

P2—N2	1.584 (3)	C1—C2	1.346 (4)
P2—N1	1.585 (3)	C1—C9	1.429 (4)
P2—O4	1.594 (2)	C2—C3	1.397 (4)
P3—N3	1.579 (3)	C3—C4	1.356 (4)
P3—N2	1.582 (3)	C4—C10	1.420 (4)
P3—O5	1.584 (2)	C5—C6	1.360 (5)
P3—O6	1.587 (2)	C5—C10	1.425 (4)
F14—C14	1.367 (4)	C6—C7	1.392 (6)
F20—C20	1.365 (4)	C7—C8	1.362 (5)
F26—C26	1.363 (3)	C8—C9	1.412 (5)
F32—C32	1.374 (4)	C9—C10	1.416 (4)
O1—C2	1.401 (3)		
N1—P1—N3	117.22 (14)	N2—P3—O5	110.36 (12)
N1—P1—O1	110.70 (13)	N3—P3—O6	109.58 (12)
N3—P1—O1	109.30 (13)	N2—P3—O6	110.75 (13)
N1—P1—O2	110.12 (13)	O5—P3—O6	95.38 (11)
N3—P1—O2	110.80 (13)	C2—O1—P1	110.4 (2)
O1—P1—O2	96.82 (11)	C3—O2—P1	110.3 (2)
O3—P2—N2	112.11 (13)	C11—O3—P2	122.6 (2)
O3—P2—N1	106.24 (13)	C17—O4—P2	119.5 (2)
N2—P2—N1	117.53 (13)	C23—O5—P3	121.7 (2)
O3—P2—O4	99.46 (11)	C29—O6—P3	122.0 (2)
N2—P2—O4	109.33 (12)	P1—N1—P2	122.6 (2)
N1—P2—O4	110.66 (13)	P3—N2—P2	122.2 (2)
N3—P3—N2	117.02 (14)	P1—N3—P3	123.3 (2)
N3—P3—O5	111.64 (13)		

The diffraction data were collected on a Siemens three-circle diffractometer (χ axis fixed at 54.74°) equipped with a CCD detector maintained at 218.6 K, using the ω -scan technique (Campana, Shepard & Litchman, 1980). The initial cell constants were determined from reflection data obtained by collecting 60×10 s frames at a detector resolution of 512×512 pixels. The final unit-cell values, however, are based on the least-squares refinement of all the observed reflections [4645 for (1) and 3449 for (2)]. A complete hemisphere of data was scanned on ω (0.3°), with a run time of 10 s frames for a total of 1271 frames collected in three sets plus a final set of 50 frames using the *SMART Software* (Siemens, 1995c). The crystal decay was monitored through reflection data from 50 frames collected at the beginning and at the end of data collection. The data reduction was accomplished by processing the frames data using *SAINT Software* (Siemens, 1995a) to give the raw file corrected for Lp and decay. Since the raw file contains information about directional cosines, it was used for empirical absorption correction. The structures were solved by direct methods using *SHELXS86* (Sheldrick, 1990) in *SHELXTL-Plus* (Siemens, 1995b) and refined by full-matrix least-squares methods using *SHELXTL-Plus* and *SHELXL93* (Sheldrick, 1993). H atoms were located from difference Fourier syntheses and refined with isotropic displacement parameters. All computations were performed on a Silicon Graphics workstation.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry, and torsion angles have been deposited with the IUCr (Reference: FG1172). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Multiple Hydrogen Bonds in Pyridine-2,6-dimethanol and Benzene-1,3,5-trimethanol

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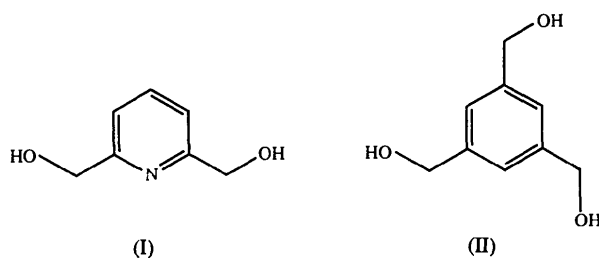
(Received 28 March 1996; accepted 8 May 1996)

Abstract

Pyridine-2,6-dimethanol, C₇H₉NO₂, forms a chain structure in which the molecules are linked by O—H···O hydrogen bonds into dimeric units lying across centres of inversion, these dimers being linked by O—H···N hydrogen bonds into chains around other centres of inversion. In the structure of benzene-1,3,5-trimethanol, C₉H₁₂O₃, the molecules form a continuous three-dimensional network in which each molecule is hydrogen-bonded to six others.

Comment

The structure of furan-2,5-dimethanol, $\text{HOCH}_2(2,5\text{-C}_4\text{H}_2\text{O})\text{CH}_2\text{OH}$, consists of highly puckered rhomboidal nets of molecules held together by $\text{O—H}\cdots\text{O}$ hydrogen bonds in which only the hydroxyl O atoms participate (Glidewell, Zakaria & Ferguson, 1996). Pyridine is π isoelectronic with furan, but the N atom is much more basic than the O atom of furan. Accordingly, there is the possibility that in the structure of the analogous compound pyridine-2,6-dimethanol, $\text{HOCH}_2(2,6\text{-C}_5\text{H}_3\text{N})\text{CH}_2\text{OH}$, (I), the N atom will take part in the hydrogen bonding. We have therefore studied the structure of compound (I) and report it here together with the structure of the related compound benzene-1,3,5-trimethanol, $\text{C}_6\text{H}_3(\text{CH}_2\text{OH})_3$, (II).



In compound (I), the internal N—C—C angles at the C atoms carrying the CH_2OH substituents are both significantly larger than 120° , but there is not even approximate molecular symmetry because of the different conformations adopted by the two CH_2OH substituents (Fig. 1). The hydroxyl H atoms are fully ordered, in contrast to those in furan-2,5-dimethanol (Glidewell, Zakaria & Ferguson, 1996), one hydroxyl group (O2—H) acting as both a donor and an acceptor of hydrogen bonds, the other (O6—H) acting as just a donor, while the pyridine N atom acts as an acceptor, consistent with expectation. The O2 atom in the molecule at (x, y, z) acts as a hydrogen-bond donor to atom O6 in the molecule at $(-x, -y, -z)$, thus linking the molecules into cyclic centrosymmetric pairs whose hydrogen-bonding motif has graph set $R_2^2(16)$ (Etter, 1990; Etter, MacDonald & Bernstein, 1990; Bernstein, Davis, Shimoni & Chang, 1995). In addition, atom O6 in the molecule at (x, y, z) acts as a donor to the

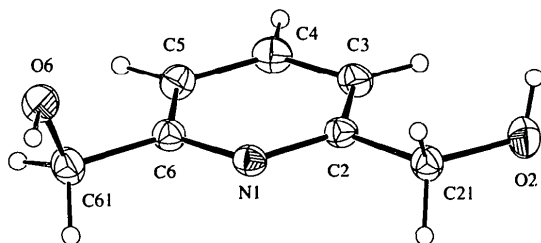


Fig. 1. A view of compound (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

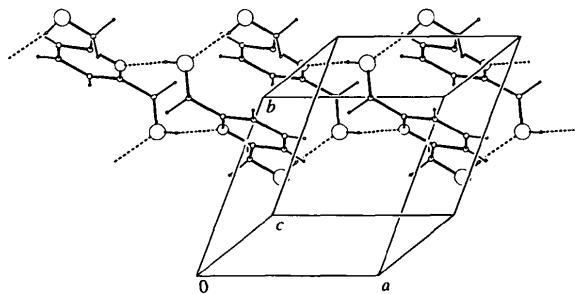


Fig. 2. A view of the chain structure of compound (I) showing the hydrogen bonds.

N atom in the molecule at $(1-x, -y, -z)$, forming a second centrosymmetric cyclic motif, this time with graph set $R_2^2(10)$. These two motifs propagate infinite chains running parallel to the *a* direction; there are only van der Waals interactions between the chains and each molecule is hydrogen bonded to only two others (Fig. 2). The overall hydrogen-bonding scheme in (I) is thus a chain of rings (Bernstein, Davis, Shimoni & Chang, 1995) whose complete graph set can be written as $C_2^2(7)[R_2^2(16)R_2^2(10)]$.

Although the pair of pyridine rings related by a centre of inversion are parallel with an interplanar separation of 3.69 Å, they are in fact almost completely offset from each other, with only the N1—C2 bonds partially overlapping. There are therefore effectively no $\pi\cdots\pi$ stacking interactions between these rings. Atom H21A in the molecule at (x, y, z) makes the closest approach to the ring C4, C5 and C6 atoms in the molecule at $(-x, -y, -z)$, but none is shorter than the sum of the van der Waals radii (Bondi, 1964).

In compound (II), although there are no significant differences between the independent C—C bond lengths within the benzene ring, the internal C—C—C angles (Table 5) show a clear alternation, with the smaller angles occurring at the C atoms carrying the CH_2OH substituents. This angle distortion is in the opposite sense from that observed in compound (I); the alternation of bond angles lowers the effective local symmetry of the ring from D_{6h} ($6/mmm$) to D_{3h} ($\bar{6}m2$). Overall, the molecules do not exhibit even approximate threefold symmetry since the conformation of the three CH_2OH groups are entirely different (Table 5, Figs. 3 and 4); the C—O bond lengths also vary widely (Table 5).

The hydroxyl H atoms in compound (II) are fully ordered and all participate in $\text{O—H}\cdots\text{O}$ hydrogen bonds which serve to link the molecules into a continuous three-dimensional network (Fig. 4). Firstly, atom O5 in the molecule at (x, y, z) acts as a hydrogen-bond donor to atom O3 in the molecule at $(x, 1+y, z)$. This generates, by repeated translation in the *b* direction, a chain motif with graph set $C(8)$. Four such chains run through each unit cell. Secondly, atom O3 in the molecule at (x, y, z) acts as donor to atom O5 in the mol-

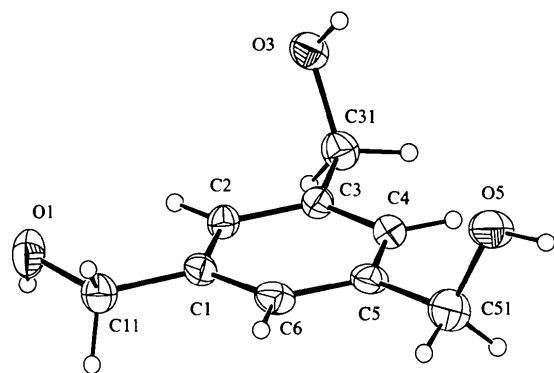


Fig. 3. A view of compound (II) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

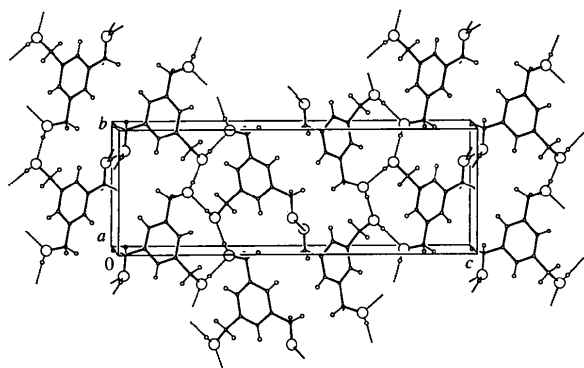


Fig. 4. A view of the crystal structure of compound (II) showing the hydrogen bonds.

ecule at $(-x, -\frac{1}{2} + y, \frac{1}{2} - z)$, thus linking the pairs of chains related by the 2_1 axis at $(0, y, \frac{1}{4})$ into a ladder with first-level graph set *DD* and second-level graph set *C(4)* (Bernstein, Davis, Shimoni & Chang, 1995). A similar ladder running in the opposite sense is generated from two other chains by the 2_1 axis at $(0, y, \frac{3}{4})$. Finally, atom O1 in the molecule at (x, y, z) acts as donor to atom O1 in the molecule at $(-\frac{1}{2} + x, -\frac{1}{2} - y, -z)$ generating a spiral motif with graph set *C(2)* around the 2_1 axis at $(x, -\frac{1}{4}, 0)$. In this way, each hydroxyl group acts as both donor and acceptor of hydrogen bonds and each molecule is hydrogen-bonded to six others in a continuous three-dimensional network.

The molecular aggregation is thus one-dimensional in pyridine-2,6-dimethanol, two-dimensional in furan-2,5-dimethanol (Glidewell, Zakaria & Ferguson, 1996) and three-dimensional in benzene-1,3,5-trimethanol.

Experimental

Compound (I) was obtained from Aldrich. Compound (II) was prepared by reduction of trimethyl 1,3,5-benzenetricarboxylate (Cochrane, Pauson & Stevens, 1968; Storck & Manecke, 1975). Crystals of (I) and (II) suitable for single-crystal diffraction analysis were grown by slow evaporation of methanol solutions.

Compound (I)

Crystal data

C₇H₉NO₂
M_r = 139.15
 Triclinic
P $\bar{1}$
a = 6.8730 (10) Å
b = 7.2268 (14) Å
c = 7.471 (2) Å
 α = 80.41 (2)°
 β = 80.27 (2)°
 γ = 67.121 (10)°
V = 334.87 (11) Å³
Z = 2
D_x = 1.380 Mg m⁻³
D_m not measured

Mo K α radiation

λ = 0.7107 Å
 Cell parameters from 25 reflections
 θ = 11.74–22.32°
 μ = 0.102 mm⁻¹
T = 294 (1) K
 Needle
 0.40 × 0.26 × 0.22 mm
 Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
 $\theta/2\theta$ scans
 Absorption correction: none
 1945 measured reflections
 1945 independent reflections
 1039 observed reflections
 $[I > 2\sigma(I)]$

θ_{\max} = 30°
h = -8 → 9
k = 0 → 10
l = -10 → 10
 3 standard reflections
 frequency: 60 min
 intensity decay: none

Refinement

Refinement on *F*²
R(*F*) = 0.0483
 $wR(F^2)$ = 0.1328
S = 0.969
 1945 reflections
 93 parameters
 H atoms riding [SHELXL93 (Sheldrick, 1993) defaults; C—H 0.93–0.97 and O—H 0.82 Å]

$w = 1/[\sigma^2(F_o^2) + (0.0644P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.249 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.157 \text{ e \AA}^{-3}$
 Extinction correction: none
 Atomic scattering factors from *International Tables for Crystallography* (1992), Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for (I)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
O2	-0.3346 (2)	0.3650 (2)	0.2479 (2)	0.0490 (4)
O6	0.5593 (2)	-0.1192 (2)	-0.2209 (2)	0.0442 (4)
N1	0.1688 (2)	0.1968 (2)	-0.0465 (2)	0.0317 (3)
C2	-0.0421 (2)	0.2715 (2)	-0.0013 (2)	0.0310 (4)
C3	-0.1843 (3)	0.3383 (2)	-0.1306 (2)	0.0367 (4)
C4	-0.1060 (3)	0.3254 (3)	-0.3126 (2)	0.0401 (4)
C5	0.1113 (3)	0.2469 (3)	-0.3608 (2)	0.0382 (4)
C6	0.2450 (2)	0.1841 (2)	-0.2243 (2)	0.0329 (4)
C21	-0.1124 (3)	0.2776 (3)	0.2013 (2)	0.0372 (4)
C61	0.4828 (3)	0.0940 (3)	-0.2669 (2)	0.0417 (4)

Table 2. Selected geometric parameters (\AA , °) for (I)

O2—C21	1.413 (2)	C2—C21	1.512 (2)
O6—C61	1.423 (2)	C3—C4	1.380 (2)
N1—C2	1.339 (2)	C4—C5	1.382 (2)
N1—C6	1.347 (2)	C5—C6	1.389 (2)
C2—C3	1.385 (2)	C6—C61	1.504 (2)

C2—N1—C6	118.63 (13)	C4—C5—C6	118.9 (2)
N1—C2—C3	122.47 (15)	N1—C6—C5	121.9 (2)
C2—C3—C4	118.8 (2)	O2—C21—C2	114.66 (14)
C3—C4—C5	119.27 (15)	O6—C61—C6	110.56 (13)
N1—C2—C21—O2	177.22 (14)	N1—C6—C61—O6	74.7 (2)

Table 3. Hydrogen-bonding geometry (\AA , $^\circ$) for (I)

D—H...A	D—H	H...A	D...A	D—H...A
O2—H2...O6 ⁱ	0.82	2.00	2.818 (2)	172
O6—H6...N1 ⁱⁱ	0.82	1.99	2.806 (2)	173

Symmetry codes: (i) $-x, -y, -z$; (ii) $1 - x, -y, -z$.**Compound (II)***Crystal data*C₉H₁₂O₃ $M_r = 168.19$

Orthorhombic

 $P2_12_12_1$ $a = 4.5660 (3) \text{\AA}$ $b = 8.1331 (5) \text{\AA}$ $c = 23.173 (3) \text{\AA}$ $V = 860.55 (14) \text{\AA}^3$ $Z = 4$ $D_x = 1.298 \text{ Mg m}^{-3}$ D_m not measuredMo $K\alpha$ radiation $\lambda = 0.7107 \text{\AA}$

Cell parameters from 25

reflections

 $\theta = 9.15\text{--}17.81^\circ$ $\mu = 0.097 \text{ mm}^{-1}$ $T = 294 (1) \text{ K}$

Needle cut from longer piece

 $0.41 \times 0.28 \times 0.28 \text{ mm}$

Colourless

Data collection

Enraf–Nonius CAD-4

diffractometer

 $\theta/2\theta$ scans

Absorption correction:

none

1134 measured reflections

1134 independent reflections

680 observed reflections

 $[I > 2\sigma(I)]$ *Refinement*Refinement on F^2 $R(F) = 0.0434$ $wR(F^2) = 0.1004$ $S = 1.050$

1134 reflections

112 parameters

H atoms riding [SHELXL93

(Sheldrick, 1993) defaults;

C—H 0.93–0.97 and O—

H 0.82 \AA] $\theta_{\text{max}} = 27^\circ$ $h = 0 \rightarrow 5$ $k = 0 \rightarrow 10$ $l = 0 \rightarrow 29$

3 standard reflections

frequency: 60 min

intensity decay: none

 $w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 0.0259P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.159 \text{ e \AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.140 \text{ e \AA}^{-3}$

Extinction correction: none

Atomic scattering factors

from *International Tables for Crystallography* (1992),

Vol. C, Tables 4.2.6.8 and

6.1.1.4)

Table 4. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for (II)
$$U_{\text{eq}} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U_{eq}
O1	0.3000 (5)	-0.1870 (3)	0.02131 (10)	0.0596 (7)
O3	-0.2286 (6)	-0.2190 (2)	0.22715 (7)	0.0507 (6)
O5	0.0190 (7)	0.4960 (2)	0.19198 (9)	0.0721 (9)
C1	0.0849 (7)	0.0444 (3)	0.07473 (11)	0.0372 (7)
C2	-0.0732 (7)	-0.0608 (3)	0.10973 (11)	0.0378 (7)
C3	-0.2460 (8)	-0.0027 (3)	0.15440 (10)	0.0378 (7)
C4	-0.2606 (9)	0.1645 (3)	0.16356 (11)	0.0479 (8)
C5	-0.1049 (8)	0.2732 (3)	0.12979 (12)	0.0477 (9)

C6	0.0669 (8)	0.2132 (3)	0.08555 (11)	0.0455 (8)
C11	0.2728 (9)	-0.0147 (3)	0.02541 (11)	0.0501 (8)
C31	-0.4153 (8)	-0.1208 (4)	0.19161 (12)	0.0506 (8)
C51	-0.1216 (10)	0.4566 (3)	0.14081 (13)	0.0739 (15)

Table 5. Selected geometric parameters (\AA , $^\circ$) for (II)

O1—C11	1.410 (3)	C2—C3	1.384 (4)
O3—C31	1.429 (3)	C3—C4	1.378 (3)
O5—C51	1.386 (4)	C3—C31	1.505 (4)
C1—C2	1.382 (4)	C4—C5	1.378 (4)
C1—C6	1.398 (4)	C5—C6	1.380 (4)
C1—C11	1.508 (4)	C5—C51	1.515 (4)
C2—C1—C6	118.1 (3)	C1—C6—C5	120.9 (3)
C1—C2—C3	121.7 (3)	O1—C11—C1	114.7 (3)
C2—C3—C4	118.6 (3)	O3—C31—C3	112.4 (3)
C3—C4—C5	121.4 (3)	O5—C51—C5	110.4 (3)
C4—C5—C6	119.2 (3)		
C2—C1—C11—O1	-6.4 (5)	C6—C5—C51—O5	-110.1 (4)
C4—C3—C31—O3	-111.9 (4)		

Table 6. Hydrogen-bonding geometry (\AA , $^\circ$) for (II)

D—H...A	D—H	H...A	D...A	D—H...A
O1—H1...O1 ⁱ	0.82	1.87	2.690 (2)	177
O3—H3...O5 ⁱⁱ	0.82	1.93	2.736 (3)	170
O5—H5...O3 ⁱⁱⁱ	0.82	1.89	2.704 (3)	174

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

In both compounds (I) and (II), the top peaks in the difference maps used to locate the H atoms were those of the hydroxyl groups. Examination of the structures with *PLATON* (Spek, 1995a) showed that there were no solvent-accessible voids in the crystal lattices. The absolute configuration for compound (II) was indeterminate.

For both compounds, data collection: *CAD-4-PC Software* (Enraf–Nonius, 1992); cell refinement: *SET4* and *CELDIM* in *CAD-4-PC Software*; data reduction: *DATRD2* in *NRCVAX94* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structures: *SHELXS86* (Sheldrick, 1990) for (I); *SOLVER* in *NRCVAX94* for (II). For both compounds, program(s) used to refine structures: *NRCVAX94* and *SHELXL93* (Sheldrick, 1993); molecular graphics: *NRCVAX94*, *PLATON* (Spek, 1995a) and *PLUTON* (Spek, 1995b); software used to prepare material for publication: *NRCVAX94*, *SHELXL93* and *WordPerfect* (macro *PREPCIF*).

GF thanks NSERC (Canada) for Research Grants.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: CF1110). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Hydrogen-Bonded Chains in 4,4'-Dihydroxybenzophenone–4,4'-Bipyridyl (1/1) and Chains of Rings in 1,3,5-Trihydroxybenzene–4,4'-Bipyridyl (2/3)

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Abstract

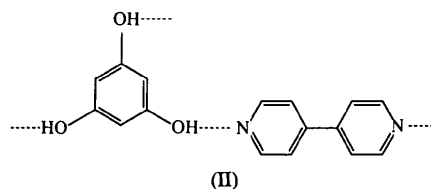
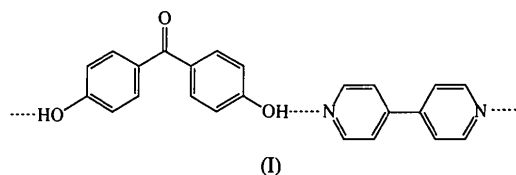
In the 1:1 adduct of 4,4'-dihydroxybenzophenone and 4,4'-bipyridyl, [OC(C₆H₄OH)₂].(NC₅H₄–C₅H₄N), the components are linked into chains by O—H···N hydrogen bonds. In the 2:3 adduct formed between 1,3,5-trihydroxybenzene and 4,4'-bipyridyl, 2[C₆H₃(OH)₃].3(NC₅H₄–C₅H₄N), pairs of molecules of each component are linked by O—H···N hydrogen bonds into macrocyclic rings, which are themselves linked by further 4,4'-bipyridyl molecules into chains of rings; these chains are cross-linked by C—H···O hydrogen bonds.

Comment

4,4'-Bipyridyl forms an adduct of 1:1 stoichiometry with the diol ferrocene-1,1'-diylbis(diphenylmethanol), Fe(C₅H₄CPh₂OH)₂, but despite the exact numerical match in this system between the number of hydroxy groups, hydrogen-bond donors and N atoms acting as hydrogen-bond acceptors, only one half of the 4,4'-bipyridyl molecules in the adduct participate in the hydrogen-bonding scheme (Glidewell, Ferguson, Lough & Zakaria, 1994). In view of this unexpected behaviour, we have now investigated the behaviour of 4,4'-

bipyridyl with some bis-phenols and tris-phenols; since phenols are somewhat more acidic than tertiary alcohols, they can be expected to be more effective hydrogen-bond donors towards 4,4'-bipyridyl. The adducts thus formed illustrate the versatility of the O—H···N synthon in crystal engineering (Subramanian & Zaworotko, 1994; Desiraju, 1995).

Co-crystallization of bis-phenols of the type X(C₆H₄OH)₂ with 4,4'-bipyridyl in methanol solution yielded analytically pure adducts of 1:1 stoichiometry for X = O, S, SO₂ and CO; with each of the tris-phenols CH₃C(C₆H₄OH)₃ and 1,3,5-trihydroxybenzene, adducts having 2:3 tris-phenol:bipyridyl stoichiometry were obtained. Few of these adducts yield crystals suitable for single-crystal X-ray diffraction, but we have obtained such crystals for two representative adducts, 4,4'-dihydroxybenzophenone–4,4'-bipyridyl (1/1), (I), and 1,3,5-trihydroxybenzene–4,4'-bipyridyl (2/3), (II), and we report here their structures.



The structure of compound (I) (Fig. 1) is dominated by the formation of simple chains consisting of alternate bis-phenol and 4,4'-bipyridyl units joined together by O—H···N hydrogen bonds (Fig. 2), as expected when the two components employ two hydrogen-bond donors and acceptors respectively. Atom O1 in the asymmetric unit at (x, y, z) acts as hydrogen-bond donor to atom N34 within the same unit, while atom O2 in this unit acts as donor to atom N44 in the bipyridyl molecule at $(-\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z)$. Repetition of these hydrogen bonds generates chains running parallel to the direction $[\bar{1}01]$, in which the chain-forming motif has graph set $C_2^2(21)$ (Bernstein, Davis, Shimoni & Chang, 1995). The chains are arranged within the unit cell such that pairs of bipyridyl rings related by centres of inversion and lying in adjacent chains form stacks parallel to the $[010]$ direction, but none of the individual C···C or C···N distances is significantly shorter than the sum of van der Waals radii. In addition to the involvement of atoms O1 and O2 as donors of hydrogen bonds, the carbonyl O atom, O3, is potentially an acceptor of hydrogen bonds and, in the absence of other donors, C—H···O hydrogen-bond formation may be expected (Hunter, 1991).