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Inclusion compound 4-methyl-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) = 0.002 Å
R factor = 0.046
wR factor = 0.127
Data-to-parameter ratio = 17.9

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

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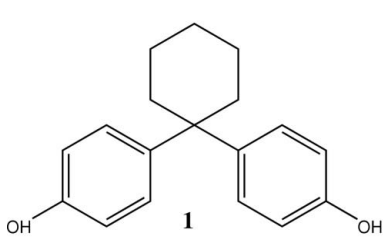
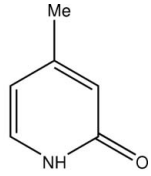
In the title compound, $C_6H_7NO{\cdot}C_{18}H_{20}O_2$, the host molecules of 1,1-bis(4-hydroxyphenyl)cyclohexane are hydrogen bonded *via* the hydroxy groups into zigzag chains extended along the *a* axis. The guest molecules of 4-methyl-2-pyridone are paired into N—H···O hydrogen-bonded dimers, which 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

In continuation of our study of the effects of photodimerization of the guest molecules in solid inclusion compounds on the crystal structure during and after the reaction takes place (Lavy & Kaftory, 2006*a*), the inclusion compound between 1,1-bis(4-hydroxyphenyl)cyclohexane and 4-methyl-2-pyridone (1 and a in the scheme, respectively) was prepared.



1



a

(I)

The title inclusion compound, (I) (Fig. 1), crystallizes in monoclinic space group $P2_1/c$. In many aspects its crystal structure is similar to that obtained with 2-pyridone as the guest (Lavy & Kaftory, 2006*b*). The host molecules in (I) are hydrogen bonded *via* the hydroxy groups (Table 1) into zigzag chains extended along the *a* axis. The guest molecules are paired into N—H···O (Table 1) hydrogen-bonded dimers, which connect two zigzag chains *via* O—H···O hydrogen bonds (Table 1) to produce a hydrogen-bonded ribbon extended along the *a* axis (Fig. 2).

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 between the potentially reacting atoms (C20···C24^{iv}) is 5.967 (2) Å [symmetry code: (iv) $-x, -y, -z$]. 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 4.73 (1) Å.

Experimental

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

Crystal data

$C_6H_7NO\cdot C_{18}H_{20}O_2$
M_r = 377.47
Monoclinic, $P2_1/c$
a = 10.931 (2) Å
b = 16.737 (3) Å
c = 11.340 (2) Å
β = 99.93 (3)°
V = 2043.6 (7) Å^3
Z = 4
D_x = 1.227 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Prism, colourless
0.30 × 0.25 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
16251 measured reflections
4630 independent reflections
2609 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.8°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.127
S = 0.97
4630 reflections
258 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.013
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.038 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O1···O3^{i}	0.82	1.81	2.615 (2)	167
O2—H2O2···O1^{ii}	0.82	1.98	2.796 (2)	177
N1—H1N1···O3^{iii}	0.86	2.02	2.877 (2)	173

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

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 and C—H = 0.93–0.97 Å. U_{iso}(H) values were set at 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other C-bound H atoms; U_{iso}(H) was refined freely for O- and N-bound H atoms.

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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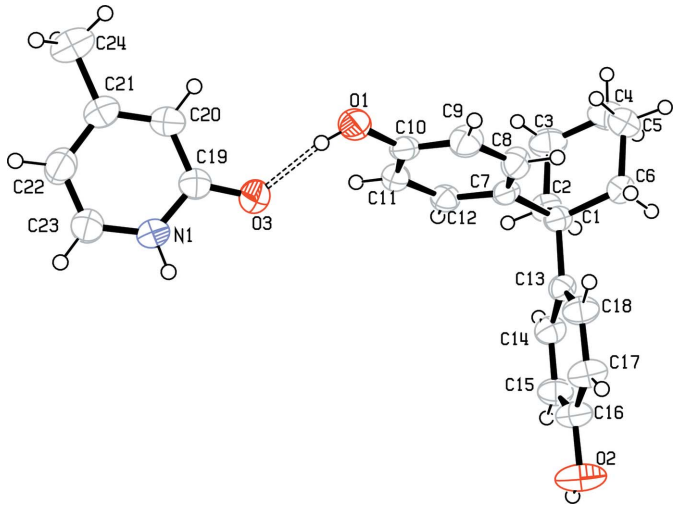

Figure 1
The asymmetric unit of inclusion compound (I), showing the atomic numbering and 50% probability displacement ellipsoids. The dashed line denotes a hydrogen bond.

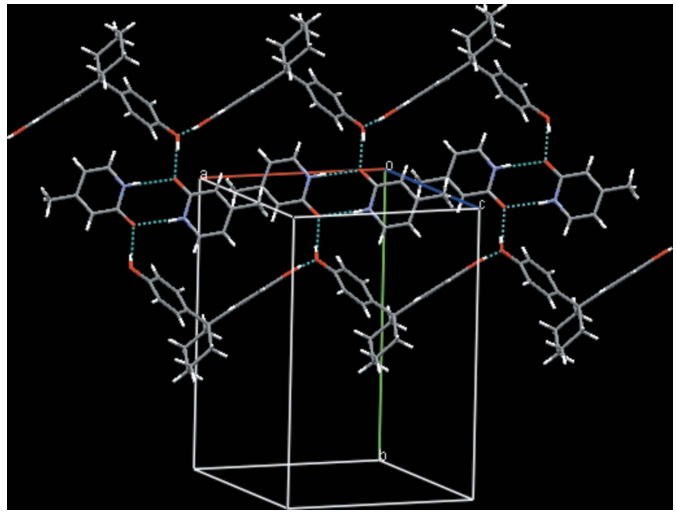

Figure 2
The crystal packing of (I), showing the hydrogen-bonded (dashed lines) ribbon.

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