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4-Pyridylmethyl 1*H*-pyrrole-2-carboxylate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.121
Data-to-parameter ratio = 15.3

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

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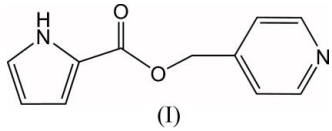
The title compound, $C_{11}H_{10}N_2O_2$, has been synthesized by the reaction of 2-(trichloroacetyl)pyrrole with 4-(hydroxymethyl)-pyridine. In the solid state, the molecules form a one-dimensional infinite ladder structure through intermolecular N—H···N and C—H···O hydrogen bonds.

Comment

Hydrogen-bond-mediated self-assembly represents an area of considerable current interest (Burrows, 2004). Recently, it was found that pyrrole-based entities are also capable of undergoing self-assembly through hydrogen bonds, especially in the solid state (Sessler *et al.*, 2003; Wang & Yin, 2006; Yin & Li, 2006). We report here the self-assembly of the title compound, (I), *via* conventional N—H···N and non-classical C—H···O hydrogen bonds.



(I)

The molecular structure of (I) is shown in Fig. 1. In the solid state, the carbonyl group is arranged *anti* to its adjacent pyrrole NH group; this is quite different from the previous observation (Yin & Li, 2006). The dihedral angle between the pyrrole ring and the pyridine ring is 75.55 (14)°. Two molecules of (I) are held together by a pair of N—H···N hydrogen bonds. The dimers are further connected by a pair of non-classical C—H···O hydrogen bonds (Table 1), forming a one-dimensional ladder-type structure (Fig. 2).

Experimental

4-(Hydroxymethyl)pyridine (109 mg, 1 mmol), 2-(trichloroacetyl)-pyrrole (316 mg, 1.5 mmol) and triethylamine (0.5 ml) were added to acetonitrile (20 ml), and the mixture was refluxed for 20 h. The

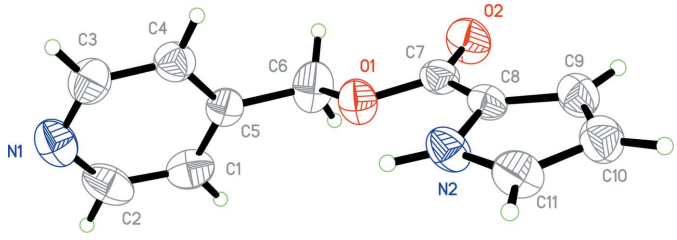


Figure 1
The molecular structure of (I), with the numbering scheme and 30% probability displacement ellipsoids.

solution was evaporated under reduced pressure and the residue was purified by column chromatography on silica gel with ethyl acetate–petroleum ether (1:2 *v*/*v*), affording the title compound (white powder, 164 mg, 81%). Analysis calculated for $C_{11}H_{10}N_2O_2$: C 65.34, H 4.98, N 13.85%; found: C 65.25, H 5.07, N 13.76%.

Crystal data

$C_{11}H_{10}N_2O_2$
M_r = 202.21
Monoclinic, $P2_1/c$
a = 7.698 (3) Å
b = 15.796 (6) Å
c = 8.789 (3) Å
β = 99.771 (7)°
V = 1053.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.977, T_{max} = 0.982
5812 measured reflections
2147 independent reflections
884 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.121
S = 0.91
2147 reflections
140 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.90 (2)	2.01 (2)	2.902 (3)	169 (3)
C11—H11···O2^{ii}	0.93	2.47	3.331 (3)	155

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

The N-bound H atom was located in a difference map and refined freely. Other H atoms were positioned geometrically (C—H = 0.93 or 0.97 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

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

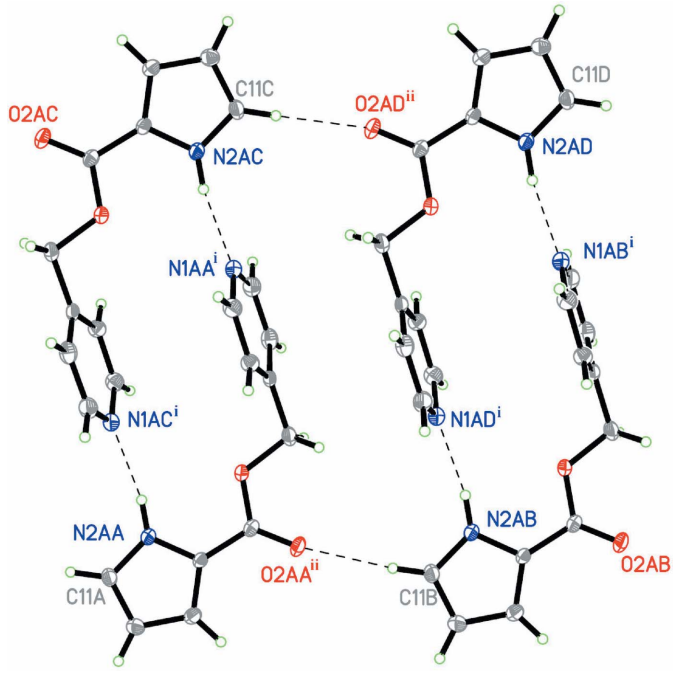


Figure 2
Part of the ladder structure of (I), with molecules connected by N—H···N($-x$, $1-y$, $2-z$) and C—H···O($x-1$, y, z) hydrogen bonds (dashed lines).

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