Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Cocrystal of 2,5-di-4-pyridyl-1,3,4-oxadiazole and malonic acid (1/1)

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Received 7 October 2005
Accepted 27 October 2005
Online 5 November 2005

Key indicators

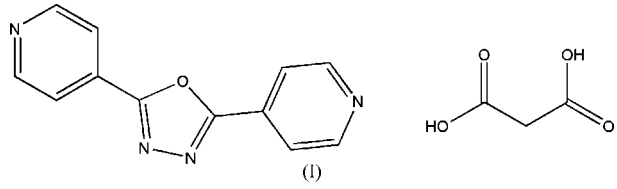
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.058
wR factor = 0.186
Data-to-parameter ratio = 10.2

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

In the title compound, $C_{12}H_8N_4O\cdot C_3H_4O_4$, a single O—H···N hydrogen bond links the two molecules. In addition, C—H···O and C—H···N hydrogen bonds link these units into a two-dimensional framework.

Comment

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-bis(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 (Wang, Tang & Qin, 2005; Dong *et al.*, 2003; Du *et al.*, 2005, and references therein). In our effort to characterize the properties of cocrystals 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 cocrystal (I), consisting of bpo and the most typical fatty carboxylic acid, malonic acid.



The asymmetric unit consists of one bpo molecule and a molecule of malonic acid (Fig. 1). The geometry of the bpo

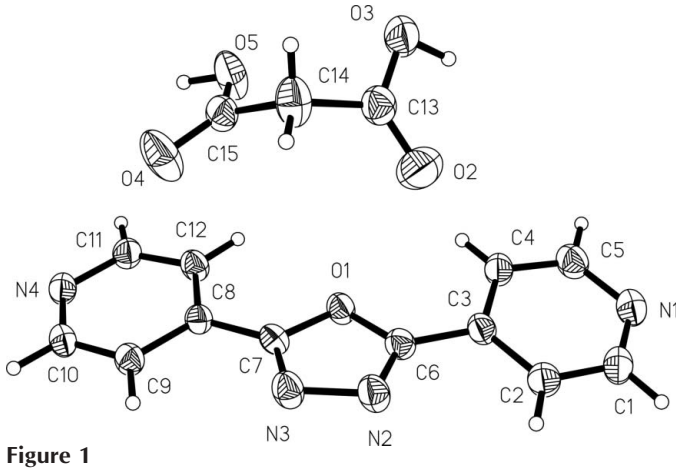


Figure 1
View of (I), showing displacement ellipsoids at the 30% probability level. H atoms are represented by circles of arbitrary size.

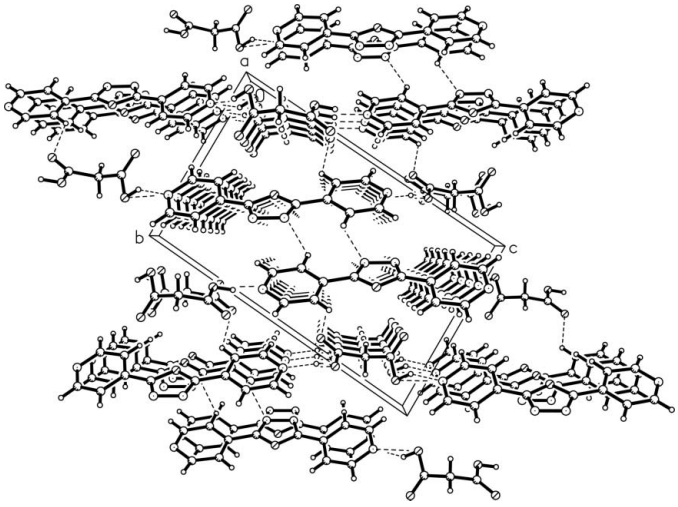


Figure 2
A packing diagram, showing hydrogen bonds as dashed lines.

molecule is very similar to that of the parent structure (Stockhause *et al.*, 2001); likewise, the malonic acid geometry is close to that of free malonic acid (Vishweshwar *et al.*, 2003). In the crystal structure, a two-dimensional framework is formed *via* O—H···N, C—H···N and C—H···O hydrogen bonds (Table 1 and Fig. 2).

Experimental

A mixture of 2,5-bis(4-pyridyl)-1,3,4-oxadiazole (112 mg, 0.5 mmol) (Wang, Tang, Qin & Duan, 2005) and malonic acid (52 mg, 0.5 mmol) was recrystallized from methanol and water in about 77% yield (126 mg); from this, a colourless block suitable for X-ray diffraction was selected. Analysis found: C 54.78, H 3.65, N 17.17%; calculated: C 54.88, H 3.68, N 17.07%; IR (KBr, cm^{-1}): ν 2452, 1708, 1602, 1570, 1534, 1418, 1271, 1211, 1018, 835, 743, 723.

Crystal data

$C_{12}H_8N_4O{\cdot}C_3H_4O_4$
M_r = 328.29
Triclinic, $P\overline{1}$
a = 5.1232 (8) Å
b = 9.5108 (15) Å
c = 15.566 (3) Å
α = 85.297 (3)°
β = 81.159 (3)°
γ = 86.289 (3)°
V = 745.9 (2) Å^3
Z = 2
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 100 reflections
θ = 17–23°
μ = 0.11 mm^{-1}
T = 293 (2) K
Block, colourless
0.26 × 0.15 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.971, T_{max} = 0.986
3788 measured reflections
2692 independent reflections
1843 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 25.5°
$h = -6 \rightarrow 4$
$k = -11 \rightarrow 11$
$l = -17 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.186
S = 1.00
2692 reflections
265 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.1148P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···N1^{i}	0.99 (7)	1.77 (7)	2.666 (4)	149 (5)
O5—H5A···N4^{ii}	0.97 (3)	1.66 (3)	2.611 (3)	166 (3)
C9—H9···N3	0.95 (3)	2.61 (3)	2.938 (3)	101 (2)
C9—H9···N3^{iii}	0.95 (3)	2.55 (3)	3.327 (3)	139 (2)
C11—H11···O4^{ii}	0.92 (3)	2.59 (3)	3.298 (4)	134 (2)
C12—H12···O4^{iv}	0.94 (3)	2.48 (3)	3.146 (4)	128 (2)

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x, -y+1, -z+1$; (iv) $x+1, y, z$.

All H atoms were refined independently with isotropic displacement parameters [O—H = 0.97 (4) and 0.99 (7) Å, C—H = 0.89 (4)–0.97 (3) Å].

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) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Starting Fund of Shandong Institute of Light Industry (to YTW).

References

Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. (1989). *Crystal Engineering: The Design of Organic Solids*. New York: Elsevier.
Dong, Y.-B., Ma, J.-P., Huang, R.-Q., Smith, M. D. & zur Loye, H.-C. (2003). *Inorg. Chem.* **42**, 294–300.
Du, M., Zhang, Z.-H. & Zhao, X.-J. (2005). *Cryst. Growth Des.* **5**, 1119–1208.
Holman, K. T., Pivovar, A. M., Swift, J. A. & Ward, M. D. (2001). *Acc. Chem. Res.* **34**, 107–118.
Jeffrey, G. A. & Saenger, W. (1991). *Hydrogen Bonding in Biological Structures*. Berlin: Springer-Verlag.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1999). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stockhause, S., Wickleder, M. S., Meyer, G., Orgzall, I. & Schulz, B. (2001). *J. Mol. Struct.* **561**, 175–183.
Vishweshwar, P., Nangia, A. & Lynch, V. M. (2003). *Cryst. Growth Des.* **3**, 783–790.
Wang, Y.-T., Tang, G.-M. & Qin, D.-W. (2005). *Acta Cryst.* E**61**, o3623–o3624.
Wang, Y.-T., Tang, G.-M., Qin, D.-W. & Duan, H.-D. (2005). *Acta Cryst.* E**61**. Submitted.