Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

4,4′-Bipyridyl *N*,*N*′-dioxide–3-hydroxy-2-naphthoic acid (1/2)

Ben-Yong Lou* and Yan-Bin Huang

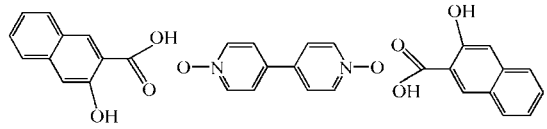
Department of Chemistry and Chemical Engineering, Minjiang University, Fuzhou, Fujian 350108, People's Republic of China
Correspondence e-mail: loubenyong@163.com

Received 31 January 2007
Accepted 28 February 2007
Online 31 March 2007

4,4′-Bipyridyl *N*,*N*′-dioxide crystallizes with 3-hydroxy-2-naphthoic acid to give a centrosymmetric three-component adduct, $C_{10}H_8N_2O_2{\cdot}2C_{11}H_8O_3$, which is engineered into a two-dimensional layer structure by two kinds of π–π interactions. Weak C—H···O interactions further link the two-dimensional structure into a three-dimensional structure.

Comment

Supramolecular heterosynthons provide an effective strategy for designing organic solids containing multiple components (Almarsson & Zaworotko, 2004). For example, the pyridine–carboxylic acid heterosynthon has been used to make several pharmaceutical cocrystals (Bailey Walsh *et al.*, 2003). The bipyridyl system is also able to provide other weak interactions, such as π–π and C—H···π interactions, as exemplified by the adduct of 4,4′-bipyridine and 3-hydroxy-2-naphthoic acid (Lou *et al.*, 2006). Here, we treated 4,4′-bipyridyl *N*,*N*′-dioxide, rather than 4,4′-bipyridine, with 3-hydroxy-2-naphthoic acid and obtained the title molecular complex, (I).



(I)

X-ray diffraction shows that the centrosymmetric three-component adduct, (I), results from the heterosynthon containing hydrogen-bonding (O2—H2···O4; Table 2) and C—H···O interactions (C14–H14···O1; Table 3) between the pyridyl ring and carboxylic acid group (Fig. 1). The phenol hydroxyl group is involved in intramolecular hydrogen bonding with the carbonyl O atom (O3—H3···O1; Table 2). Selected geometric parameters are given in Table 1.

The rings of 4,4′-bipyridyl *N*,*N*′-dioxide are coplanar and the naphthalene rings are parallel to the plane of the 4,4′-bipyridyl *N*,*N*′-dioxide molecule. The naphthalene rings C2–C4/C11/C10/C9 and C5–C8/C10/C11 of the 3-hydroxy-2-

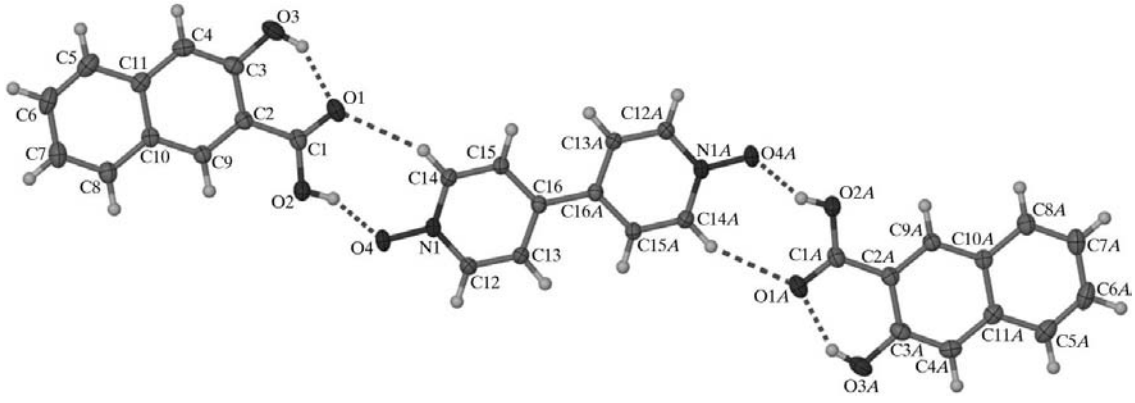


Figure 1
A plot of adduct (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Dashed lines indicate hydrogen bonds. Atoms labelled with the suffix *A* are generated by the symmetry operator ($-x$, $1-y$, $-z-1$).

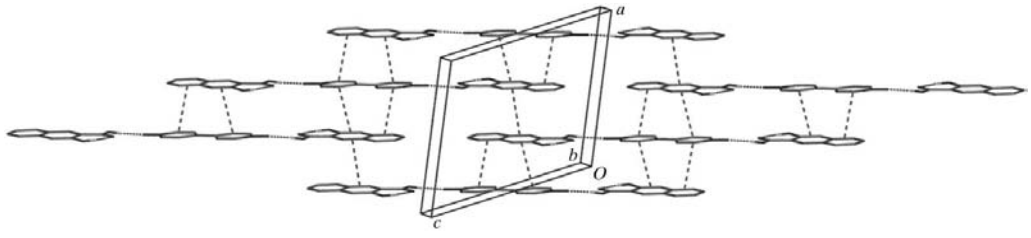


Figure 2
The π–π interactions in adduct (I). Dashed lines indicate π–π interactions and dotted lines indicate hydrogen bonds.

  DOI: 10.1107/S0108270107009717

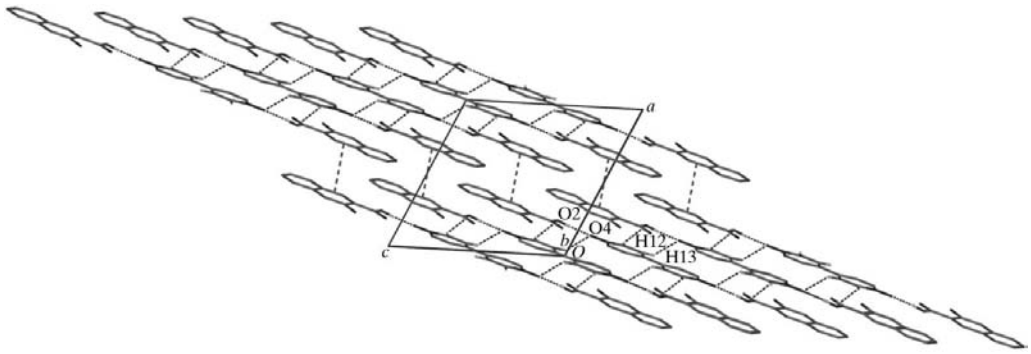


Figure 3
The three-dimensional structure of (I), viewed along the *b* axis. Dashed lines indicate C—H···O and π–π interactions.

naphthoic acid molecule are involved in π–π interactions in the *a* direction with two N1/C12–C16 pyridyl rings at $(-x, 1-y, -z)$ and $(x, y, 1+z)$, respectively (Table 3). Along the *c* axis, the adduct is linked into an infinite one-dimensional chain by face-to-face π–π stacking between pyridyl rings and naphthalene rings (Table 3). There are also π–π interactions in the *a* direction between naphthalene rings: ring C2–C4/C11/C10/C9 of the 3-hydroxy-2-naphthoic acid molecule is simultaneously involved in π–π interactions with two rings, *viz*. C2–C4/C11/C10/C9 and C5–C8/C10/C11, of another 3-hydroxy-2-naphthoic acid molecule at $(1-x, 1-y, 1-z)$ (Table 3). Thus, along the (102) direction the adduct is also linked into a one-dimensional chain by π–π stacking between naphthalene rings. As a result, the centrosymmetric adduct is engineered into a two-dimensional structure in the *ac* plane by two kinds of π–π interactions, both of which produce stacking in the *a* direction (Fig. 2).

In the adduct, two C—H groups of the same pyridyl ring are involved in C—H···O interactions with the carboxylic acid group (C12—H12···O2; Table 3) and pyridyl O atom (C13—H13···O4) from the same adduct molecule at $(x, \frac{1}{2}-y, z-\frac{1}{2})$. These weak interactions link the two-dimensional structure into a three-dimensional π–π stacking array (Fig. 3).

The structure of (I) also shows that pyridine *N*-oxide can offer more weak interactions than the pyridine ring, due to its extra O atom which can simultaneously participate in two kinds of hydrogen bonds.

Experimental

A mixture of 3-hydroxy-2-naphthoic acid (0.075 g, 0.4 mmol) and 4,4′-bipyridyl *N*,*N*′-dioxide (0.038 g, 0.2 mmol) was stirred in ethanol (10 ml). The solution was kept in air and after several days yellow crystals of (I) were obtained in 70% yield.

Crystal data

$C_{10}H_8N_2O_2{\cdot}2C_{11}H_8O_3$
$M_r = 564.54$
Monoclinic, $P2_1/c$
$a = 10.7800\ (16)$ Å
$b = 11.8800\ (11)$ Å
$c = 11.4700\ (15)$ Å
$\beta = 114.820\ (5)^\circ$
$V = 1333.2\ (3)$ Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 293\ (2)$ K
0.30 × 0.25 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
$T_{min} = 0.839$, $T_{max} = 1.000$
9907 measured reflections
3038 independent reflections
2226 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.137$
$S = 1.08$
3038 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.227 (2)	O4—N1	1.3252 (17)
O2—C1	1.306 (2)	N1—C12	1.339 (2)
O3—C3	1.362 (2)	N1—C14	1.343 (2)
O4—N1—C12	117.92 (14)	O1—C1—C2	122.98 (17)
O4—N1—C14	121.81 (14)	O2—C1—C2	114.18 (14)
O1—C1—O2	122.83 (17)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1	0.84	1.85	2.597 (2)	147
O2—H2···O4	0.84	1.70	2.489 (2)	155

Table 3
Geometric parameters for weak hydrogen bonds and π–π interactions in the title structure (Å, °).

*Cg*1 is the centroid of the C2–C4/C11/C10/C9 ring, *Cg*2 is the centroid of the C5–C8/C10/C11 ring and *Cg*3 is the centroid of the N1/C12–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O1	0.95	2.50	3.389 (7)	156
C12—H12···O2^{i}	0.95	2.47	3.204 (8)	134
C13—H13···O4^{i}	0.95	2.52	3.362 (3)	147
*Cg*1···*Cg*1^{ii}		3.44†	3.861 (4)‡	27§
*Cg*1···*Cg*2^{ii}		3.45	3.886 (3)	27
*Cg*1···*Cg*3^{iii}		3.49	3.712 (4)	19
*Cg*2···*Cg*3^{iv}		3.58	3.685 (5)	13

† Perpendicular distance between *Cgx* and *Cgy*. ‡ Distance between ring centroids. § Angle between the *Cgx*···*Cgy* vector and the normal to the plane of *Cgy*. Symmetry codes: (i) $x, \frac{1}{2}-y, z-\frac{1}{2}$; (ii) $1-x, 1-y, 1-z$; (iii) $-x, 1-y, -z$; (iv) $x, y, 1+z$.

All H atoms were located geometrically and refined as riding, with C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the Research Fund (grant No. YKQ05008) of Minjiang University for the support of this research.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV3073). Services for accessing these data are described at the back of the journal.

References

Almarsson, Ö. & Zaworotko, M. J. (2004). *Chem. Commun.* pp. 1889–1896.
Bailey Walsh, R. D., Bradner, M. W., Fleischman, S., Morales, L. A., Moulton, B., Rodriguez-Hornedo, N. & Zaworotko, M. J. (2003). *Chem. Commun.* pp. 186–187.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Lou, B.-Y., Huang, X.-D. & Lin, X.-C. (2006). *Acta Cryst.* C**62**, o310–o311.
Rigaku (2000). *CrystalClear*. Version 1.3. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.