H···O(2')	$x - 1, 1.5 - y, 0.5 + z$	3.007	0.99	2.17	141
(III)					
O1—H···O2')	$x + 1, y, z$	3.016	0.85	2.51	119
O1'—H···O2)	$x - 1, y, z$	2.887	0.85	2.35	121
O3—H···O2')	$x - 1, 1.5 - y, 0.5 + z$	2.786	0.85	1.97	160
O3—H···O2)	$x + 1, 1.5 - y, -0.5 - z$	3.123	0.85	2.62	119
(IV)					
O(1W)—H···O(2)	$x, 1 + y, z$	2.998	1.10	2.01	147
O(1W)—H—O(2')	$0.5 - x, y - 0.5, 0.5 - z$	3.000	0.99	2.16	123
O(3)—H···O(1W)	$0.5 - x, -0.5 - y, 1 - z$	2.816	1.00	1.82	174
O(3')—H···O(1W)	$x, -y, -0.5 - z$	2.821	1.04	2.16	120
O(2W)—H···O(2)	$0.5 - x, 1.5 + y, 0.5 - z$	2.827	0.99	2.16	123
O(2W)—H···O(2')	x, y, z	2.840	0.71	2.20	151
O(1)—H···O(2W)	$x, y - 1, z$	2.710	0.79	2.09	135
O(1')—H···O(2W)	$0.5 - x, -0.5 + y, 0.5 - z$	2.704	0.96	1.78	160

molecule I(x, y, z) is hydrogen bonded with molecule II($-x, 1 - y, 1 - z$) by a pair of centrosymmetrically related bonds O(3)—H···O(2) closing 10-membered rings. Simultaneously molecule I is hydrogen bonded to molecule III($-x, y, 0.5 - z$) by a pair of bonds O(1)—H···O(2) related through a twofold axis closing 12-membered pseudorings (Table III). Oxygen atoms O(1) and O(3) show only proton donor abilities whereas atom O(2) is a double proton acceptor. By these H-bonds each gossindane molecule is bonded to four other molecules and bilayers parallel to the xz plane are formed. All polar groups of gossindane molecules are hidden inside the bilayers while their surface are covered by hydrophobic parts of the host molecules. The surfaces of the bilayer are not smooth and there are pits on it. During packing of the bilayers channels are formed between these pits which are occupied with guest molecules (Figure 2).

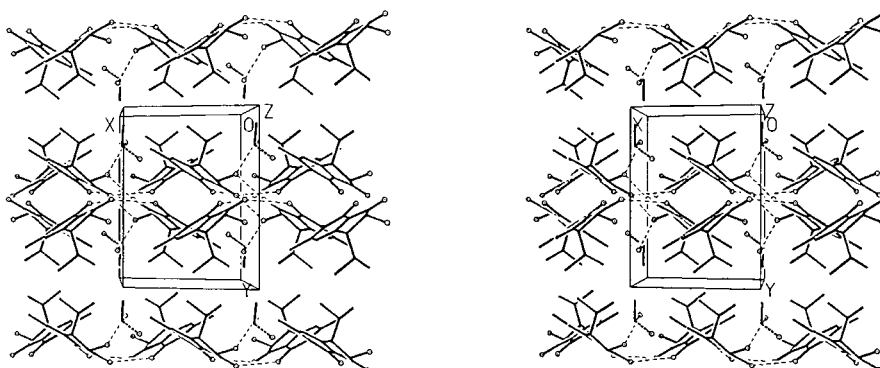


Figure 2. Crystal structure of the gossindane complex with ethanol.

Ethanol molecules (exactly their CH_2 -groups) are located on the twofold axes and disordered in the two positions with approximately equal site occupation factors. Guest molecules are H-bonded to O(3) atoms of the host molecules situated on the pits (Table III). In this case the O(3) atom exhibits proton acceptor properties.

In the solvate of the aprotic guest ethylacetate the crystal loses the twofold symmetry axis and the asymmetric part of the unit cell contains a whole host molecule. In order to form a bilayer structure a less symmetric system of H-bonds is used. Two symmetric H-bonds observed in the ethanol complex are separated by four bonds (Table III). These H-bonds form bilayers, whose structure is very similar to the one found in the above complexes (Figure 3). Ethylacetate molecules are disordered and situated on the inversion centre (the ether oxygen atom occupies the inversion center). They are placed in channels running along the direction of the x -axis. In the host-guest complex of gossindane with dichloromethane the structure of the bilayers is identical to the one in the ethylacetate complex but here two neighbouring bilayers contact by a slightly different mode in order to form a more voluminous space for enclathrating two dichloromethane molecules (Figure 4).

The dihydrate is related to the second group of gossindane complexes. In it each water molecule is H-bonded with the four host molecules entirely using their H-bonding capability and showing in two bonds proton acceptor abilities and in the other two proton donor properties (Table III). Water molecules locating between gossindane layers incorporate host molecules into bilayers parallel to the yz plane. In the bilayers no H-bonds exist between host molecules. The packing of these bilayers with hydrophobic surfaces gives rise to the crystal structure of the hydrate (Figure 5).

Thus, two types of gossindane host-guest complexes are identified. In the complexes of the first group guest molecules are enclathrated between bilayers whereas in the case of the second group water molecules situated inside host monolayers gives rise to bilayers.

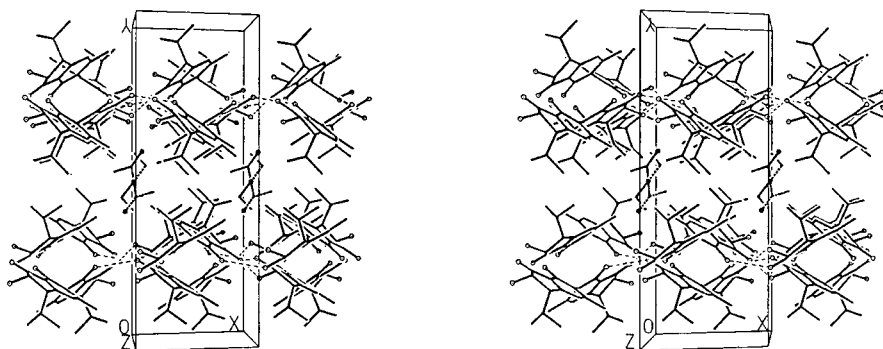


Figure 3. Crystal structure of the gossindane complex with ethylacetate (the ethylacetate molecules are disordered and situated on the inversion centre).

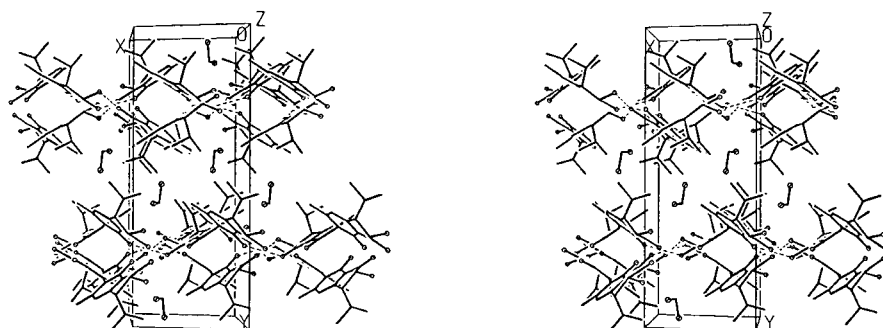


Figure 4. Crystal structure of the gossindane complex with dichloromethane.

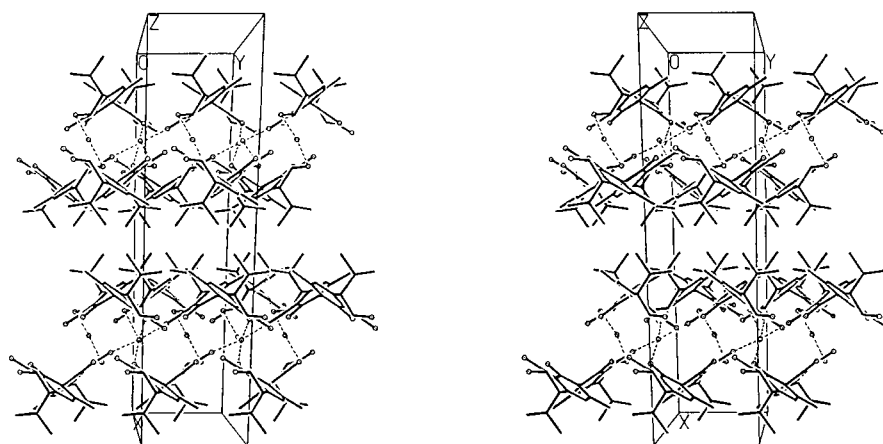


Figure 5. Crystal structure of the gossindane complex with water.

Gossindane shows inclusion ability towards the four solvents chosen accidentally. The host versatility of this compound relatively to other substances is a matter of new investigations which are now in progress.

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