Table 2. *Selected bond lengths* (Å) *and angles* (°)

	Molecule *A*	Molecule *B*	Molecule *C*
N1—C2	1·463 (3)	1·457 (4)	1·464 (4)
N1—C43	1·344 (3)	1·342 (4)	1·343 (4)
C2—C3	1·540 (5)	1·530 (6)	1·522 (4)
C2—C10	1·528 (4)	1·523 (4)	1·541 (4)
C10—O11	1·218 (4)	1·226 (4)	1·228 (4)
C10—N12	1·346 (4)	1·347 (4)	1·343 (4)
N12—C13	1·457 (4)	1·457 (4)	1·467 (4)
C13—C14	1·530 (6)	1·544 (4)	1·547 (5)
C13—C21	1·548 (4)	1·548 (4)	1·547 (5)
C21—O22	1·222 (4)	1·213 (4)	1·215 (5)
C21—N23	1·357 (4)	1·363 (4)	1·357 (5)
N23—C24	1·483 (6)	1·482 (6)	1·483 (7)
N23—C28	1·455 (4)	1·466 (4)	1·460 (4)
C28—C29	1·534 (4)	1·543 (4)	1·538 (4)
C29—O30	1·226 (4)	1·226 (4)	1·222 (4)
C29—N31	1·339 (4)	1·338 (4)	1·346 (4)
N31—C32	1·464 (4)	1·461 (4)	1·466 (4)
C37—C38	1·453 (9)	1·519 (17)	1·501 (8)
C38—O39	1·202 (9)	1·246 (20)	1·193 (9)
C38—C40	1·491 (10)	1·491 (19)	1·491 (10)
C40—O41	1·405 (11)	1·383 (17)	1·405 (11)
C40—C42	1·405 (14)	1·352 (20)	1·431 (20)
O41—C42	1·428 (14)	1·338 (19)	1·302 (20)
C43—O44	1·232 (4)	1·231 (4)	1·231 (4)
C2—N1—C43	123·5 (2)	121·5 (2)	122·7 (3)
N1—C2—C3	108·6 (2)	111·9 (3)	108·7 (3)
N1—C2—C10	109·5 (2)	110·1 (3)	107·0 (3)
C3—C2—C10	114·0 (3)	112·3 (3)	116·8 (3)
C2—C3—C4	115·5 (3)	112·5 (4)	117·5 (3)
C2—C10—O11	121·2 (3)	121·1 (3)	120·7 (3)
C2—C10—N12	115·8 (3)	116·7 (3)	116·2 (3)
O11—C10—N12	123·0 (3)	122·2 (3)	123·0 (3)
C10—N12—C13	123·3 (3)	122·8 (3)	122·5 (3)
N12—C13—C14	110·4 (3)	111·4 (3)	109·9 (3)
N12—C13—C21	118·0 (3)	117·3 (3)	120·9 (3)
C14—C13—C21	110·2 (3)	110·4 (2)	109·5 (3)
C13—C14—C15	114·2 (4)	113·1 (3)	111·8 (3)
C13—C21—O22	116·2 (3)	116·0 (3)	113·9 (3)
C13—C21—N23	121·9 (3)	121·5 (3)	124·7 (3)
O22—C21—N23	121·6 (3)	121·9 (3)	120·9 (4)
C21—N23—C24	118·0 (3)	115·5 (3)	115·7 (4)
C21—N23—C28	124·6 (3)	123·0 (3)	124·1 (3)
C24—N23—C28	116·2 (3)	115·8 (3)	116·3 (3)
N23—C24—C25	111·5 (4)	111·7 (4)	112·0 (5)
N23—C28—C27	111·5 (3)	111·7 (3)	110·6 (3)
N23—C28—C29	110·5 (3)	108·9 (3)	110·0 (3)
C27—C28—C29	113·5 (3)	113·7 (3)	113·5 (3)
C28—C29—O30	121·3 (3)	121·2 (3)	121·0 (3)
C28—C29—N31	118·2 (3)	117·6 (3)	117·6 (3)
O30—C29—N31	120·3 (3)	121·2 (3)	121·3 (3)
C29—N31—C32	118·4 (3)	118·1 (3)	117·2 (3)
N31—C32—C33	111·9 (3)	112·1 (3)	111·5 (3)
N31—C32—C43	108·7 (3)	109·3 (3)	109·5 (3)
C33—C32—C43	111·6 (3)	113·3 (3)	113·3 (3)
C32—C33—C34	101·4 (4)	113·6 (4)	111·9 (3)
C37—C38—O39	124·0 (6)	117·2 (12)	124·8 (6)
C37—C38—C40	114·4 (6)	122·7 (11)	118·8 (5)
O39—C38—C40	121·6 (6)	119·4 (13)	116·4 (6)
C38—C40—O41	118·0 (7)	116·0 (11)	117·9 (7)
C38—C40—C42	121·3 (8)	121·4 (13)	118·7 (9)
O41—C40—C42	61·1 (7)	58·6 (10)	54·7 (8)
C40—O41—C42	59·4 (6)	59·6 (10)	63·7 (9)
C40—C42—O41	59·5 (6)	61·9 (10)	61·7 (9)
N1—C43—C32	115·3 (2)	115·6 (3)	116·3 (3)
N1—C43—O44	123·2 (3)	123·2 (3)	122·3 (3)
C32—C43—O44	121·5 (3)	121·2 (3)	121·4 (3)

respectively, in molecule *B* from the values of their thermal parameters. The accuracy of bond lengths in these disordered sites is relatively poor. Conformations of the 12-membered rings in the molecules *A*, *B* and *C* are almost the same.

In each main-chain ring all the three NH groups are on one side of the ring and the four CO groups are on the opposite side. The molecules are linked to each other along the *a* axis through intermolecular NH···O hydrogen bonds between the rings. O30*A*···N31*B* = 2·951 (4) [O···H = 2·25 (5)], O44*A*···N1*B* = 3·017 (4) [2·34 (3)], O44*A*···N12*B* = 3·038 (4) [2·16 (3)], O11*B*···N31*C* = 2·928 (4) [2·05 (5)], O44*B*···N12*C* = 3·008 (4) [2·27 (5)], O11*C*···N31*A* $(1 + x, y, z)$ = 3·188 (4) [2·53 (5)], O44*C*···N1*A* = 3·020 (3) [2·17 (5)], O44*C*···N12*A* = 3·000 (4) Å [2·11 (5) Å].

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Lattice Inclusion Compounds of Gossypol. Structure of the 1:2 Gossypol/Salicylaldehyde Coordinatoclathrate

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Abstract. $C_{30}H_{30}O_8.2C_7H_6O_2$, $M_r = 762·81$, monoclinic, $P2_1/n$, $a = 11·130$ (2), $b = 29·542$ (5), $c = 11·744$ (2) Å, $\beta = 98·45$ (1)°, $V = 3820$ (1) Å^3, $Z = 4$, $D_x = 1·33$ g cm^{-3}, μ(Cu $K\alpha$) = 8·09 cm^{-1}, $\lambda = 1·51478$ Å, $F(000) = 1608$, $T = 293$ K, $R = 0·059$ for 3541 observed reflections. The gossypol molecules

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form, *via* a pair of O(5)—H···O(3) hydrogen bonds, typical centrosymmetric dimers. Two salicylaldehyde molecules, *B*, related by a symmetry centre, are enclosed in a cage whose four walls are formed by naphthyl rings. The guest molecules in the cage are disordered and adopt two coplanar orientations where they are hydrogen bonded to the gossypol O(1)—H hydroxyl group. Gossypol and salicylaldehyde molecule *B* form a layer analogous to that observed in the gossypol/benzaldehyde 2:3 inclusion compound [Gdaniec, Ibragimov & Talipov (1991), *Acta Cryst.* C**47**, 573–577]. The salicylaldehyde molecules *A* are accommodated in channels formed between the nearest layers related by the *n*-glide plane. In these channels they are hydrogen bonded to the gossypol O(8)—H hydroxyl group.

Introduction. Gossypol [1,1′,6,6′,7,7′-hexahydroxy-5,5′-diisopropyl-3,3′-dimethyl(2,2′-binaphthalene)-8,8′-dicarboxaldehyde] shows remarkable inclusion ability towards a number of chemically different guest substrates (Ibragimov, Talipov, Dadabaev, Nazarov & Aripov, 1988). The structure is easily rearranged to accommodate guests of proper shape, size and chemical nature. Sometimes, a change of crystallization conditions can lead to different inclusion compounds of gossypol with the same guest species. For example, crystallization of gossypol from salicyladehyde gives triclinic crystals, $a = 13{\cdot}838$ (3), $b = 14{\cdot}874$ (3), $c = 18{\cdot}403$ (2) Å, $\alpha = 66{\cdot}60$ (1), $\beta = 109{\cdot}12$ (1), $\gamma = 109{\cdot}63$ (2)°, $V = 3189$ Å^3, $Z = 4$, $D_x = 1{\cdot}33$ g cm^{-3}; host:guest molecular ratio 1:1. When gossypol is crystallized from salicylaldehyde/benzene mixture, monoclinic crystals with host:guest molecular ratio of 1:2 are formed. In both cases, two new forms of gossypol inclusion compounds are obtained. The crystal structure of 1:2 gossypol/salicylaldehyde presented in this paper is closely related to the 2:3 gossypol/benzaldehyde coordinatoclathrate (Gdaniec, Ibragimov & Talipov, 1991).

Experimental. Gossypol was obtained from the Institute of Bioorganic Chemistry, Tashkent, USSR. Pale-yellow elongated plates crystallized when benzene was diffused into salicylaldehyde/benzene mixture containing gossypol. Unit-cell parameters were determined on a Syntex $P2_1$ diffractometer by a least squares fitting of the setting angles of 15 reflections within 2θ range 19–23°. Diffraction data were collected from a crystal of dimensions $0{\cdot}5 \times 0{\cdot}3 \times 0{\cdot}2$ mm in the θ–2θ mode to a maximum 2θ value of 115° using Cu $K\alpha$ radiation with a graphite monochromator (h: $0\rightarrow 11$; k: $0\rightarrow 32$; l: $-12\rightarrow 12$). Two standard reflections were monitored every 100 intensity measurements; maximum variation of their intensity was 3·5%. Final data set consisted of 5647 unique reflections ($R_{\rm int} = 0{\cdot}025$) of which 3541 had $I > 1{\cdot}5\sigma(I)$ and were considered observed. No corrections for extinction or absorption were used. The structure was solved with *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). All atoms of the host with the exception of isopropyl methyl groups were located on the 'best' *E* map. These methyl groups and the guest molecules were found from subsequent ΔF maps. One of the salicylaldehyde molecules is disordered. It adopts two different coplanar orientations in the crystal with occupancy factor 0·657 (6) for orientation *B* and 0·343 (6) for orientation *B*′. The structure was refined by full-matrix least-squares methods with the program *SHELX*76 (Sheldrick, 1976). Positional and anisotropic thermal parameters of non-H atoms of the host and of the salicylaldehyde *A* molecule and positional and isotropic thermal parameters of non-H atoms of salicylaldehyde *B* and *B*′ were refined. The H atoms of the guest *B* and *B*′ were not determined. The H atoms attached to the O atoms and those of the methyl groups C(21) and C(26) were found from ΔF maps. The remaining H atoms were placed in idealized positions, assuming C—H distance of 1·08 Å. The positional parameters of the H atoms located from the ΔF maps and isotropic thermal parameters of all H atoms were included in the refinement. An empirical extinction parameter x was applied to correct F_c according to $F_c' = F_c(1 - xF_c^2/\sin\theta)$; x converged at $59\,(5) \times 10^{-5}$. Weights were assigned as $w = 1/[\sigma^2(F) + 0{\cdot}0001F^2]$ and the quantity minimized was $\sum w(F_o - F_c)^2$. The refinement converged to give final residuals $R = 0{\cdot}059$ and $wR = 0{\cdot}065$. The max. Δ/σ value in the final cycle of refinement was 0·1, final $\Delta\rho$ max. and min. were 0·33 and $-0{\cdot}21$ e Å^{-3}, respectively. Atomic scattering factors were those incorporated in *SHELX*76 (Sheldrick, 1976). The atomic parameters are given in Table 1.* An XT IBM PC computer was used to carry out all crystallographic calculations.

Discussion. An *ORTEP* (Johnson, 1976) representation of the complex with atom labelling is shown in Fig. 1. The gossypol molecule is in the aldehyde form (Kamaev, Baram, Ismailov, Leontev & Sadykov, 1979; Reyes, Wyrick, Borriero & Benas, 1986). Bond lengths and bond angles of the two halves of the gossypol molecule agree within 3σ with the exception of four angles which are within 5σ. They are also in good agreement with the values found in

* Lists of structure factors, anisotropic thermal parameters, bond lengths and bond angles, least-squares-planes data and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53804 (31 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* ($Å^2$) *with e.s.d.'s in parentheses*

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
C(1)	0·2540 (3)	0·9524 (1)	−0·0111 (3)	0·049 (1)
C(2)	0·2357 (3)	0·9064 (1)	0·0037 (3)	0·048 (1)
C(3)	0·2969 (3)	0·8756 (1)	−0·0584 (3)	0·061 (1)
C(4)	0·3709 (3)	0·8915 (1)	−0·1344 (3)	0·062 (1)
C(5)	0·4729 (3)	0·9531 (1)	−0·2283 (3)	0·055 (1)
C(6)	0·5015 (3)	0·9980 (1)	−0·2283 (3)	0·056 (1)
C(7)	0·4487 (3)	1·0297 (1)	−0·1607 (3)	0·053 (1)
C(8)	0·3620 (3)	1·0172 (1)	−0·0926 (3)	0·047 (1)
C(9)	0·3342 (3)	0·9700 (1)	−0·0842 (3)	0·044 (1)
C(10)	0·3914 (3)	0·9383 (1)	−0·1498 (3)	0·050 (1)
C(21)	0·2835 (7)	0·8249 (2)	−0·0395 (7)	0·113 (2)
C(22)	0·3094 (4)	1·0537 (1)	−0·0359 (4)	0·068 (1)
C(23)	0·5262 (4)	0·9195 (1)	−0·3064 (3)	0·067 (1)
C(24)	0·5117 (5)	0·9349 (2)	−0·4329 (4)	0·095 (2)
C(25)	0·6586 (4)	0·9087 (2)	−0·2609 (4)	0·085 (2)
O(1)	0·1939 (3)	0·9833 (1)	0·0468 (2)	0·069 (1)
O(2)	0·3409 (3)	1·0945 (1)	−0·0415 (3)	0·074 (1)
O(3)	0·4851 (2)	1·0728 (1)	−0·1699 (3)	0·070 (1)
O(4)	0·5845 (3)	1·0140 (1)	−0·2949 (3)	0·076 (1)
C(11)	0·1937 (3)	0·8764 (1)	0·1932 (3)	0·050 (1)
C(12)	0·1498 (3)	0·8898 (1)	0·0810 (3)	0·046 (1)
C(13)	0·0252 (3)	0·8850 (1)	0·0406 (3)	0·051 (1)
C(14)	−0·0508 (3)	0·8670 (1)	0·1117 (3)	0·051 (1)
C(15)	−0·0896 (3)	0·8322 (1)	0·2958 (3)	0·049 (1)
C(16)	−0·0433 (3)	0·8185 (1)	0·4040 (3)	0·054 (1)
C(17)	0·0810 (3)	0·8236 (1)	0·4486 (3)	0·055 (1)
C(18)	0·1643 (3)	0·8416 (1)	0·3836 (3)	0·054 (1)
C(19)	0·1197 (3)	0·8568 (1)	0·2683 (3)	0·046 (1)
C(20)	−0·0066 (3)	0·8522 (1)	0·2259 (3)	0·044 (1)
C(26)	−0·0248 (4)	0·8981 (2)	−0·0810 (4)	0·072 (1)
C(27)	0·2896 (4)	0·8418 (2)	0·4369 (4)	0·080 (1)
C(28)	−0·2233 (3)	0·8244 (1)	0·2507 (3)	0·059 (1)
C(29)	−0·3098 (4)	0·8474 (2)	0·3220 (4)	0·082 (2)
C(30)	−0·2518 (4)	0·7737 (1)	0·2378 (4)	0·080 (1)
O(5)	0·3153 (2)	0·8824 (1)	0·2345 (2)	0·067 (1)
O(6)	0·3237 (3)	0·8287 (1)	0·5378 (3)	0·088 (1)
O(7)	0·1120 (3)	0·8088 (1)	0·5581 (2)	0·074 (1)
O(8)	−0·1165 (3)	0·7984 (1)	0·4735 (3)	0·077 (1)
O(1*A*)	0·0902 (3)	0·2406 (1)	0·3065 (3)	0·100 (1)
O(2*A*)	−0·0186 (3)	0·2401 (1)	0·0937 (3)	0·108 (1)
C(1*A*)	0·1918 (4)	0·2256 (1)	0·1438 (3)	0·059 (1)
C(2*A*)	0·1931 (4)	0·2311 (1)	0·2621 (4)	0·067 (1)
C(3*A*)	0·3008 (4)	0·2268 (2)	0·3364 (4)	0·079 (1)
C(4*A*)	0·4058 (4)	0·2171 (2)	0·2930 (5)	0·088 (2)
C(5*A*)	0·4061 (5)	0·2125 (2)	0·1762 (5)	0·094 (2)
C(6*A*)	0·2991 (5)	0·2162 (1)	0·1018 (4)	0·082 (1)
C(7*A*)	0·0799 (5)	0·2306 (2)	0·0651 (4)	0·082 (2)
C(1*B*)	0·4460 (8)	0·4529 (2)	0·0804 (7)	0·057 (2)*
C(2*B*)	0·5760 (7)	0·4414 (2)	0·0830 (6)	0·061 (2)*
C(3*B*)	0·6320 (11)	0·4307 (4)	−0·0058 (11)	0·120 (5)*
C(4*B*)	0·5350 (12)	0·4216 (3)	−0·1017 (9)	0·072 (3)*
C(5*B*)	0·4107 (15)	0·4296 (6)	−0·1151 (16)	0·124 (7)*
C(6*B*)	0·3774 (12)	0·4461 (3)	−0·0071 (14)	0·114 (5)*
C(7*B*)	0·3933 (08)	0·4694 (3)	0·1815 (9)	0·106 (3)*
O(1*B*)	0·6497 (5)	0·4517 (2)	0·1829 (4)	0·103 (2)*
O(2*B*)	0·4671 (6)	0·4763 (2)	0·2791 (5)	0·090 (2)*
C(1*B*′)	0·5037 (16)	0·4520 (4)	0·1009 (11)	0·052 (4)*
C(2*B*′)	0·3465 (22)	0·4540 (7)	0·0275 (19)	0·102 (7)*
C(3*B*′)	0·3434 (14)	0·4406 (5)	−0·0770 (15)	0·077 (5)*
C(4*B*′)	0·4375 (28)	0·4235 (8)	−0·1257 (21)	0·077 (8)*
C(5*B*′)	0·5630 (41)	0·4182 (14)	−0·1070 (37)	0·200 (23)*
C(6*B*′)	0·5873 (18)	0·4278 (6)	−0·0080 (17)	0·075 (6)*
C(7*B*′)	0·5196 (15)	0·4651 (5)	0·2144 (15)	0·101 (5)*
O(1*B*′)	0·2779 (11)	0·4653 (4)	0·0835 (10)	0·119 (4)*
O(2*B*′)	0·4105 (10)	0·4782 (3)	0·2557 (9)	0·066 (3)*

* Isotropic temperature factor.

other gossypol inclusion compounds (Changfu, Cunheng, Guanghong & Shantian, 1982; Gdaniec, Imbragimov & Talipov, 1991; Gdaniec, Ibragimov & Talipov, 1990; Ibragimov, Gdaniec & Dadabaev, 1990; Ibragimov, Talipov, Aripov & Sadykov, 1990). The two naphthyl moieties are nearly perpendicular, the dihedral angle between their least-squares planes

Table 2. *Geometry of hydrogen bonds*

D—H···*A*	*D*···*A* (Å)	*D*—H (Å)	H···*A* (Å)	*D*—H···*A* (°)
(a) Intramolecular hydrogen bonds				
O(3)—H(30)···O(2)	2·444 (5)	0·97 (6)	1·53 (6)	153 (5)
O(7)—H(70)···O(6)	2·474 (5)	0·97 (6)	1·58 (6)	153 (5)
O(4)—H(40)···O(3)	2·622 (5)	0·90 (6)	2·01 (6)	123 (5)
O(8)—H(80)···O(7)	2·609 (5)	0·95 (5)	2·12 (6)	111 (4)
O(1*A*)—H(1*A*)···O(2*A*)	2·612 (5)	1·02 (6)	1·70 (7)	147 (6)
(*b*) Intermolecular hydrogen bonds				
O(5)—H(50)···O(3^{i})	2·785 (4)	0·92 (6)	1·97 (6)	146 (5)
O(4)—H(40)···O(5^{i})	3·299 (4)	0·90 (6)	2·46 (6)	154 (5)
O(1)—H(10)···O(2*B*^{ii})	2·918 (13)	0·87 (5)	2·13 (6)	151 (5)
O(1)—H(10)···O(2*B*′^{ii})	2·747 (13)	0·87 (5)	2·01 (6)	143 (5)
O(8)—H(80)···O(1*A*^{iii})	2·805 (5)	0·95 (5)	1·99 (5)	143 (5)

Symmetry codes: (i) $1 - x, 2 - y, -z$; (ii) $0{\cdot}5 - x, 0{\cdot}5 + y, 0{\cdot}5 - z$; (iii) $-x, 1 - y, 1 - z$.

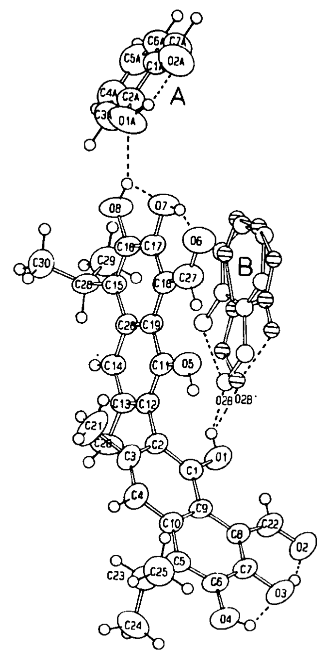

Fig. 1. Atom-numbering scheme.

being 87·6 (3)°. The ring C(11)–C(20) is more planar ($\chi^2 = 112$, max. dev. = 0·015 Å) than the ring C(1)–C(10) ($\chi^2 = 2378$, max. dev. = 0·088 Å). The geometries of the four intramolecular O—H···O hydrogen bonds (Table 2) are close to those observed for gossypol in other inclusion compounds. The intramolecular hydrogen bond in salicylaldehyde *A* has a donor–acceptor distance more than 0·1 Å longer than the analogous O(3)—H(30)···O(2) and O(7)—H(70)···O(6) hydrogen bonds in gossypol.

The hydroxyl group O(5)—H(50) acts as a hydrogen donor to O(3^{i}) of the molecule related by the inversion centre and a typical gossypol dimer is formed. The dimer is further stabilized by a weak O(4)—H(40)···O(5^{i}) interaction. As in the gossypol/benzaldehyde inclusion compound (Gdaniec, Imbragimov & Talipov, 1991), the dimers are the only hydrogen-bond associates of the host in the structure. The hydroxyl groups O(1)—H(10) and O(8)—H(80) are involved, as donors, in hydrogen-bond interactions with salicylaldehyde molecules. The hydroxyl group of the guest *A* interacts with the O(8)—H(8) of gossypol. The second guest was found in the crystal structure in two coplanar orientations, *B* and *B′*, with occupancy factors 0·657 (6) and 0·343 (6), respectively. It is hydrogen bonded (in both orientations) through the aldehyde group to the gossypol O(1)—H(10). The hydrogen bond of salicylaldehyde in the orientation with the lower occupation factor (*B′*) has a donor–acceptor distance 0·17 Å shorter than that of the guest in the alternative orientation.

In 1:2 gossypol/salicylaldehyde and 2:3 gossypol/benzaldehyde there is a common packing motif of the host–guest elements. The gossypol dimers and the guest *B* molecules pack into layers parallel to (010). The structure of the layer for gossypol/salicylaldehyde is shown in Fig. 2. The guest molecules *B* are accommodated in centrosymmetric cages. The two rings, C(1)–C(10) and C(11)–C(20), which form lipophilic walls of the cage are at a distance of 11·41 and 10·36 Å, respectively, in the salicylaldehyde complex and 11·92 and 10·26 Å, respectively, in the benzaldehyde complex. The phenyl rings of the guests located in this cage are nearly parallel to the gossypol C(11)–C(20) moiety. The distance and dihedral angle between the gossypol C(11)–C(20) plane and the guest C(1*B*)–C(6*B*) best plane is 3·47 Å and 5·3°, respectively, in the salicylaldehyde complex and 3·40 Å and 2·5°, respectively, in the benzaldehyde complex.

While the construction of the layers is similar in both inclusion compounds, in gossypol/salicylaldehyde the guest molecule enclosed in the cage is disordered. In orientation *B* the line O(1*B*)···O(2*B*) is nearly parallel to the gossypol C(1)–C(10) ring and H(1*B*) (not localized owing to the disorder), which takes part in the intramolecular hydrogen bond, can interact with π electrons of this naphthyl ring. In orientation *B′* the line O(1*B′*)···O(2*B′*) is nearly perpendicular to the C(1)–C(10) ring; however, in this orientation the hydrogen bond between the host and the guest is stronger than in orientation *B*. The actual occupancy of these two orientations is probably a result of the interplay between the stabilizing effect of these two interactions.

These layers are building blocks of the structure. However, they are not able to form a close-packed structure. The packing diagrams of 1:2 gossypol/salicylaldehyde and 2:3 gossypol/benzaldehyde are compared in Fig. 3. In gossypol/benzaldehyde, close packing is achieved by enclosing additional guest

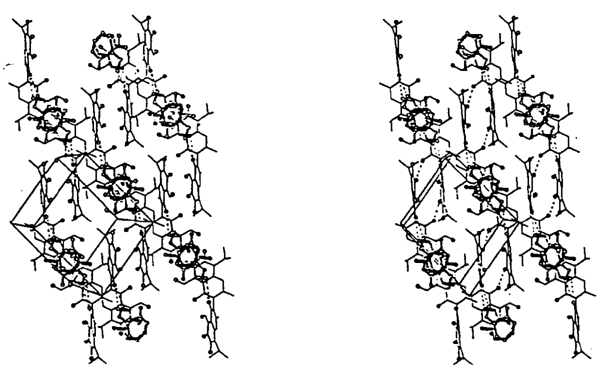

Fig. 2. Structure of the host–guest *B* layer in gossypol/salicylaldehyde 1:2 viewed along [010].

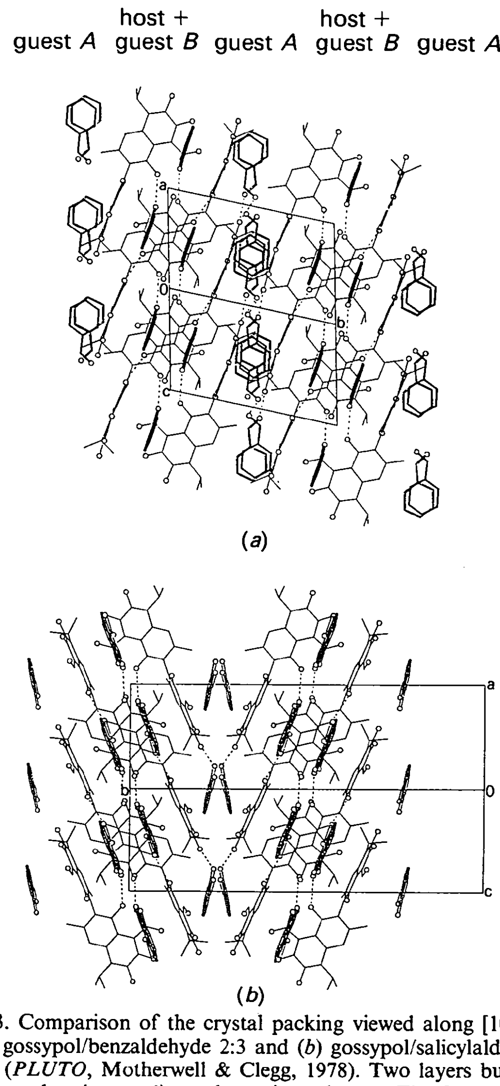

Fig. 3. Comparison of the crystal packing viewed along [101] of (*a*) gossypol/benzaldehyde 2:3 and (*b*) gossypol/salicylaldehyde 1:2 (*PLUTO*, Motherwell & Clegg, 1978). Two layers built by gossypol and guest *B* are shown in each case. The O atoms are marked with circles. H atoms have been omitted for clarity. Hydrogen bonds are drawn with dashed lines.

molecules in cages formed between the two nearest layers related by translation along **b**. These guest molecules show four different coplanar orientations in the cage in which they are hydrogen bonded to the host O(8)—H(80) hydroxyl. In gossypol/salicylaldehyde, channels accommodating guest molecules *A* are formed between the two nearest layers related by an *n*-glide plane. The guest molecules located in the channels are hydrogen bonded to the host O(8)—H(80). The best plane C(1*A*)–C(6*A*) forms a dihedral angle of 15·7° with the naphthyl moiety C(11)–C(20), and the local stacks consisting of six aromatic rings can be distinguished in this structure.

The inclusion compounds of gossypol with benzaldehyde and salicylaldehyde are examples of inclusion compounds with guest:host ratio exceeding 1. In this case one of the solvent molecules and gossypol are used to build 'an inclusion aggregate' (a layer), stabilized by hydrogen bonds and stacking interactions, with the solvent molecule enclosed within a cage formed by gossypol molecules. However, because these aggregates are not able to form a close-packed crystal, an additional solvent molecule is included on crystallization. In this case the inclusion aggregate plays the role of host. It can be expected that a lattice inclusion compound with a structure similar to gossypol/benzaldehyde or gossypol/salicylaldehyde can be obtained with two different guest species: guest *A* will be accommodated in voids formed between the inclusion aggregates of gossypol and guest *B*.

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Structure of D-*glycero*-L-*galacto*-Heptitol

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Abstract. $C_7H_{16}O_7$, $M_r = 212{\cdot}20$, monoclinic, $P2_1$, $a = 4{\cdot}748$ (3), $b = 8{\cdot}362$ (6), $c = 11{\cdot}428$ (7) Å, $\beta = 92{\cdot}01$ (3)°, $V = 453{\cdot}4$ (5) Å^3, $Z = 2$, $D_x = 1{\cdot}554$ g cm^{-3}, λ(Cu $K\alpha_1$) = 1·54051 Å, $\mu = 11{\cdot}7$ cm^{-1}, $F(000) = 228$, $T = 293$ K, final $R = 0{\cdot}049$ for 993 unique observed data. The molecules adopt a

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