Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,4′-Bipyridine–2-methoxybenzoic acid (1/2)

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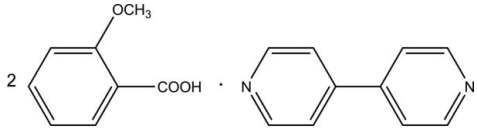
Received 12 January 2012; accepted 25 January 2012

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.052; wR factor = 0.154; data-to-parameter ratio = 12.0.

The asymmetric unit of the title compound, $C_{10}H_8N_2\cdot 2C_8H_8O_3$, contains two 2-methoxybenzoic acid molecules and one 4,4′-bipyridine molecule. The 4,4′-bipyridine molecule is disordered over two positions in a 1:1 ratio. In the crystal, the 2-methoxybenzoic acid and 4,4′-bipyridine molecules are connected by intermolecular O—H···N hydrogen bonds. The dihedral angle between the carboxy group and its attached ring is 26.823 (2)°.

Related literature

For the use and related structures of 2-methoxybenzoic acid in coordination chemistry, see: Vollano *et al.* (1984); Smith *et al.* (1986); Li (2005); Andrews *et al.* (2006); Ren *et al.* (2006); Zhao *et al.* (2008); Sharma *et al.* (2009).



Experimental

Crystal data

$C_{10}H_8N_2\cdot 2C_8H_8O_3$
M_r = 460.47
Monoclinic, $P2_1/c$
a = 7.7090 (15) Å
b = 25.620 (5) Å
c = 6.3624 (13) Å
β = 112.08 (3)°
V = 1164.4 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.30 × 0.28 × 0.25 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.972, T_{max} = 0.977
5991 measured reflections
2060 independent reflections
1540 reflections with $I > 2\sigma(I)$
R_{int} = 0.088

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.154
S = 1.06
2060 reflections
172 parameters
9 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	1.85	2.673 (2)	177

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2171).

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supplementary materials

Acta Cryst. (2012). E**68**, o597 [doi:10.1107/S1600536812003194]

4,4′-Bipyridine–2-methoxybenzoic acid (1/2)

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Comment

Bipyridine is a well known molecule often used as a linker in polymeric coordination complexes. 2-Methoxybenzoic acid is also sometimes used as a common ligand in coordination polymers (Vollano *et al.*, 1984; Smith *et al.*, 1986; Li, 2005; Andrews *et al.*, 2006; Ren *et al.*, 2006; Zhao *et al.*, 2008; Sharma *et al.*, 2009.). The title compound, (I), is a 1:2 cocrystal of the aforementioned linkers. Herewith we present its crystal structure. The asymmetric unit of the title compound (Fig. 1) contains two 2-methoxybenzoic acid molecules and one 4,4′-bipyridine molecule. The dihedral angle of carboxy group to its ring is 26.823 (2)°. The 4,4′-bipyridine molecule is disordered over two positions in a 1:1 ratio. In the crystal structure, the 2-methoxybenzoic acid and 4,4′-bipyridine are held together by intermolecular O—H···N hydrogen bonds.

Experimental

An ethanol solution (20 ml) of 2-methoxybenzoic acid (0.1 mmol) and 4,4′-bipyridine (0.1 mmol) was heated at 333 K for 2 h. Then the mixture was cooled to room temperature. After two weeks colorless crystals were obtained that were suitable for X-ray diffraction study.

Refinement

Four C atoms of bipyridyl group are disordered over two sites. The occupancy factors refined to 0.761 (2) and 0.239 (2). H atoms were positioned geometrically and refined as riding groups, with O—H = 0.82 Å, $C_{aromatic}$—H = 0.93 Å and C_{methyl}—H = 0.96 Å and with U_{iso}(H) = 1.2U_{eq}(C_{methyl},O) and U_{iso}(H) = 1.5U_{eq}($_{aromatic}$), respectively.

Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

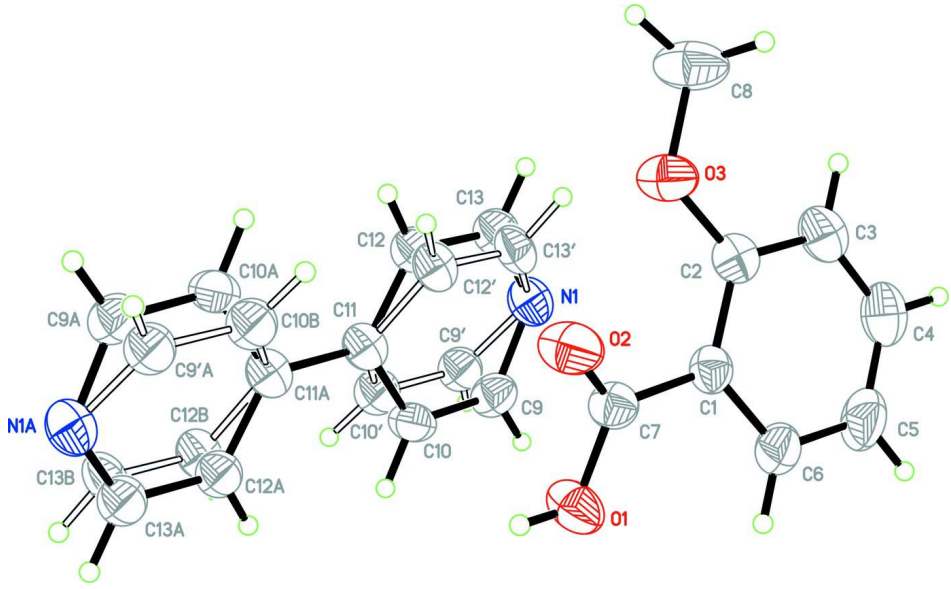

Figure 1

View of the title compound showing the atomic labeling and 30% probability displacement ellipsoids.

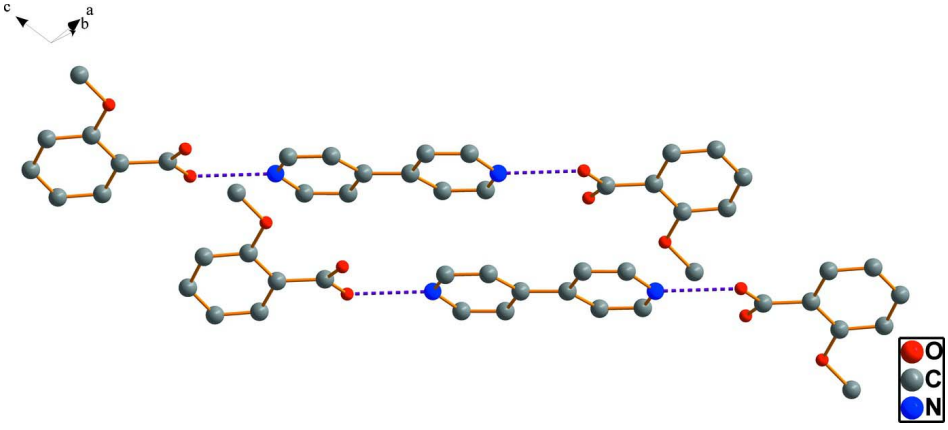

Figure 2

The O—H···N hydrogen bonds of (I). All H atoms have been omitted for clarity. The dashed lines indicate the O—H···N hydrogen bonds.

4,4′-Bipyridine–2-methoxybenzoic acid (1/2)

Crystal data

$C_{10}H_8N_2·2C_8H_8O_3$
M_r = 460.47
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.7090 (15) Å
b = 25.620 (5) Å
c = 6.3624 (13) Å
β = 112.08 (3)°
V = 1164.4 (4) Å^3
Z = 2
$F(000)$ = 484
D_x = 1.313 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2567 reflections
θ = 2.4–23.4°
μ = 0.09 mm^{-1}
T = 298 K
Block, colourless
0.30 × 0.28 × 0.25 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.972, T_{max} = 0.977
5991 measured reflections
2060 independent reflections
1540 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 25.1°, θ_{min} = 2.9°
$h = -6 \rightarrow 9$
$k = -30 \rightarrow 29$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.154
S = 1.06
2060 reflections
172 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0805P)^2 + 0.1072P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.4229 (2)	0.58341 (6)	0.9083 (3)	0.0771 (5)	
H1	0.3645	0.5715	0.9816	0.116*	
C1	0.4341 (3)	0.65024 (7)	0.6614 (3)	0.0525 (5)	
O2	0.1962 (2)	0.64201 (7)	0.8143 (3)	0.0791 (5)	
C2	0.3393 (3)	0.68089 (7)	0.4708 (3)	0.0562 (5)	
O3	0.1512 (2)	0.68604 (6)	0.4068 (2)	0.0717 (5)	
C3	0.4378 (4)	0.70402 (9)	0.3514 (4)	0.0751 (7)	
H3	0.3747	0.7242	0.2241	0.090*	
C4	0.6271 (4)	0.69715 (11)	0.4209 (5)	0.0877 (8)	
H4	0.6916	0.7131	0.3408	0.105*	
C5	0.7227 (3)	0.66730 (11)	0.6053 (6)	0.0875 (8)	
H5	0.8513	0.6627	0.6505	0.105*	
C6	0.6260 (3)	0.64391 (9)	0.7248 (4)	0.0702 (6)	
H6	0.6912	0.6235	0.8505	0.084*	
C7	0.3370 (3)	0.62529 (8)	0.7980 (3)	0.0545 (5)	
C8	0.0540 (4)	0.71555 (13)	0.2045 (4)	0.0945 (9)	
H8A	0.0982	0.7509	0.2256	0.142*	

H8B	−0.0779	0.7151	0.1734	0.142*	
H8C	0.0767	0.7004	0.0793	0.142*	
N1	0.2439 (3)	0.54252 (7)	0.1570 (3)	0.0661 (5)	
C11	0.0512 (3)	0.50894 (7)	0.4279 (3)	0.0556 (5)	
C9	0.3203 (7)	0.5048 (2)	0.3112 (9)	0.0635 (12)	0.50
H9	0.4362	0.4910	0.3277	0.076*	0.50
C10	0.2284 (7)	0.48633 (19)	0.4455 (9)	0.0616 (11)	0.50
H10	0.2804	0.4593	0.5474	0.074*	0.50
C12	−0.0112 (8)	0.5490 (2)	0.2734 (9)	0.0581 (18)*	0.50
H12	−0.1225	0.5658	0.2568	0.070*	0.50
C13	0.0872 (8)	0.5649 (3)	0.1426 (10)	0.063 (2)*	0.50
H13	0.0406	0.5923	0.0411	0.075*	0.50
C9′	0.2515 (7)	0.49348 (19)	0.2343 (9)	0.0625 (16)*	0.50
H9′	0.3280	0.4698	0.1990	0.075*	0.50
C10′	0.1531 (8)	0.4757 (2)	0.3634 (9)	0.0645 (16)*	0.50
H10′	0.1587	0.4407	0.4043	0.077*	0.50
C12′	0.0289 (8)	0.55892 (18)	0.3415 (9)	0.0554 (13)	0.50
H12′	−0.0516	0.5823	0.3710	0.066*	0.50
C13′	0.1266 (8)	0.57342 (19)	0.2127 (10)	0.0599 (14)	0.50
H13′	0.1112	0.6075	0.1585	0.072*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0796 (11)	0.0708 (10)	0.0986 (12)	0.0224 (8)	0.0536 (9)	0.0295 (9)
C1	0.0532 (11)	0.0469 (10)	0.0603 (11)	−0.0023 (8)	0.0247 (9)	−0.0035 (9)
O2	0.0730 (10)	0.0971 (12)	0.0823 (11)	0.0283 (8)	0.0465 (8)	0.0295 (9)
C2	0.0632 (12)	0.0525 (10)	0.0581 (11)	0.0013 (9)	0.0287 (9)	−0.0044 (9)
O3	0.0667 (9)	0.0895 (11)	0.0631 (9)	0.0218 (7)	0.0292 (7)	0.0171 (8)
C3	0.0904 (17)	0.0689 (14)	0.0751 (14)	−0.0069 (12)	0.0413 (13)	0.0071 (11)
C4	0.0878 (19)	0.0886 (17)	0.103 (2)	−0.0228 (14)	0.0550 (16)	0.0040 (15)
C5	0.0574 (13)	0.0915 (18)	0.121 (2)	−0.0166 (12)	0.0426 (14)	−0.0042 (17)
C6	0.0533 (12)	0.0671 (13)	0.0882 (15)	−0.0044 (10)	0.0244 (11)	0.0036 (11)
C7	0.0532 (11)	0.0563 (11)	0.0562 (11)	0.0063 (9)	0.0231 (9)	0.0015 (9)
C8	0.0963 (18)	0.126 (2)	0.0663 (14)	0.0422 (16)	0.0362 (13)	0.0282 (15)
N1	0.0785 (12)	0.0605 (10)	0.0678 (11)	−0.0008 (9)	0.0373 (9)	0.0010 (9)
C11	0.0683 (12)	0.0470 (10)	0.0550 (11)	−0.0013 (9)	0.0272 (9)	−0.0049 (8)
C9	0.054 (3)	0.076 (3)	0.060 (3)	0.003 (2)	0.022 (2)	−0.001 (2)
C10	0.059 (3)	0.067 (3)	0.059 (3)	0.013 (2)	0.022 (2)	0.018 (2)
C12′	0.072 (3)	0.042 (2)	0.055 (3)	−0.005 (2)	0.028 (2)	−0.010 (2)
C13′	0.083 (3)	0.043 (2)	0.054 (3)	−0.012 (2)	0.026 (3)	−0.002 (2)

Geometric parameters (Å, º)

O1—C7	1.316 (2)	N1—C9′	1.343 (5)
O1—H1	0.8200	N1—C9	1.345 (4)
C1—C6	1.389 (3)	N1—C13′	1.346 (5)
C1—C2	1.398 (3)	C11—C10′	1.325 (6)
C1—C7	1.488 (3)	C11—C12	1.377 (6)

O2—C7	1.207 (2)	C11—C12′	1.378 (5)
C2—O3	1.357 (2)	C11—C10	1.448 (4)
C2—C3	1.392 (3)	C11—C11^{i}	1.490 (4)
O3—C8	1.437 (3)	C9—C10	1.382 (5)
C3—C4	1.368 (3)	C9—H9	0.9300
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.362 (4)	C12—C13	1.381 (7)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.385 (4)	C13—H13	0.9300
C5—H5	0.9300	C9′—C10′	1.388 (6)
C6—H6	0.9300	C9′—H9′	0.9300
C8—H8A	0.9600	C10′—H10′	0.9300
C8—H8B	0.9600	C12′—C13′	1.357 (6)
C8—H8C	0.9600	C12′—H12′	0.9300
N1—C13	1.309 (6)	C13′—H13′	0.9300

C7—O1—H1	109.5	C10′—C11—C12	110.4 (4)
C6—C1—C2	118.00 (18)	C10′—C11—C12′	118.3 (3)
C6—C1—C7	119.65 (19)	C12—C11—C10	114.8 (3)
C2—C1—C7	122.34 (17)	C12′—C11—C10	112.0 (3)
O3—C2—C3	122.4 (2)	C10′—C11—C11^{i}	120.4 (3)
O3—C2—C1	117.74 (17)	C12—C11—C11^{i}	123.0 (3)
C3—C2—C1	119.9 (2)	C12′—C11—C11^{i}	121.0 (3)
C2—O3—C8	117.29 (17)	C10—C11—C11^{i}	122.1 (3)
C4—C3—C2	120.2 (2)	N1—C9—C10	120.8 (4)
C4—C3—H3	119.9	N1—C9—H9	119.6
C2—C3—H3	119.9	C10—C9—H9	119.6
C5—C4—C3	121.1 (2)	C9—C10—C11	120.2 (4)
C5—C4—H4	119.4	C9—C10—H10	119.9
C3—C4—H4	119.4	C11—C10—H10	119.9
C4—C5—C6	119.1 (2)	C11—C12—C13	121.7 (5)
C4—C5—H5	120.4	C11—C12—H12	119.1
C6—C5—H5	120.4	C13—C12—H12	119.1
C5—C6—C1	121.6 (2)	N1—C13—C12	122.0 (6)
C5—C6—H6	119.2	N1—C13—H13	119.0
C1—C6—H6	119.2	C12—C13—H13	119.0
O2—C7—O1	122.15 (18)	N1—C9′—C10′	124.5 (5)
O2—C7—C1	124.29 (18)	N1—C9′—H9′	117.7
O1—C7—C1	113.52 (17)	C10′—C9′—H9′	117.7
O3—C8—H8A	109.5	C11—C10′—C9′	119.4 (5)
O3—C8—H8B	109.5	C11—C10′—H10′	120.3
H8A—C8—H8B	109.5	C9′—C10′—H10′	120.3
O3—C8—H8C	109.5	C13′—C12′—C11	118.7 (4)
H8A—C8—H8C	109.5	C13′—C12′—H12′	120.6
H8B—C8—H8C	109.5	C11—C12′—H12′	120.6
C13—N1—C9′	110.4 (4)	N1—C13′—C12′	125.4 (4)
C13—N1—C9	120.3 (4)	N1—C13′—H13′	117.3
C9′—N1—C13′	113.3 (3)	C12′—C13′—H13′	117.3
C9—N1—C13′	112.6 (3)		

C6—C1—C2—O3	178.65 (17)	C10′—C11—C12—C13	−28.0 (6)
C7—C1—C2—O3	−2.3 (3)	C12′—C11—C12—C13	88.6 (12)
C6—C1—C2—C3	−0.2 (3)	C10—C11—C12—C13	1.7 (7)
C7—C1—C2—C3	178.92 (18)	C11^{i}—C11—C12—C13	179.7 (4)
C3—C2—O3—C8	1.7 (3)	C9′—N1—C13—C12	24.7 (7)
C1—C2—O3—C8	−177.1 (2)	C9—N1—C13—C12	−3.9 (8)
O3—C2—C3—C4	−179.2 (2)	C13′—N1—C13—C12	−77.4 (12)
C1—C2—C3—C4	−0.4 (3)	C11—C12—C13—N1	0.5 (9)
C2—C3—C4—C5	0.7 (4)	C13—N1—C9′—C10′	−23.9 (7)
C3—C4—C5—C6	−0.5 (4)	C9—N1—C9′—C10′	93.1 (9)
C4—C5—C6—C1	−0.1 (4)	C13′—N1—C9′—C10′	−1.4 (7)
C2—C1—C6—C5	0.4 (3)	C12—C11—C10′—C9′	28.7 (6)
C7—C1—C6—C5	−178.7 (2)	C12′—C11—C10′—C9′	7.6 (7)
C6—C1—C7—O2	151.7 (2)	C10—C11—C10′—C9′	−76.1 (7)
C2—C1—C7—O2	−27.4 (3)	C11^{i}—C11—C10′—C9′	−178.2 (4)
C6—C1—C7—O1	−26.2 (3)	N1—C9′—C10′—C11	−3.8 (8)
C2—C1—C7—O1	154.75 (18)	C10′—C11—C12′—C13′	−6.4 (7)
C13—N1—C9—C10	4.8 (8)	C12—C11—C12′—C13′	−78.6 (12)
C9′—N1—C9—C10	−70.7 (8)	C10—C11—C12′—C13′	23.5 (7)
C13′—N1—C9—C10	26.7 (7)	C11^{i}—C11—C12′—C13′	179.4 (5)
N1—C9—C10—C11	−2.5 (9)	C13—N1—C13′—C12′	89.0 (13)
C10′—C11—C10—C9	86.1 (8)	C9′—N1—C13′—C12′	2.6 (8)
C12—C11—C10—C9	−0.7 (7)	C9—N1—C13′—C12′	−27.3 (8)
C12′—C11—C10—C9	−23.2 (7)	C11—C12′—C13′—N1	1.2 (10)
C11^{i}—C11—C10—C9	−178.8 (4)		

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{ii}	0.82	1.85	2.673 (2)	177

Symmetry code: (ii) *x*, *y*, *z*+1.