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5,5′-Diallylbiphenyl-2,2′-diol–1,4-diazabicyclo[2.2.2]octane (2/1)

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.123
Data-to-parameter ratio = 14.5

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

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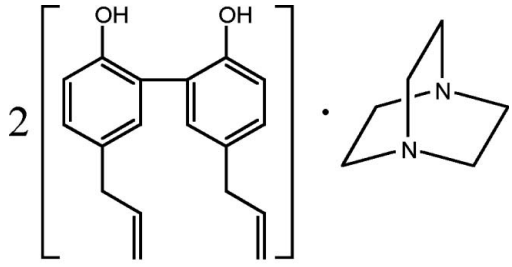
In the title compound, $2C_{18}H_{18}O_2\cdot C_6H_{12}N_2$, 5,5′-diallylbiphenyl-2,2′-diol and 1,4-diazabicyclo[2.2.2]octane molecules are linked by O—H···O and O—H···N hydrogen bonds.

Comment

5,5′-Diallylbiphenyl-2,2′-diol, also known as magnolol, an active principal component isolated from the Chinese herb 'Houpu' (*Magnolia officinalis*), has been shown to be an anti-platelet aggregation (Teng *et al.*, 1988), vessel dilation (Teng *et al.*, 1990) and anti-inflammatory (Wang *et al.*, 1992) agent. The extract of *Magnolia officinalis* contains mainly magnolol and its isomer honokiol. The crystal structure of magnolol has been reported (Wang *et al.*, 1982). In our laboratory, honokiol has been separated from the *Magnolia officinalis* extract by applying molecular recognition of 1,4-diazabicyclo[2.2.2]-octane (DABCO) (Jin *et al.*, 2005). Recently, we obtained a 2:1 complex of magnolol and DABCO, (I). We report here the structure of (I).



(I)

The asymmetric unit of (I) contains two magnolol and one DABCO molecules (Fig. 1). The geometry of the magnolol molecule in the title compound (Table 1) is consistent with that observed in the crystal structure of magnolol (Wang *et al.*, 1982). An intramolecular O—H···O hydrogen bond is observed in both magnolol molecules (Table 2). In the crystal structure, the two magnolol molecules are linked by O—H···O hydrogen bonds and the DABCO molecule is linked to them *via* an O—H···N hydrogen bond (Fig. 2).

Experimental

5,5′-Diallylbiphenyl-2,2′-diol (3 mol) and 1,4-diazabicyclo[2.2.2]-octane (1 mol) were dissolved in sufficient ethanol by heating to a temperature where a clear solution resulted. Crystals of (I) were formed by gradual evaporation of the ethanol solution over a period of 7 d at 293 K.

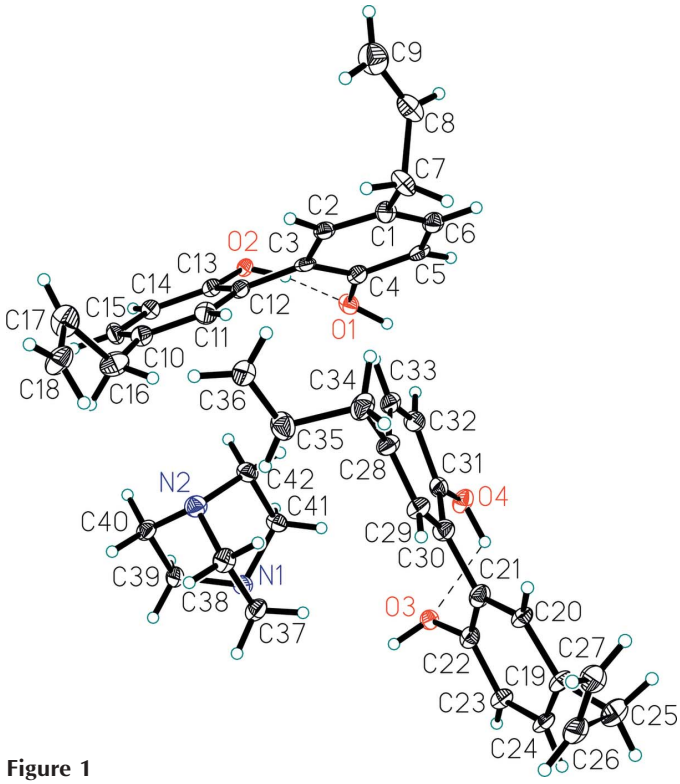


Figure 1
The asymmetric unit of (I), showing the atomic numbering scheme and 40% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

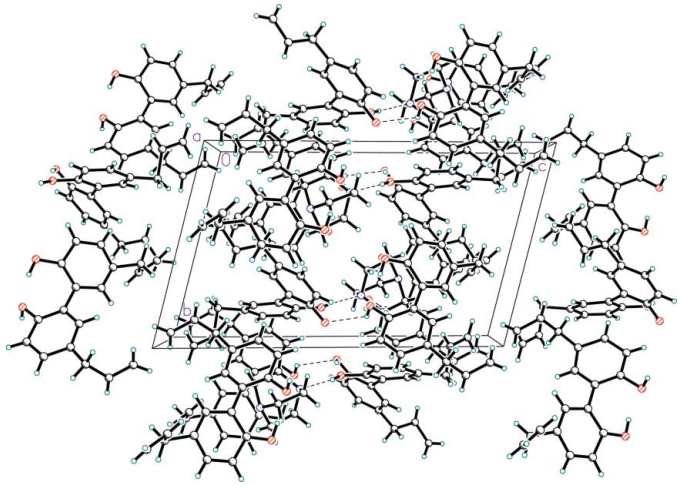


Figure 2
The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

Crystal data

$2C_{18}H_{18}O_2{\cdot}C_6H_{12}N_2$
M_r = 644.82
Triclinic, $P\overline{1}$
a = 10.272 (3) Å
b = 10.646 (3) Å
c = 17.697 (5) Å
α = 103.948 (5)°
β = 95.457 (5)°
γ = 92.632 (5)°
V = 1864.9 (9) Å^3
Z = 2
D_x = 1.148 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 977 reflections
θ = 2.4–18.5°
μ = 0.07 mm^{-1}
T = 273 (2) K
Block, colourless
0.32 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.98, T_{max} = 0.98
9357 measured reflections
6454 independent reflections
4865 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°
$h = -11 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -16 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.123
S = 1.07
6454 reflections
445 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 1.2457P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.329 (3)	C12—C13	1.392 (3)
C1—C6	1.373 (4)	C13—O2	1.346 (3)
C1—C7	1.486 (3)	C13—C14	1.395 (3)
C2—C3	1.395 (3)	C14—C15	1.391 (3)
C3—C4	1.428 (3)	C16—C17	1.543 (4)
C3—C12	1.477 (3)	C17—C18	1.407 (4)
C4—O1	1.374 (3)	C37—N1	1.520 (3)
C4—C5	1.398 (3)	C37—C38	1.523 (3)
C5—C6	1.344 (3)	C38—N2	1.459 (3)
C7—C8	1.560 (4)	C39—N1	1.471 (3)
C8—C9	1.345 (4)	C39—C40	1.520 (3)
C10—C15	1.387 (4)	C40—N2	1.420 (3)
C10—C11	1.392 (4)	C41—N1	1.502 (3)
C10—C16	1.443 (4)	C41—C42	1.508 (3)
C11—C12	1.386 (3)	C42—N2	1.506 (3)

C2—C1—C6	116.2 (2)	C13—C12—C3	128.5 (2)
C2—C1—C7	122.2 (2)	O2—C13—C12	119.2 (2)
C6—C1—C7	121.6 (2)	O2—C13—C14	120.8 (2)
C1—C2—C3	128.2 (2)	C12—C13—C14	119.9 (2)
C2—C3—C4	112.1 (2)	C15—C14—C13	119.9 (2)
C2—C3—C12	128.0 (2)	C10—C15—C14	120.3 (2)
C4—C3—C12	120.0 (2)	C10—C16—C17	120.1 (2)
O1—C4—C5	116.7 (2)	C18—C17—C16	103.2 (3)
O1—C4—C3	121.9 (2)	N1—C37—C38	106.07 (19)
C5—C4—C3	121.4 (2)	N2—C38—C37	110.9 (2)
C6—C5—C4	119.5 (2)	N1—C39—C40	108.3 (2)
C5—C6—C1	122.4 (2)	N2—C40—C39	110.0 (2)
C1—C7—C8	94.5 (2)	N1—C41—C42	110.92 (19)
C9—C8—C7	115.4 (3)	N2—C42—C41	106.16 (19)
C15—C10—C11	119.6 (2)	C39—N1—C41	110.70 (18)
C15—C10—C16	129.8 (2)	C39—N1—C37	112.50 (18)
C11—C10—C16	110.5 (2)	C41—N1—C37	105.40 (19)
C12—C11—C10	120.5 (2)	C40—N2—C38	110.4 (2)
C11—C12—C13	119.8 (2)	C40—N2—C42	111.07 (19)
C11—C12—C3	111.6 (2)	C38—N2—C42	110.7 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*O*···O1	0.90 (3)	1.58 (3)	2.444 (2)	162 (3)
O4—H4*O*···O3	0.96 (3)	2.00 (3)	2.575 (3)	116 (2)
O1—H1*O*···N1^{i}	0.98 (3)	1.84 (3)	2.634 (3)	136 (2)
O3—H3*O*···O2^{i}	0.89 (3)	2.25 (3)	2.498 (3)	96 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydroxy H atoms were located in a difference Fourier map and refined with $U_{iso}(H) = 1.2U_{eq}(O)$. All other H atoms were placed in calculated positions and allowed to ride on their parent atoms with C—H distances of 0.93 (phenyl and alkene) and 0.97 Å (methylene), and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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