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Methyl 1*H*-pyrrole-2-carboxylate

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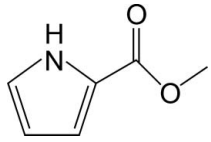
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.005 Å; R factor = 0.070; wR factor = 0.176; data-to-parameter ratio = 13.3.

The title compound, $C_6H_7NO_2$, is essentially planar with a dihedral angle of 3.6 (3)° between the pyrrole ring and the methoxycarbonyl O/C/O/C plane. In the crystal structure, the N atom is a hydrogen-bond donor to the carboxylate C=O O atom of the neighboring molecule. These intermolecular hydrogen bonds lead to the formation of helical chains along the *b* axis.

Related literature

For related structures, see: Kerscher, Klüfers, Kügel & Müller (2007); Kerscher, Klüfers & Kügel (2007). For graph-set analysis, see: Bernstein *et al.* (1995); Etter *et al.* (1990).



Experimental

Crystal data

$C_6H_7NO_2$
M_r = 125.13
Monoclinic, $P2_1/c$
a = 7.5346 (19) Å
b = 5.4598 (14) Å
c = 14.730 (4) Å
β = 100.55 (2)°
V = 595.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 200 K
0.38 × 0.16 × 0.06 mm

Data collection

Oxford Xcalibur KappaCCD diffractometer
Absorption correction: none
2591 measured reflections
1103 independent reflections
528 reflections with $I > 2\sigma(I)$
R_{int} = 0.112

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.176
S = 0.95
1103 reflections
83 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.88	2.06	2.933 (4)	171
C4—H4···$Cg1^{ii}$	0.95	2.63	3.401 (5)	139

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$. $Cg1$ is the centroid of the pyrrole ring.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2445).

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supplementary materials

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Comment

The title compound was prepared, in the attempt to create new complexing ligands, as a byproduct. The compound is quite simular to other compounds already published by our group (Kerscher, Klüfers, Kügel & Müller, 2007; Kerscher, Klüfers & Kügel, 2007).

In the molecule, a formic acid methyl ester is in the 2 position of the pyrrole ring (Fig. 1). With a torsion angle for C2–C1–C5–O1 of only about 2.9°, the molecule is, with the exception of the H atoms of the methyl group, nearly planar. Because of this small torsion angle, the molecule is not C_s symmetric.

The hydrogen bonds of the nitrogen to the carboxylate oxygen lead to a chain like hydrogen bonding system which can be described according to graph-set analysis (Etter *et al.*, 1990; Bernstein *et al.*, 1995) with a C(5) descriptor on the unitary level [the rpluto program (Cambridge Crystallographic Data Centre, England) was used for the graph set analyses; one of these strands is shown in Fig. 2].

Considering contacts whose range falls below the sum of van der Waals radii by only about 0.1 Å, a set of weak C–H···π interactions leads to the formation of a second system of strands along [0 1 0] which can be described by a C(2) descriptor (see Fig. 3).

The two strand systems alternate, which means two hydrogen bonding strands are interconnected by a strand of weak C–H···π contacts (this situation is illustrated in Fig. 4) and *vice versa*, two strands made of weak C–H···π contacts are interconnected by hydrogen bonding strands. This bonding pattern leads to sheet like structures normal to [0 0 1].

The molecular packing of the title compound is shown in Figure 5.

Experimental

The title compound was obtained by reaction of 228 mg (3.40 mmol) of pyrrole with 280 mg (1.70 mmol) phosgene iminium chloride in 6 ml of dry acetonitrile. After removal of the solvent, the remaining green solid was purified by column chromatoghraphy on silica with chloroform as eluent. Sublimation of fraction five yielded the title compound as colorless crystals.

Refinement

H atoms were calculated in ideal geometry, with U_{iso}(H) = 1.2U_{eq}(C or N) for all aromatic C- and N-bound H atoms, and with U_{iso}(H) = 1.5U_{eq}(C) for the methylgroup H atoms.

Figures

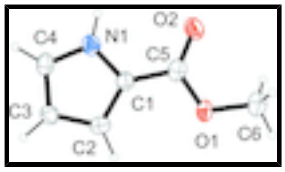

Fig. 1. The molecular structure of the title compound with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

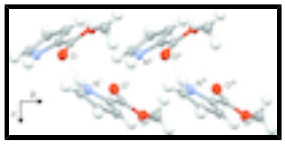

Fig. 2. Strands formed by N–H···O hydrogen bonds along [0 1 0] in the crystal structure of the title compound, viewed along [1 0 0]. Symmetry codes: (i) -*x*, *y* + 1/2, 1/2 - *z*; (ii) *x*, *y* + 1, *z*; (iii) -*x*, *y* + 3/2, 1/2 - *z*.

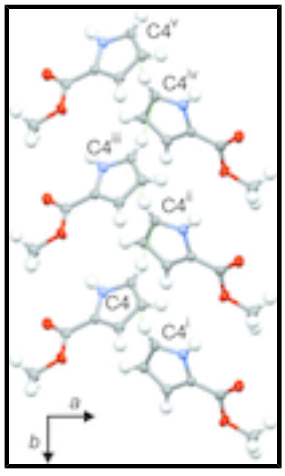

Fig. 3. Strands formed by C–H···π contacts along [0 1 0] in the crystal structure of the title compound, viewed along [0 0 1]. Symmetry codes: (i) 1 - *x*, *y* + 1/2, 1/2 - *z*; (ii) 1 - *x*, *y* - 1/2, *z* - 1/2; (iii) *x*, *y* - 1, *z*; (iv) 1 - *x*, *y* - 3/2, 1/2 - *z*; (v) *x*, *y* - 2, *z*.

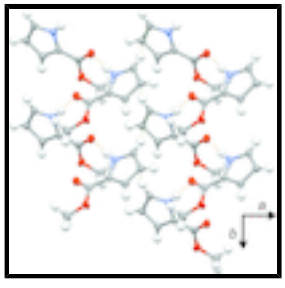

Fig. 4. The strands formed by hydrogen bonding in the crystal structure are interconnected by the strands formed by C–H···π contacts.

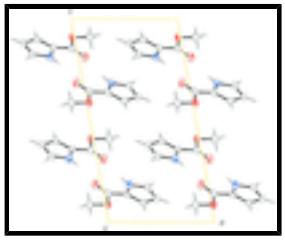

Fig. 5. The packing of the title compound, viewed along [0 1 0].

Methyl 1*H*-pyrrole-2-carboxylate

Crystal data

$C_6H_7NO_2$	F_{000} = 264
M_r = 125.13	D_x = 1.395 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å

Hall symbol: -P 2ybc
a = 7.5346 (19) Å
b = 5.4598 (14) Å
c = 14.730 (4) Å
β = 100.55 (2)º
V = 595.7 (3) Å^3
Z = 4

Cell parameters from 1091 reflections
θ = 4.0–27.5º
μ = 0.11 mm^{-1}
T = 200 K
Platelet, colourless
0.38 × 0.16 × 0.06 mm

Data collection

Oxford Xcalibur KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
T = 200 K
ω–scans
Absorption correction: none
2591 measured reflections
1103 independent reflections

528 reflections with $I > 2\sigma(I)$
R_{int} = 0.112
θ_{max} = 25.5º
θ_{min} = 4.0º
h = −9→9
k = −6→6
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.176
S = 0.95
1103 reflections
83 parameters
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0745P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.0203 (3)	0.7534 (4)	0.08955 (19)	0.0312 (8)
O2	−0.0644 (3)	0.4755 (5)	0.18723 (19)	0.0331 (8)
N1	0.2637 (4)	0.2221 (6)	0.1856 (2)	0.0286 (9)
H1	0.1960	0.1417	0.2183	0.034*
C1	0.2176 (5)	0.4370 (7)	0.1405 (3)	0.0248 (10)
C5	0.0452 (5)	0.5519 (7)	0.1425 (3)	0.0276 (10)
C6	−0.1459 (5)	0.8847 (7)	0.0877 (3)	0.0378 (12)
H6A	−0.2475	0.7701	0.0753	0.057*
H6B	−0.1594	1.0093	0.0391	0.057*
H6C	−0.1439	0.9640	0.1476	0.057*

C3	0.4923 (5)	0.3236 (7)	0.1182 (3)	0.0275 (10)
H3	0.6054	0.3212	0.0984	0.033*
C4	0.4295 (5)	0.1506 (7)	0.1726 (3)	0.0300 (10)
H4	0.4914	0.0065	0.1967	0.036*
C2	0.3585 (5)	0.5042 (7)	0.0975 (3)	0.0276 (10)
H2	0.3638	0.6461	0.0608	0.033*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0235 (16)	0.0309 (17)	0.0388 (19)	0.0084 (12)	0.0042 (12)	0.0051 (13)
O2	0.0241 (16)	0.0352 (17)	0.041 (2)	0.0013 (13)	0.0090 (14)	−0.0012 (14)
N1	0.025 (2)	0.0251 (19)	0.036 (2)	−0.0002 (15)	0.0059 (15)	−0.0020 (16)
C1	0.024 (2)	0.022 (2)	0.028 (2)	−0.0012 (18)	0.0041 (18)	−0.0015 (17)
C5	0.028 (2)	0.022 (2)	0.030 (2)	0.0005 (18)	−0.0009 (19)	−0.0072 (18)
C6	0.034 (3)	0.037 (3)	0.041 (3)	0.009 (2)	0.004 (2)	0.001 (2)
C3	0.026 (2)	0.031 (2)	0.026 (2)	0.0016 (18)	0.0079 (17)	−0.0016 (19)
C4	0.023 (2)	0.029 (2)	0.035 (3)	0.0024 (19)	−0.0013 (18)	−0.0029 (19)
C2	0.030 (2)	0.026 (2)	0.026 (3)	−0.0026 (19)	0.0051 (19)	0.0019 (19)

Geometric parameters (Å, °)

O1—C5	1.341 (4)	C6—H6A	0.9800
O1—C6	1.439 (4)	C6—H6B	0.9800
O2—C5	1.221 (5)	C6—H6C	0.9800
N1—C4	1.356 (5)	C3—C4	1.377 (5)
N1—C1	1.362 (5)	C3—C2	1.403 (5)
N1—H1	0.8800	C3—H3	0.9500
C1—C2	1.382 (5)	C4—H4	0.9500
C1—C5	1.447 (5)	C2—H2	0.9500
C5—O1—C6	116.6 (3)	O1—C6—H6C	109.5
C4—N1—C1	109.8 (3)	H6A—C6—H6C	109.5
C4—N1—H1	125.1	H6B—C6—H6C	109.5
C1—N1—H1	125.1	C4—C3—C2	107.4 (3)
N1—C1—C2	107.7 (3)	C4—C3—H3	126.3
N1—C1—C5	120.9 (3)	C2—C3—H3	126.3
C2—C1—C5	131.4 (4)	N1—C4—C3	108.0 (3)
O2—C5—O1	123.9 (4)	N1—C4—H4	126.0
O2—C5—C1	124.1 (4)	C3—C4—H4	126.0
O1—C5—C1	112.0 (4)	C1—C2—C3	107.2 (3)
O1—C6—H6A	109.5	C1—C2—H2	126.4
O1—C6—H6B	109.5	C3—C2—H2	126.4
H6A—C6—H6B	109.5		
C4—N1—C1—C2	0.0 (4)	C2—C1—C5—O1	2.9 (6)
C4—N1—C1—C5	179.3 (3)	C1—N1—C4—C3	0.3 (4)
C6—O1—C5—O2	0.7 (5)	C2—C3—C4—N1	−0.4 (4)
C6—O1—C5—C1	−179.0 (3)	N1—C1—C2—C3	−0.2 (4)
N1—C1—C5—O2	4.1 (6)	C5—C1—C2—C3	−179.4 (4)

C2—C1—C5—O2	−176.8 (4)	C4—C3—C2—C1	0.4 (4)
N1—C1—C5—O1	−176.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.88	2.06	2.933 (4)	171
C4—H4···Cg1^{ii}	0.95	2.63	3.401 (5)	139

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) −*x*+1, *y*−1/2, −*z*+1/2.

Fig. 1

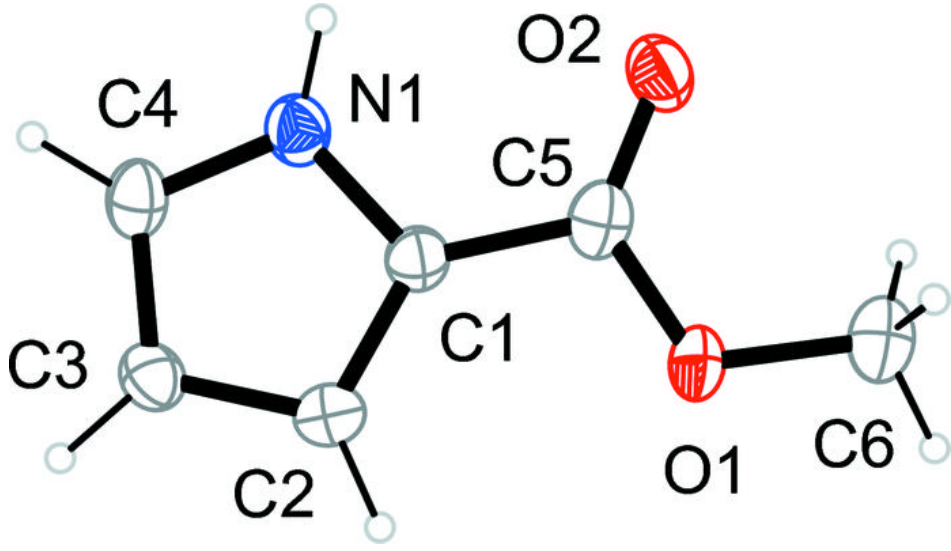

Fig. 2

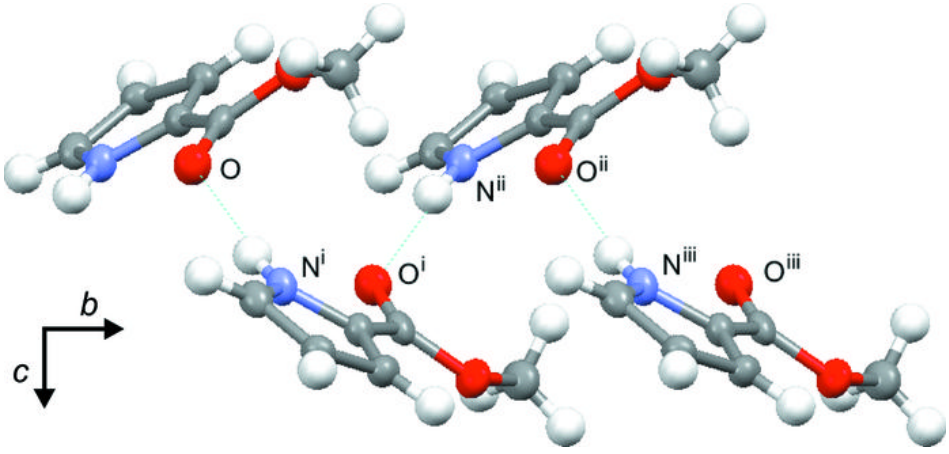

Fig. 3

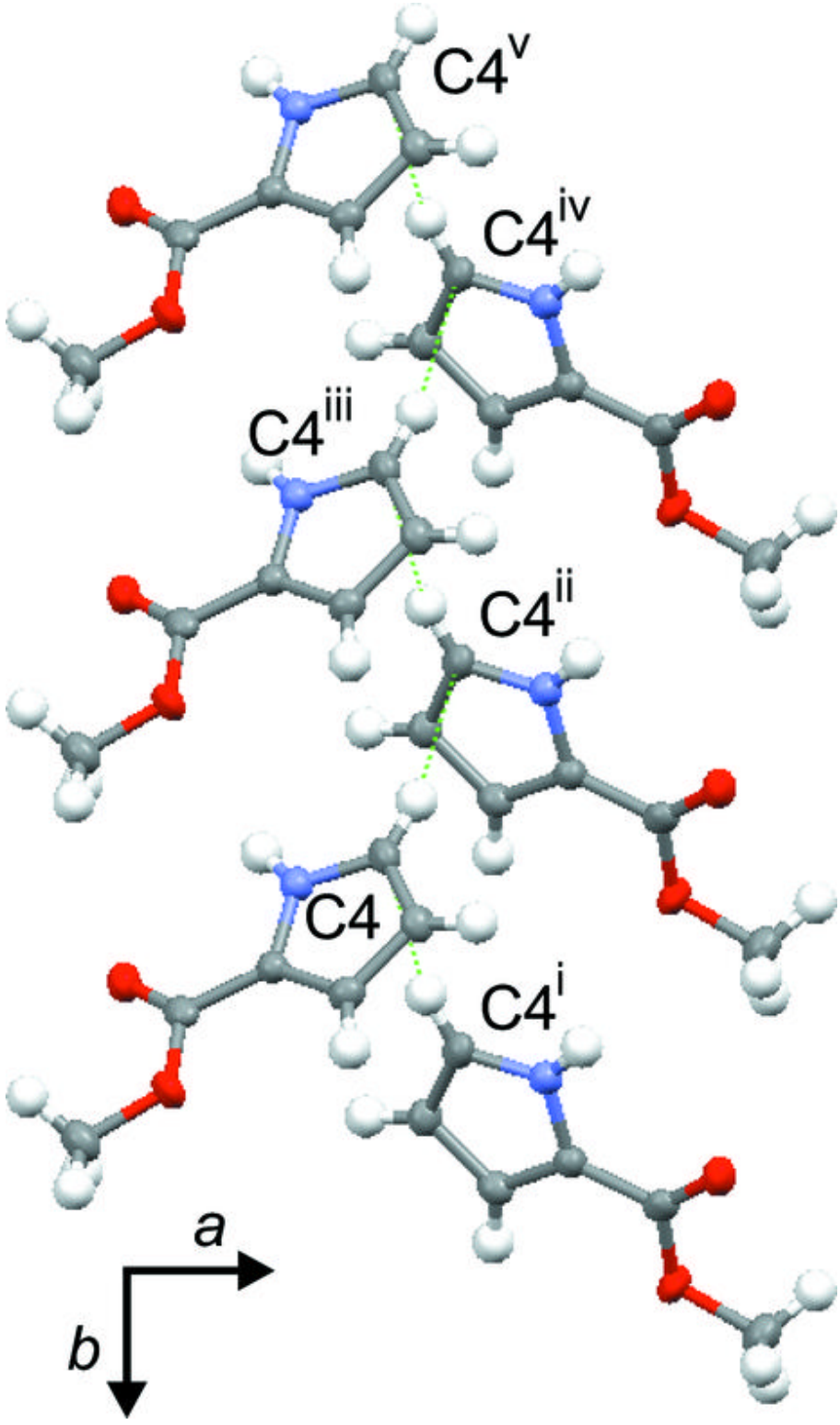

Fig. 4

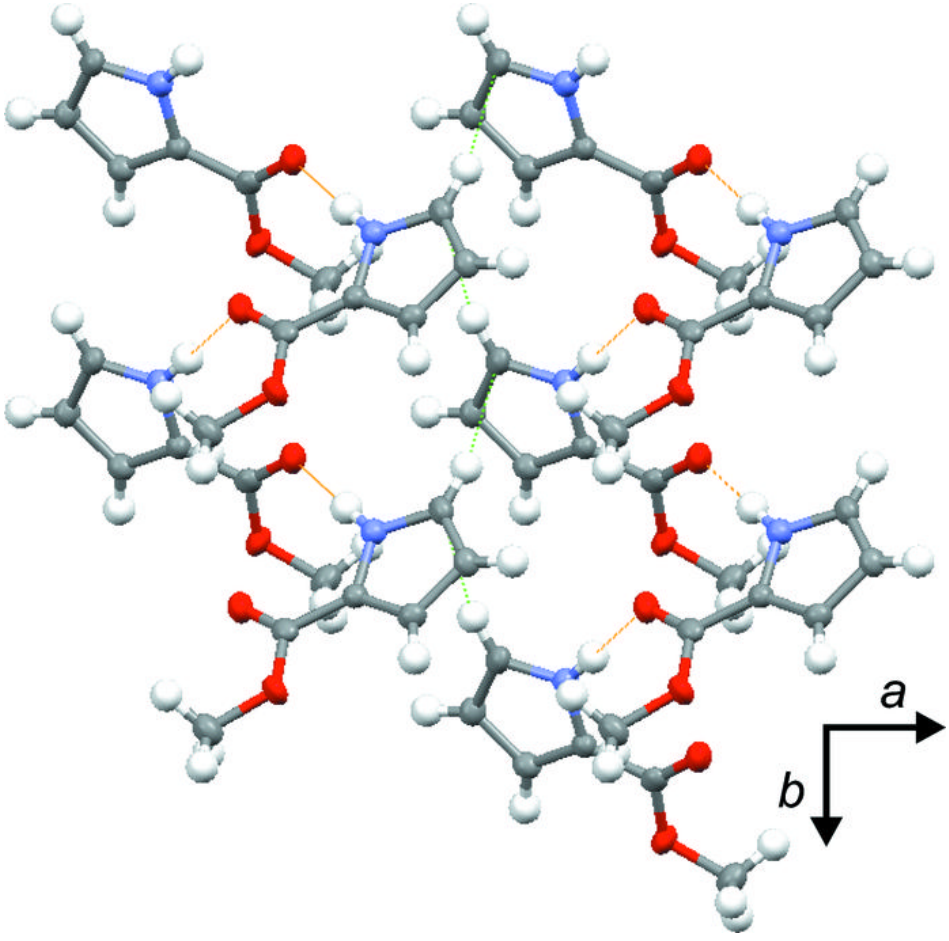

Fig. 5