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

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Key indicators

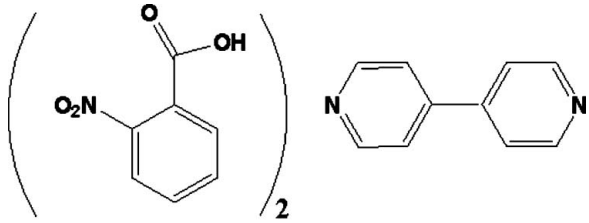
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.074
wR factor = 0.156
Data-to-parameter ratio = 15.6

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

The title compound, $C_{10}H_8N_2\cdot 2C_7H_5NO_4$, was obtained as a by-product of the hydrothermal reaction of $ZnSO_4$ with 2-nitrobenzoic acid and 4,4′-bipyridine. The 4,4′-bipyridine molecule lies on an inversion centre. There are O—H···N and C—H···O hydrogen bonds between the components in the crystal structure.

Comment

Much effort has focused on the design and synthesis of coordination polymeric frameworks, due not only to their potential applications in microelectronics, nonlinear optics, porous materials and catalysis, but also to their intriguing variety of architectures and topologies (Evans *et al.*, 1999; Fujita *et al.*, 1994). As a linear bifunctional ligand, 4,4′-bipyridine (4,4′-bipy) has been widely used in the study of the crystal engineering of coordination polymers (Dai *et al.*, 2005; Tang *et al.*, 2004). The title compound, (I), was obtained unexpectedly during our attempt to react 2-nitrobenzoic acid and 4,4′-bipy with metal ions.



(I)

The asymmetric unit of (I) consists of a 2-nitrobenzoic acid molecule and half of a 4,4′-bipy molecule (Fig. 1).

There are O—H···N and C—H···O hydrogen bonds between the components (Table 1), as well as a π–π interaction between the pyridine rings (Fig. 2). The centroid (*Cg* is the centroid of atoms C1, C2, 3, C4, C5 and N1) separation, $Cg\cdots Cg$ $(-x, 1-y, 2-z)$, is 4.010 (2) Å, and the interplanar spacing is 3.439 (2) Å.

Experimental

$ZnSO_4\cdot 7H_2O$ (0.145 g, 0.5 mmol), 2-nitrobenzoic acid (0.167 g, 1.0 mmol) and 4,4′-bipy (0.075 g, 0.5 mmol) were mixed in water (15 ml) and heated at 433 K for 3 d in a sealed 25 ml Teflon-lined stainless steel vessel under autogenous pressure. After cooling to room temperature at 5 K h^{-1}, orange prismatic crystals of (I) were isolated, and these were washed with water and dried in air.

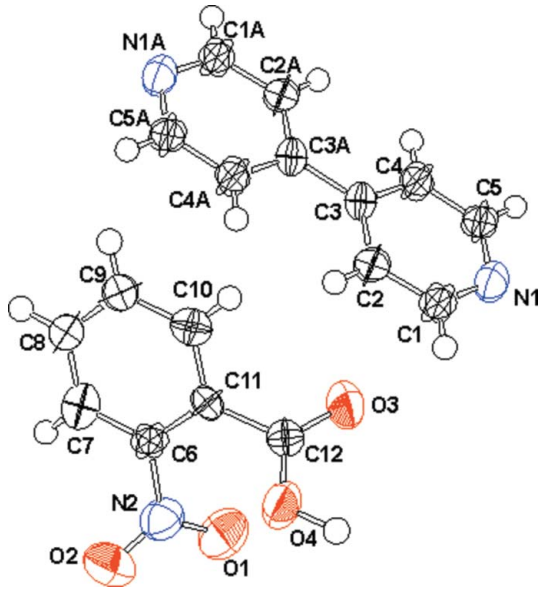


Figure 1
The molecular structure of (I), showing the atom-labelling scheme, and with displacement ellipsoids at the 40% probability level. Symmetry code: (A) $1-x, 1-y, 2-z$.

Crystal data

$C_{10}H_8N_2\cdot 2C_7H_5NO_4$
$M_r = 490.42$
Monoclinic, $P2_1/c$
$a = 7.0788\ (13)$ Å
$b = 18.660\ (3)$ Å
$c = 8.6256\ (16)$ Å
$\beta = 96.649\ (9)^\circ$
$V = 1131.7\ (3)$ Å^3
$Z = 2$
$D_x = 1.439$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1782 reflections
$\theta = 3.1$–27.5°
$\mu = 0.11$ mm^{-1}
$T = 293\ (2)$ K
Prism, orange
0.55 × 0.20 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.974$, $T_{max} = 0.993$
8485 measured reflections
2600 independent reflections
2018 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5^\circ$
$h = -9 \rightarrow 6$
$k = -24 \rightarrow 22$
$l = -11 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.074$
$wR(F^2) = 0.156$
$S = 1.19$
2600 reflections
166 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.3073P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ 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
O4—H11···N1^{i}	1.02 (3)	1.57 (3)	2.578 (2)	169 (3)
C10—H10A···O3^{ii}	0.93	2.55	3.454 (3)	166

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

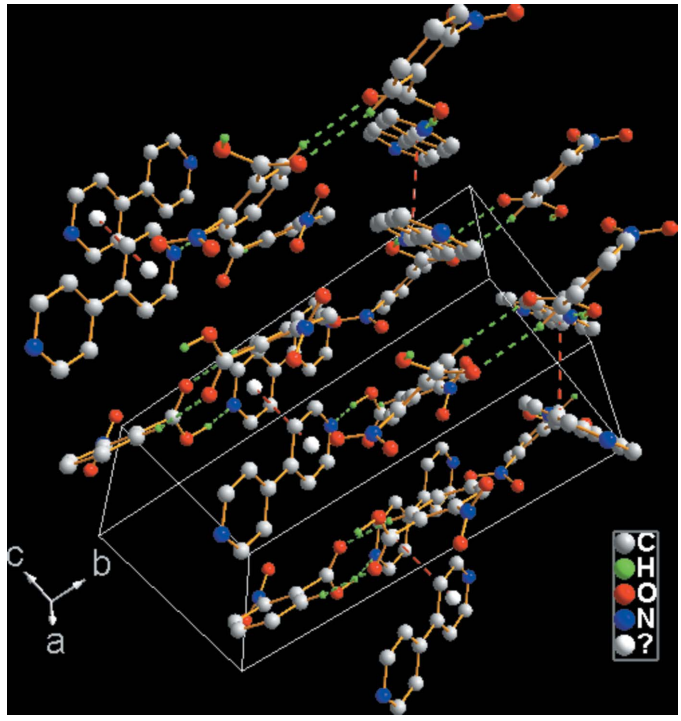


Figure 2
A packing diagram for (I) viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

The carboxyl H atom was located in a difference Fourier map and its coordinates were refined, with $U_{iso}(H) = 1.2U_{eq}(O)$. Other H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*

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References

Dai, Y. M., Ma, E. Tang, E., Zhang, J., Li, Z. J., Huang, X. D. & Yao, Y. G. (2005). *Cryst. Growth Des.* **5**, 1313–1315.
Evans, O. R., Xiong, R., Wang, Z., Wong, G. K. & Lin, W. (1999). *Angew. Chem. Int. Ed.* **38**, 536–538.
Fujita, M., Kwon, Y. J., Washizu, S. & Ogura, K. (1994). *J. Am. Chem. Soc.* **116**, 1151–1152.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Siemens (1994). *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tang, E., Dai, Y. M. & Lin, S. (2004). *Acta Cryst.* C**60**, m433–m434.