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(*E*)-4,4′-Diazastilbene–4,4′-oxydibenzoic acid (1/1)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.092
wR factor = 0.178
Data-to-parameter ratio = 12.7

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

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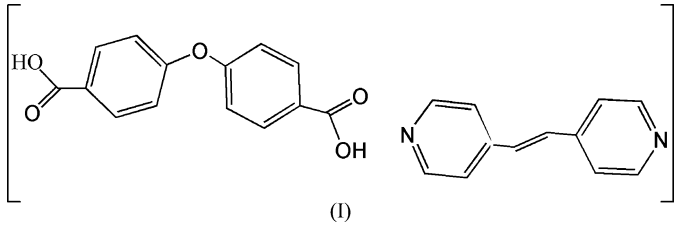
The title compound, $C_{12}H_{10}N_2{\cdot}C_{14}H_{10}O_5$, is a cocrystal of (*E*)-4,4′-diazastilbene and 4,4′-oxydibenzoic acid, lying on an inversion centre and a twofold axis, respectively. Molecules are linked by strong intermolecular O—H···N hydrogen bonds, resulting in a one-dimensional architecture.

Comment

Cocrystallization reactions provide helpful means for probing the importance and balance between different intermolecular interactions, and thus offer practical guidelines for developing new methodologies in supramolecular synthesis (Desiraju, 2003; Shan *et al.*, 2002). The role of hydrogen bonding and π–π stacking for these purposes is well established (Shattock *et al.*, 2005). The reaction of $CdSO_4{\cdot}8H_2O$, 4,4′-oxydibenzoic acid (4,4′-dicarboxydiphenyl ether, H_2oba) and 1,2-bis(4-pyridyl)ethylene (4,4′-diazastilbene, bpe) affords the zigzag chain polymer $[Cd(bpe)(Hoba)_2]_n$ (Yin & Xiao, 2005). We attempted to isolate the corresponding Mn^{II} complex, replacing $CdSO_4{\cdot}8H_2O$ by $Mn(CH_3COO)_2{\cdot}4H_2O$ and using the same hydrothermal synthesis conditions. However, we were not successful and a new cocrystal, (bpe)(H_2oba), (I), was isolated instead (Fig. 1 and Table 1).



(I)

In (I), each molecule lies on a special position, an inversion centre for bpe and a twofold axis for H_2oba. The dihedral angle between the two benzene rings of the flexible H_2oba molecule is 51.2 (1)°, which is more acute than that reported for $[Cd(bpe)(Hoba)_2]_n$. Meanwhile, in (I), the protonated carboxylate O1 atom of the flexible H_2oba molecule forms a strong intermolecular hydrogen bond with atom N1 of the rigid bpe molecule (Table 2), linking the molecules into zigzag chains (Fig. 2).

Experimental

H_2oba (0.5 mmol, 0.129 g), $Mn(CH_3COO)_2{\cdot}4H_2O$ (1.5 mmol, 0.367 g) and bpe (0.5 mmol, 0.092 g) were placed in a 30 ml Teflon-lined stainless steel Parr bomb together with water (18 ml). The bomb was heated at 423 K for six days, and then cooled slowly to 298 K, to furnish colourless crystals.

Crystal data

$C_{12}H_{10}N_2{\cdot}C_{14}H_{10}O_5$
M_r = 440.44
Monoclinic, $C2/c$
a = 13.308 (5) Å
b = 6.080 (2) Å
c = 26.143 (10) Å
β = 92.603 (7)°
V = 2113.1 (13) Å^3
Z = 4
D_x = 1.384 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 662 reflections
θ = 2.5–22.2°
μ = 0.10 mm^{-1}
T = 298 (2) K
Rod, colourless
0.21 × 0.10 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.975, T_{max} = 0.990
5391 measured reflections
1919 independent reflections
1401 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 25.3°
$h = -14 \rightarrow 16$
$k = -6 \rightarrow 7$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.092
$wR(F^2)$ = 0.178
S = 1.23
1919 reflections
151 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2 + 1.8866P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.309 (4)	C4—C5	1.378 (4)
O2—C7	1.208 (4)	C7—C8	1.485 (4)
O3—C11	1.387 (3)	C8—C13	1.383 (5)
N1—C5	1.326 (4)	C8—C9	1.388 (4)
N1—C1	1.328 (4)	C9—C10	1.379 (4)
C1—C2	1.371 (4)	C10—C11	1.377 (4)
C2—C3	1.394 (4)	C11—C12	1.373 (4)
C3—C4	1.389 (5)	C12—C13	1.371 (5)
C3—C6	1.466 (4)		
C5—N1—C1	117.4 (3)	O1—C7—C8	113.9 (3)
C11—O3—C11^{i}	117.4 (3)	C13—C8—C9	118.5 (3)
N1—C1—C2	123.3 (3)	C13—C8—C7	118.8 (3)
C1—C2—C3	120.0 (4)	C9—C8—C7	122.7 (3)
C4—C3—C2	116.2 (3)	C10—C9—C8	120.7 (3)
C4—C3—C6	120.7 (3)	C11—C10—C9	119.5 (3)
C2—C3—C6	123.1 (3)	C12—C11—C10	120.5 (3)
C5—C4—C3	119.9 (3)	C12—C11—O3	115.1 (3)
N1—C5—C4	123.2 (4)	C10—C11—O3	124.2 (3)
C6^{ii}—C6—C3	127.5 (4)	C13—C12—C11	119.8 (3)
O2—C7—O1	122.7 (3)	C12—C13—C8	121.0 (3)
O2—C7—C8	123.4 (4)		

Symmetry codes: (i) $-x+1, y, -z+\frac{3}{2}$; (ii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+2$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{iii}	0.82	1.81	2.629 (4)	172

Symmetry code: (iii) $x+\frac{1}{2}, y+\frac{1}{2}, z$.

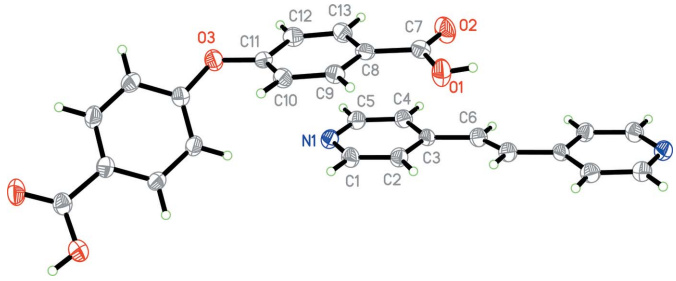


Figure 1
The structure of (I), with the atom-numbering scheme for the asymmetric unit, showing displacement ellipsoids at the 30% probability level. Unlabelled atoms in bpe are related to labelled atoms by $(\frac{3}{2}-x, \frac{3}{2}-y, 2-z)$. Unlabelled atoms in H~2~oba are related to labelled atoms by $(1-x, y, \frac{3}{2}-z)$.

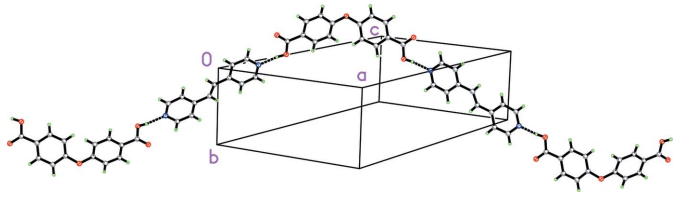


Figure 2
A zigzag chain formed by hydrogen-bonding interactions (shown as dashed lines).

All H atoms were positioned geometrically (C—H = 0.93 Å and O—H = 0.82 Å) and allowed to ride on their parent atoms, with U_{iso}(H) values equal to $1.2U_{eq}$(C) or $1.5U_{eq}$(O). The high final residuals, for example R = 0.092 for observed data, may be related to the poor quality of the crystals, the mean $I/\sigma(I)$ for the selected crystal being 6.65 (computed on merged data, excluding systematically absent reflections).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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