Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,3-Di-4-pyridylbutane-2,3-diol

Yun-Yin Niu,[a] Xiu-Cun Liu,[a] Sharifuddin M. Zain[b] and Seik Weng Ng[b]*

[a]Department of Chemistry, Zhengzhou University, Zhengzhou 450052, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.103
Data-to-parameter ratio = 12.1

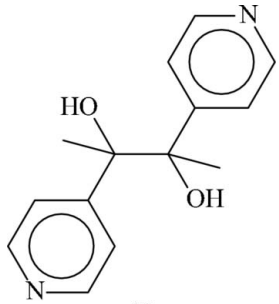
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 7 November 2005
Accepted 18 November 2005
Online 26 November 2005

The molecule of the title compound, $C_{14}H_{16}N_2O_2$, lies on a centre of inversion located at the mid-point of the central C—C bond. O–H···N hydrogen bonds link adjacent molecules into a layer motif.

Comment

Following the study of a copper complex of di(4-pyridyl)glycol (Kitaura *et al.*, 2002), we have used the related title ligand, (I), in an unsuccessful attempt to synthesize its adduct with cadmium iodide. An earlier study describes the isolation of the 1,4-(4*H*-1,2,4-triazol-1-methyl)benzene adduct (Niu *et al.*, 2005).



(I)

The molecule of (I) lies on a centre of inversion at the mid-point of the C2—C2^{i} bond (Fig. 1). O–H···N hydrogen bonds [O1—H···N1^{i} = 2.829 (2) Å; symmetry code: (i) $x, \frac{3}{2} - y, z - \frac{1}{2}$] link adjacent molecules into a layer motif (Fig. 2). The central C—C single bond is surprisingly long [1.591 (3) Å]; the geometry-optimized structure, as calculated by *GAUSSIAN98* (Frisch *et al.*, 1998), also has a similarly long bond [1.603 Å]. On the other hand, the C—C_{methyl} distances in the crystal structure and geometry-optimized structure are normal (Table 1).

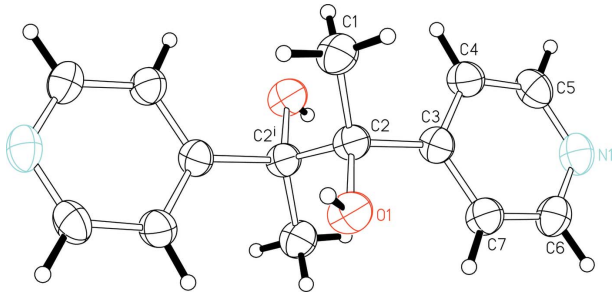


Figure 1
A plot of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii [Symmetry code (i) and for unlabelled atoms: $1 - x, 1 - y, 1 - z$.]

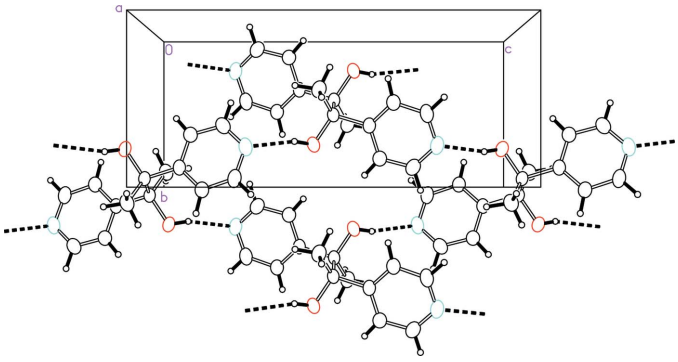


Figure 2
A plot showing the hydrogen-bonded layer structure in (I). Hydrogen bonds are shown as dashed lines.

Experimental

The title compound, which was purchased from Fluka, remained unreacted in an attempt to synthesize the adduct with cadmium iodide. Cadmium iodide (0.037 g, 0.1 mmol) and the reagent (0.024 g, 0.1 mmol) were dissolved in dimethyl sulfoxide (10 ml). Colourless crystals of (I) deposited from the solution after several days. For the density functional theory quantum-chemical calculations, the ground state electronic state was calculated at the B3LYP/6–31G* level using the *GAUSSIAN98* program suite (Frisch *et al.*, 1998).

Crystal data

$C_{14}H_{16}N_2O_2$
$M_r = 244.29$
Orthorhombic, *Pbca*
$a = 12.408\ (1)$ Å
$b = 6.4174\ (6)$ Å
$c = 15.004\ (2)$ Å
$V = 1194.8\ (2)$ Å^3
$Z = 4$
$D_x = 1.358$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1618 reflections
$\theta = 2.7$–$26.3°$
$\mu = 0.09$ mm^{-1}
$T = 291\ (2)$ K
Block, colourless
0.26 × 0.14 × 0.06 mm

Data collection

Bruker APEX-II area-detector diffractometer
φ and ω scans
Absorption correction: none
6611 measured reflections
1376 independent reflections
1049 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$
$h = -11 \rightarrow 16$
$k = -8 \rightarrow 7$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.103$
$S = 1.02$
1376 reflections
114 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.2502P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C2	1.421 (2)	C2—C2^{i}	1.591 (3)
N1—C5	1.329 (2)	C3—C7	1.386 (2)
N1—C6	1.335 (2)	C3—C4	1.392 (2)
C1—C2	1.526 (2)	C4—C5	1.386 (2)
C2—C3	1.532 (2)	C6—C7	1.381 (2)
C5—N1—C6	116.2 (1)	C7—C3—C4	116.8 (1)
O1—C2—C1	110.8 (1)	C7—C3—C2	120.8 (1)
O1—C2—C3	107.1 (1)	C4—C3—C2	122.4 (1)
C1—C2—C3	110.6 (1)	C5—C4—C3	119.3 (1)
O1—C2—C2^{i}	108.0 (1)	N1—C5—C4	124.0 (1)
C1—C2—C2^{i}	111.6 (1)	N1—C6—C7	124.1 (1)
C3—C2—C2^{i}	108.6 (1)	C6—C7—C3	119.5 (1)

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

The diffraction measurements were of a quality that allowed all H atom parameters to be refined, albeit with O—H = 0.85 (1) and C—H = 0.95 (1) Å distance restraints. Their displacement parameters were freely refined.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the National Natural Science Foundation of China (grant No 20371042), the Henan Province Excellent Young Persons Foundation (grant Nos. 2005002800 and 0612002800), the China Postdoctoral Science Foundation (grant No. 2003033525) and the University of Malaya for supporting this work. We also thank Luoyang Normal College for the diffraction measurements.

References

Bruker (2004). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Zakrzewski, V. G., Montgomery, Jr, J. A., Stratmann, R. E., Burant, J. C., Dapprich, S., Millam, J. M., Daniels, A. D., Kudin, K. N., Strain, M. C. *et al.* (1998). *GAUSSIAN98*. Revision A9. Gaussian Inc., Pittsburgh, Pennsylvania, USA.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Kitaura, R., Fujimoto, K., Noro, S., Kondo, M. & Kitagawa, S. (2002). *Angew. Chem. Int. Ed.* **41**, 133–135.
Niu, Y.-Y., Zhang, H.-L., Hou, H.-W. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m2536–m2537.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.