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Inclusion compound 2-pyridone–1,1-bis(4-hydroxyphenyl)cyclohexane (1/1)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.122
Data-to-parameter ratio = 13.6

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

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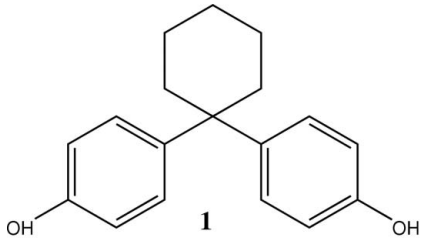
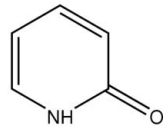
In the title compound, $C_5H_5NO{\cdot}C_{18}H_{20}O_2$, the host molecules of 1,1-bis(4-hydroxyphenyl)cyclohexane are hydrogen bonded *via* the hydroxy groups into zigzag chains extending along the *b* axis. The guest molecules of 2-pyridone are paired into N—H···O hydrogen-bonded dimers, which connect two zigzag chains *via* O—H···O hydrogen bonds to produce a hydrogen-bonded ribbon. Structure analysis reveals that the mutual relation between two successive guest molecules does not enable photodimerization.

Comment

1,1-Bis(4-hydroxyphenyl)cyclohexane (1 in scheme) forms inclusion compounds with various guest molecules (Goldberg *et al.*, 1987). It was successively used for the separation of similar isomers (Caira *et al.*, 1997; Tanaka *et al.*, 2001). It was found that the host-to-guest ratio with xylidine isomers depends on the crystalization temperture (Nassimbeni & Su, 2002). We crystallized the inclusion compound consisting of 1 as host molecule and 2-pyridone (a in scheme) as guest molecule as part of comprehensive investigation (Lavy & Kaftory, 2006) concerning the effects of photodimerization of guest molecules in solid inclusion compounds on the crystal structure during and after the reaction takes place.



1



a

(I)

The title inclusion compound, (I) (Fig. 1), crystallizes in the triclinic space group $P\overline{1}$. The host molecules are hydrogen bonded *via* the hydroxy groups (Table 1) into zigzag chains extending along the *b* axis. The guest molecules are paired into N—H···O hydrogen-bonded dimers (Table 1), which connect two zigzag chains *via* O—H···O hydrogen bonds (Table 1) to produce a hydrogen-bonded ribbon extending along the *b* axis (Fig. 2). 2*H*-Pyridone derivatives tend to form hydrogen-bonded dimers. From 240 2*H*-pyridone derivatives in the Cambridge Structural database (Version 5.27; Allen, 2002), 108 were found to have such hydrogen-bonded dimers.

This inclusion compound was crystallized in order to study the effect of photodimerization of the guest molecules in the solid state on the crystal structure. The closest distance

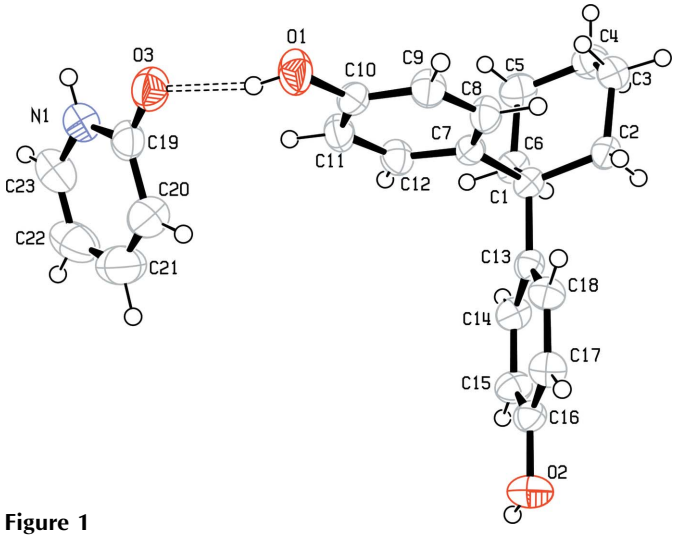


Figure 1
The asymmetric unit of inclusion compound (I), showing the atomic numbering and 50% probability displacement ellipsoids. The dashed line denotes a hydrogen bond.

between potentially reacting atoms (C20–C23^{i}) is 5.188 (4) Å [symmetry code: (i) $-x$, $-y$, $-z$]. This distance is above the limit of 4.2 Å set by Schmidt (1971) for photodimerization in the solid state. Moreover, the efficiency of the orbital overlap using the definition given by Kearsley (1987) is very poor. The distance between the two lobes is 4.08 (2) Å.

Experimental

The host and the guest substances were purchased from Sigma. The inclusion compound crystal was obtained from an ethyl acetate solution of a 1:1 mixture of host and guest.

Crystal data

$C_5H_5NO.C_{18}H_{20}O_2$
M_r = 363.44
Triclinic, $P\overline{1}$
a = 6.2860 (2) Å
b = 10.6530 (4) Å
c = 15.2150 (6) Å
α = 103.1470 (14)°
β = 96.5620 (14)°
γ = 104.143 (3)°
V = 946.40 (6) Å^3
Z = 2
D_x = 1.275 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Prism, colourless
0.20 × 0.20 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
9892 measured reflections
3356 independent reflections
2115 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.122
S = 1.01
3356 reflections
246 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.050 (5)

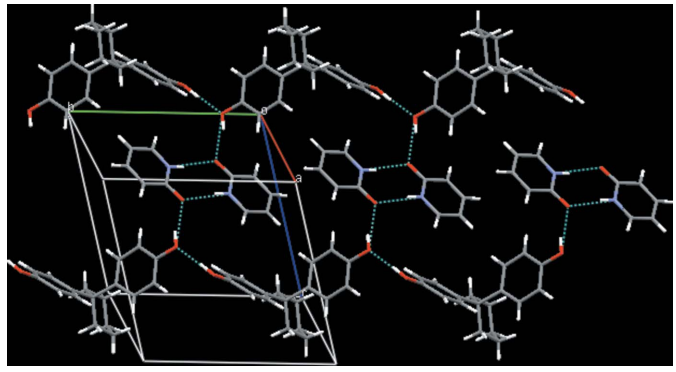


Figure 2
The crystal packing of (I), showing the hydrogen-bonded (dashed lines) ribbon.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O1···O3^{i}	0.82	1.85	2.648 (2)	162
O2—H1O2···O1^{ii}	0.82	1.94	2.762 (2)	176
N1—H1N1···O3^{iii}	0.86	2.00	2.846 (3)	166

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $x, y+1, z$; (iii) $-x+2, -y+1, -z$.

All H atoms were located in a difference Fourier map and allowed to ride on their parent atoms, with N—H = 0.86 Å, O—H = 0.82 Å, C—H = 0.96 Å and U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *COLLECT* (Nonius, 2000); 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* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *MERCURY* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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