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2,5-Di-4-pyridyl-1,3,4-oxadiazole–succinic acid (2/1)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.108
Data-to-parameter ratio = 10.7

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

In the title structure, $2C_{12}H_8N_4O\cdot 0C_4H_6O_4$, succinic acid molecules lie on crystallographic inversion centers and a pair of O—H···N hydrogen bonds links the three molecules. In addition, C—H···O and C—H···N hydrogen bonds link this unit into a two-dimensional framework.

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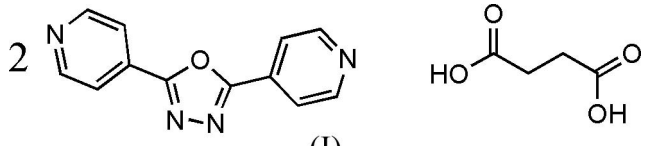
Comment

Currently, hydrogen bonding is important in the areas of crystal engineering, supramolecular chemistry, materials science, and biological recognition (Desiraju, 1989; Jeffrey & Saenger, 1991; Holman *et al.*, 2001). Recently, angular dipyridyl-donor basic compounds, such as 2,5-di-4-pyridyl-1,3,4-oxadiazole (bpo), have been used to produce a series of infinite/discrete coordination polymers/supramolecules with interesting structures and properties (Dong *et al.*, 2003; Du *et al.*, 2005*a*,b, and references therein). In our search to identify the properties of co-crystal materials of fatty diacids with linear/angular base components and to further understand the role of synthons in crystal engineering, we have prepared and determined the crystal structure of the acid–base co-crystal, (I), consisting of bpo and the most typical fatty carboxylic acid, succinic acid (Fig. 1).



(I)

A view of the title structure is shown in Fig. 1. The asymmetric unit consists of one bpo molecule and half a molecule of succinic acid; a crystallographic inversion center generates the full molecule of succinnic acid. In the crystal structure, a two-dimensional framework is formed *via* O—H·N, C—H·N and C—H···O hydrogen bonds (Table 2 and Fig. 2).

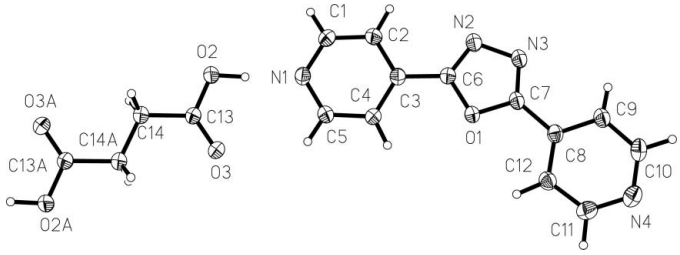


Figure 1
View of (I), showing displacement ellipsoids at the 30% probability level. H atoms are represented by circles of arbitrary size. Atoms labelled with the suffix A are generated by the symmetry code (−1 − *x*, 2 − *y*, −*z*).

Experimental

A mixture of 2,5-di-4-pyridyl-1,3,4-oxadiazole (112 mg, 0.5 mmol) (Dong *et al.*, 2002) and succinic acid (29 mg, 0.25 mmol) was recrystallized from methanol and water in 70% yield (98 mg), from which a colourless needle-shaped crystal suitable for X-ray diffraction was selected. Analysis found (%): C 59.01, H 3.90, N 19.85, O 16.84; requires (%): C 59.36, H 3.91, N 19.78, O 16.94; IR (KBr, ν cm^{-1}): 2450, 1705, 1612, 1569, 1537, 1413, 1276, 1206, 1011, 836, 741, 723.

Crystal data

$2C_{12}H_8N_4O{\cdot}C_4H_6O_4$	$Z = 1$
$M_r = 566.54$	$D_x = 1.444$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 6.4389$ (9) Å	Cell parameters from 400 reflections
$b = 9.5462$ (13) Å	$\theta = 7.5$–$23.0°$
$c = 11.0415$ (15) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 94.803$ (2)°	$T = 293$ (2) K
$\beta = 103.666$ (2)°	Block, pale yellow
$\gamma = 96.213$ (2)°	0.43 × 0.34 × 0.24 mm
$V = 651.39$ (15) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2499 independent reflections
φ and ω scans	2227 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.010$
$T_{min} = 0.956$, $T_{max} = 0.975$	$\theta_{max} = 26.0°$
3585 measured reflections	$h = -7 \rightarrow 7$
	$k = -11 \rightarrow 11$
	$l = -10 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0682P)^2 + 0.0637P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	
$wR(F^2) = 0.108$	
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
2499 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
234 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
All H-atom parameters refined	

Table 1
Selected torsion angles (°).

C2—C3—C6—N2	−5.9 (2)	N3—C7—C8—C9	9.7 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2B···N1	0.98 (2)	1.70 (2)	2.6741 (15)	174 (2)
C1—H1A···O3^{i}	0.94 (2)	2.44 (1)	3.2912 (18)	151 (1)
C10—H10A···N4^{ii}	0.98 (2)	2.60 (2)	3.433 (2)	143 (2)

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

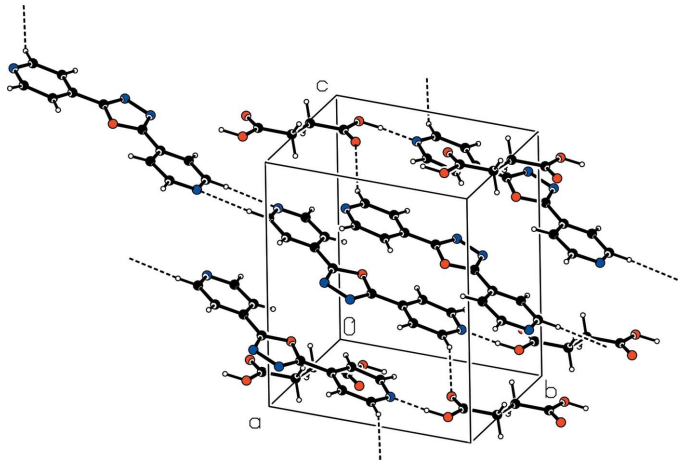


Figure 2
Packing diagram (Spek, 2003), showing hydrogen bonds as dashed lines.

All H atoms were refined independently with isotropic displacement parameters.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL*.

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