Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Inclusion of acetone by 9-(1-naphthyl)-9*H*-xanthen-9-ol

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Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.005 Å
R factor = 0.049
wR factor = 0.124
Data-to-parameter ratio = 7.2

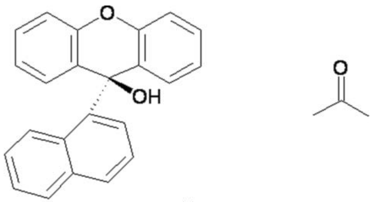
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 13 December 2005
Accepted 23 January 2006

The host compound 9-(1-naphthyl)-9*H*-xanthen-9-ol, forms an inclusion compound with acetone, $C_{23}H_{16}O_2 \cdot C_3H_6O$; two independent molecules of each comprise the asymmetric unit. Despite both host and guest molecules being achiral, the resultant host–guest crystal structure is chiral. The structure is stabilized by O(host)—H···O(guest) hydrogen bonds.

Comment

The characterization of the title compound, (I), arose out of a systematic study of inclusion compounds formed between xanthenol hosts and a variety of volatile organic guests. In a recent publication, we elucidated the structures of a series of inclusion compounds formed between the host 9-(4-methoxyphenyl)-9*H*-xanthen-9-ol and a series of related aromatic guests (Jacobs *et al.*, 2005). The structures and their kinetics of desorption were evaluated and the phenomenon of guest exchange was investigated. We have also reported the inclusion compound formed between 9-(1-naphthyl)-9*H*-xanthen-9-ol and the guest dioxane that was successfully solved in $Pna2_1$ (Jacobs *et al.*, 2004).



(I)

In the current structure, the inclusion compound formed between the achiral host 9-(1-naphthyl)-9*H*-xanthen-9-ol and acetone crystallized in the polar space group $P2_1$, with two host and two guest molecules in the asymmetric unit. The host–guest ratio of 1:1 was confirmed by thermogravimetric analysis which showed a single mass-loss step (calculated mass loss = 14.5%, experimental mass loss = 15.0%).

During structure solution, attempts were made to solve the structure in $P2_1/m$ but these were unsuccessful. The intensity statistics were inconclusive and upon careful analysis of the atomic coordinates of the refined structure, we noted a pseudo-centre of symmetry between pairs of the host molecules, but this symmetry element was not obeyed by the positions of the acetone guests. It is the latter molecules, therefore, which force the structure to crystallize in the chiral space group $P2_1$.

The important feature in the structure is the O(host)—H···O(guest) hydrogen bonds, with O···O distances of 2.730 (1) and 2.857 (1) Å. The topology shows the guest

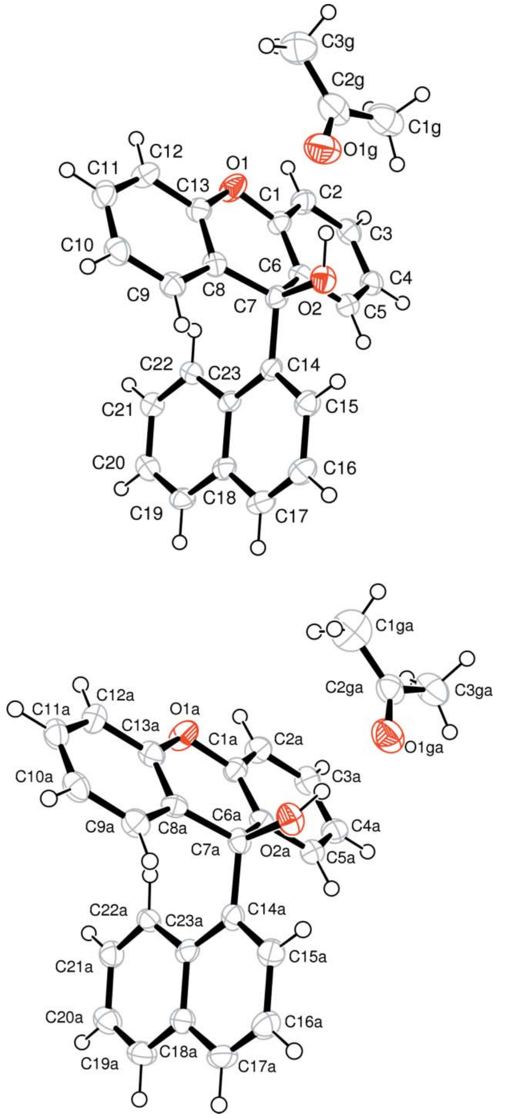


Figure 1
The two host–guest components of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level.

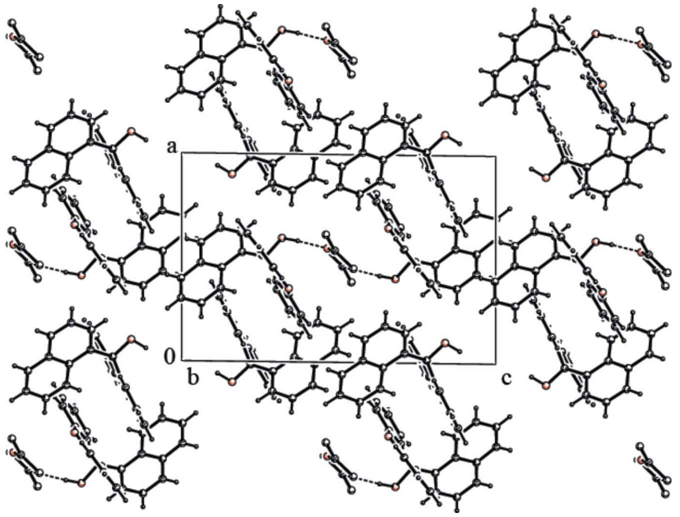


Figure 2
Packing diagram, viewed down [010]. Dashed lines indicate hydrogen bonds.

molecules to be located in channels parallel to [010]. This suggests that this compound should prove easy to desorb and to guest-exchange with such molecules as dimethyl sulfoxide, dimethylformamide and other small volatile organic compounds.

Experimental

Dilute solutions were prepared of the solid host and liquid guest. The mixture was allowed to evaporate slowly at low temperatures until suitable crystals were obtained. The resultant crystals were analysed thermogravimetrically using a Perkin–Elmer TGA6 system.

Crystal data

$C_{23}H_{16}O_2 \cdot C_3H_6O$
$M_r = 382.44$
Monoclinic, $P2_1$
$a = 11.580\ (2)$ Å
$b = 9.7036\ (19)$ Å
$c = 17.489\ (4)$ Å
$\beta = 90.70\ (3)^\circ$
$V = 1965.1\ (7)$ Å^3
$Z = 4$

$D_x = 1.293$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7121 reflections
$\theta = 3.5$–25.3°
$\mu = 0.08$ mm^{-1}
$T = 113\ (2)$ K
Rectangular block, colourless
0.39 × 0.32 × 0.27 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
7121 measured reflections
3789 independent reflections
2768 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.037$
$\theta_{\rm max} = 25.3^\circ$
$h = -13 \rightarrow 13$
$k = -11 \rightarrow 11$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.124$
$S = 1.06$
3789 reflections
528 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0759P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.26$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.25$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O1G	0.970 (18)	1.767 (17)	2.730 (1)	172 (2)
O2A—H1A···O1GA	0.971 (19)	1.897 (18)	2.857 (1)	171 (2)

The aromatic and methyl H atoms were geometrically constrained, with C—H distances fixed at 0.95 and 0.98 Å, respectively, and with $U_{\rm iso}({\rm H}) = 1.2$ and $1.5U_{\rm eq}({\rm C})$, respectively. The hydroxy H atoms were fixed in positions with torsion angles chosen to match the maximum electron density in the difference map. Thereafter, they were geometrically constrained based on the relationship between O—H and O···O distances (Olovsson & Jönsson, 1975). In the absence of significant anomalous scattering effects, Friedel pairs were merged in the final refinement.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*

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(Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 1999) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

The authors thank the National Research Foundation (Pretoria) for research grants.

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