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Dimethyl 1*H*-pyrazole-3,5-dicarboxylate

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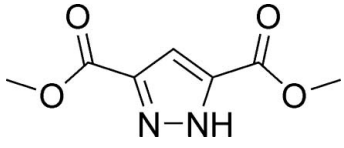
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.106; data-to-parameter ratio = 10.0.

The title compound, $C_7H_8N_2O_4$, is an important precursor of bi- or multidentate ligands. The structure contains two molecules linked together *via* intermolecular N—H···O and N—H···N hydrogen bonds and intermolecular C—H···O contacts, resulting in a two-dimensional network. All atoms except for methyl H atoms lie on crystallographic mirror planes.

Related literature

For general background, see: Zheng *et al.*, 2003; Peng *et al.*, 2006; Schenck *et al.*, 1985; Ardizzoia *et al.*, 2002. For structure analysis tools used, see: Taylor *et al.*, 1982; Desiraju *et al.*,1999.



Experimental

Crystal data

$C_7H_8N_2O_4$
M_r = 184.15
Orthorhombic, *Pnma*
a = 10.9563 (14) Å
b = 6.4983 (8) Å
c = 23.589 (3) Å
V = 1679.5 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 (2) K
0.49 × 0.34 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.943, T_{max} = 0.985
8106 measured reflections
1614 independent reflections
1196 reflections with $I > 2\sigma(I)$
R_{int} = 0.116

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.106
S = 0.97
1614 reflections
162 parameters
5 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O3	0.86	2.13	2.796 (2)	134
N1—H1···N4	0.86	2.06	2.919 (2)	176
C2—H2···O5^{i}	0.93	2.55	3.467 (3)	167
C7—H7*A*···O8^{i}	0.96	2.54	3.431 (3)	155
C5—H5*C*···O1^{ii}	0.96	2.56	3.243 (3)	128
C14—H14*C*···O7^{iii}	0.96	2.56	3.424 (3)	150

Symmetry codes: (i) $x+1, y, z$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997*b*).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2164).

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supplementary materials

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Dimethyl 1*H*-pyrazole-3,5-dicarboxylate

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Comment

Recently, there has been much interest in the study of crystal engineering of supramolecular architectures using N-donor ligands (Zheng *et al.*, 2003; Peng *et al.*, 2006). The title compound, $C_7H_8N_2O_4$, is an important organic intermediate and precursor of bi- or polydentate ligands which have been reported (Schenck *et al.*, 1985; Ardizzoia *et al.*, 2002).

The asymmetric unit contains two molecules linked together via intermolecular N—H. . .O(2.80 Å) and N—H. . .N (2.92 Å) hydrogen bonds and forming a pseudo dimer(Fig. 1). Futhermore intermolecular C—H. . .O contacts (3.24–3.47 Å) satisfy the definition of weak hydrogen bonds as proposed by Taylor *et al.* (1982) and Desiraju *et al.* (1999), and resulted in a two dimensional network (Fig. 2). Interestingly, all of the nonH atoms are coplanar. Although the interpalanar distances, 3.25 Å, between stacked pyrazole molecules might indicate π···π stacking, the centroid to centroid distance between pyrazlole rings, 3.70Å , corresponds to a large offset angle of 28.6 ° which prevents such π···π stacking.

Experimental

All reagents were of analytical grade and used without further purification. Dimethyl-1*H*-pyrazole-3,5-dicarboxylate was prepared by the general procedure of Schenck *et al.* (1985). Colorless single crystals were grown from slow evaporation of the saturated MeOH solution of the compound. Analysis found: C 45.64, H 4.40, N 15.25%.; calculated for $C_7H_8N_2O_4$: C 45.66, H 4.38, N 15.21%.

Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C—H = 0.93Å (aromatic) or 0.96Å (methyl) and N—H = 0.86Å with Uiso(H) = 1.2Ueq(CH or NH) or Uiso(H) = 1.5Ueq(CH_3).

Figures

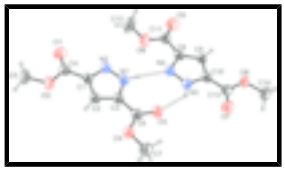


Fig. 1. The molecular structure of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii and H bonds are represented as dashed lines.

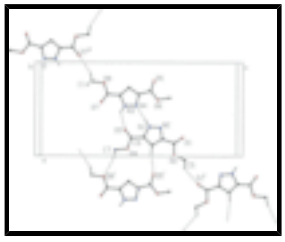


Fig. 2. Partial packing view showing the hydrogen bonding interactions. H atoms are represented as small spheres of arbitrary radii and H bonds are shown as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) 1 + x, y, z; (ii) 1/2 + x, 1/2 -y, 3/2 - z; (iii) x - 1/2, 1/2 - y, 1/2 -z].

Dimethyl 1*H*-pyrazole-3,5-dicarboxylate

Crystal data

$C_7H_8N_2O_4$	F_{000} = 768
M_r = 184.15	D_x = 1.457 Mg m^{-3}
Orthorhombic, *Pnma*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2n	Cell parameters from 2089 reflections
a = 10.9563 (14) Å	θ = 5.1–51.9º
b = 6.4983 (8) Å	μ = 0.12 mm^{-1}
c = 23.589 (3) Å	*T* = 293 (2) K
V = 1679.5 (4) Å^3	Prismatic, colorless
Z = 8	0.49 × 0.34 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1614 independent reflections
Radiation source: fine-focus sealed tube	1196 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.116
T = 293(2) K	θ_{max} = 25.1º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −13→11
T_{min} = 0.943, T_{max} = 0.985	*k* = −7→7
8106 measured reflections	*l* = −26→28

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.106	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
S = 0.97	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
1614 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
162 parameters	Extinction coefficient: 0.020 (3)
5 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. Highest peak 0.17 at 0.6417 0.2500 0.6281 [0.90 A from N2] Deepest hole -0.24 at 0.3595 0.2500 0.4390 [0.95 A from C10]

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.80198 (16)	0.2500	0.71010 (7)	0.0603 (5)	
O2	0.98429 (15)	0.2500	0.66789 (6)	0.0566 (5)	
O3	0.71755 (15)	0.2500	0.42420 (7)	0.0554 (5)	
O4	0.91928 (14)	0.2500	0.43727 (7)	0.0509 (5)	
O5	0.19936 (16)	0.2500	0.56690 (7)	0.0651 (6)	
O6	0.40030 (16)	0.2500	0.58550 (7)	0.0633 (6)	
O7	0.42515 (16)	0.2500	0.30600 (7)	0.0669 (6)	
O8	0.22351 (14)	0.2500	0.32051 (6)	0.0489 (5)	
N1	0.68713 (16)	0.2500	0.54353 (8)	0.0391 (5)	
H1	0.6186	0.2500	0.5258	0.047*	
N2	0.69628 (17)	0.2500	0.59972 (8)	0.0405 (5)	
N3	0.46241 (17)	0.2500	0.42244 (8)	0.0437 (5)	
H3	0.5287	0.2500	0.4029	0.052*	
N4	0.46048 (16)	0.2500	0.47848 (8)	0.0426 (5)	
C1	0.8175 (2)	0.2500	0.60908 (9)	0.0377 (6)	
C2	0.8834 (2)	0.2500	0.55897 (9)	0.0391 (6)	
H2	0.9678	0.2500	0.5548	0.047*	
C3	0.79727 (19)	0.2500	0.51709 (10)	0.0386 (6)	
C4	0.8624 (2)	0.2500	0.66784 (10)	0.0418 (6)	
C5	1.0440 (3)	0.2500	0.72248 (10)	0.0685 (9)	
H5A	1.0381	0.1155	0.7391	0.103*	0.50
H5B	1.0052	0.3486	0.7468	0.103*	0.50
H5C	1.1284	0.2859	0.7178	0.103*	0.50
C6	0.8042 (2)	0.2500	0.45525 (10)	0.0404 (6)	
C7	0.9345 (2)	0.2500	0.37656 (11)	0.0694 (9)	
H7A	1.0165	0.2097	0.3673	0.104*	0.50
H7B	0.9192	0.3856	0.3621	0.104*	0.50
H7C	0.8781	0.1547	0.3598	0.104*	0.50
C8	0.3416 (2)	0.2500	0.49172 (9)	0.0361 (5)	
C9	0.2694 (2)	0.2500	0.44305 (9)	0.0366 (5)	
H9	0.1846	0.2500	0.4411	0.044*	
C10	0.3500 (2)	0.2500	0.39891 (10)	0.0385 (6)	

C11	0.3041 (2)	0.2500	0.55114 (10)	0.0439 (6)	
C12	0.3778 (3)	0.2500	0.64513 (11)	0.0934 (12)	
H12A	0.3561	0.1137	0.6571	0.140*	0.50
H12B	0.3122	0.3429	0.6536	0.140*	0.50
H12C	0.4501	0.2934	0.6648	0.140*	0.50
C13	0.3392 (2)	0.2500	0.33725 (10)	0.0439 (6)	
C14	0.2036 (3)	0.2500	0.25984 (11)	0.0634 (8)	
H14A	0.2585	0.1541	0.2422	0.095*	0.50
H14B	0.2183	0.3854	0.2451	0.095*	0.50
H14C	0.1209	0.2104	0.2520	0.095*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0492 (11)	0.0942 (14)	0.0374 (10)	0.000	0.0117 (9)	0.000
O2	0.0354 (10)	0.1019 (14)	0.0326 (9)	0.000	−0.0037 (7)	0.000
O3	0.0294 (10)	0.0929 (14)	0.0440 (10)	0.000	−0.0048 (8)	0.000
O4	0.0277 (9)	0.0867 (13)	0.0382 (9)	0.000	0.0004 (7)	0.000
O5	0.0399 (12)	0.1052 (16)	0.0502 (11)	0.000	0.0107 (9)	0.000
O6	0.0440 (11)	0.1088 (15)	0.0371 (10)	0.000	−0.0066 (9)	0.000
O7	0.0404 (11)	0.1171 (17)	0.0433 (11)	0.000	0.0096 (9)	0.000
O8	0.0360 (10)	0.0784 (12)	0.0325 (9)	0.000	−0.0066 (7)	0.000
N1	0.0261 (10)	0.0509 (12)	0.0402 (11)	0.000	−0.0041 (8)	0.000
N2	0.0329 (12)	0.0504 (12)	0.0384 (11)	0.000	0.0005 (9)	0.000
N3	0.0260 (11)	0.0687 (14)	0.0365 (11)	0.000	0.0016 (8)	0.000
N4	0.0284 (11)	0.0613 (13)	0.0380 (11)	0.000	−0.0027 (9)	0.000
C1	0.0273 (12)	0.0474 (14)	0.0384 (13)	0.000	−0.0028 (10)	0.000
C2	0.0257 (12)	0.0530 (15)	0.0387 (13)	0.000	−0.0004 (10)	0.000
C3	0.0285 (12)	0.0452 (14)	0.0421 (13)	0.000	−0.0005 (10)	0.000
C4	0.0334 (13)	0.0479 (15)	0.0441 (14)	0.000	0.0032 (11)	0.000
C5	0.0526 (18)	0.115 (3)	0.0380 (15)	0.000	−0.0143 (13)	0.000
C6	0.0289 (13)	0.0527 (15)	0.0396 (13)	0.000	−0.0010 (11)	0.000
C7	0.0432 (17)	0.121 (3)	0.0442 (16)	0.000	0.0064 (13)	0.000
C8	0.0279 (12)	0.0412 (13)	0.0391 (13)	0.000	−0.0016 (10)	0.000
C9	0.0267 (12)	0.0448 (13)	0.0384 (13)	0.000	−0.0040 (10)	0.000
C10	0.0278 (12)	0.0459 (14)	0.0418 (13)	0.000	−0.0034 (11)	0.000
C11	0.0370 (15)	0.0541 (15)	0.0406 (14)	0.000	−0.0031 (11)	0.000
C12	0.086 (3)	0.161 (3)	0.0332 (16)	0.000	−0.0088 (17)	0.000
C13	0.0353 (14)	0.0579 (16)	0.0384 (14)	0.000	0.0014 (11)	0.000
C14	0.0646 (19)	0.088 (2)	0.0374 (14)	0.000	−0.0151 (14)	0.000

Geometric parameters (Å, °)

O1—C4	1.197 (3)	C1—C4	1.471 (3)
O2—C4	1.335 (3)	C2—C3	1.366 (3)
O2—C5	1.444 (3)	C2—H2	0.9300
O3—C6	1.199 (3)	C3—C6	1.461 (3)
O4—C6	1.330 (3)	C5—H5A	0.9600
O4—C7	1.442 (3)	C5—H5B	0.9600

O5—C11	1.206 (3)	C5—H5C	0.9600
O6—C11	1.330 (3)	C7—H7A	0.9600
O6—C12	1.428 (3)	C7—H7B	0.9600
O7—C13	1.196 (3)	C7—H7C	0.9600
O8—C13	1.327 (3)	C8—C9	1.394 (3)
O8—C14	1.448 (3)	C8—C11	1.461 (3)
N1—N2	1.329 (3)	C9—C10	1.366 (3)
N1—C3	1.358 (3)	C9—H9	0.9300
N1—H1	0.8600	C10—C13	1.459 (3)
N2—C1	1.347 (3)	C12—H12A	0.9600
N3—N4	1.322 (3)	C12—H12B	0.9600
N3—C10	1.351 (3)	C12—H12C	0.9600
N3—H3	0.8600	C14—H14A	0.9600
N4—C8	1.340 (3)	C14—H14B	0.9600
C1—C2	1.385 (3)	C14—H14C	0.9600
C4—O2—C5	116.98 (19)	O4—C7—H7A	109.5
C6—O4—C7	115.25 (18)	O4—C7—H7B	109.5
C11—O6—C12	117.6 (2)	H7A—C7—H7B	109.5
C13—O8—C14	115.95 (19)	O4—C7—H7C	109.5
N2—N1—C3	113.02 (18)	H7A—C7—H7C	109.5
N2—N1—H1	123.5	H7B—C7—H7C	109.5
C3—N1—H1	123.5	N4—C8—C9	111.1 (2)
N1—N2—C1	103.76 (18)	N4—C8—C11	119.8 (2)
N4—N3—C10	113.34 (19)	C9—C8—C11	129.1 (2)
N4—N3—H3	123.3	C10—C9—C8	105.1 (2)
C10—N3—H3	123.3	C10—C9—H9	127.4
N3—N4—C8	104.40 (18)	C8—C9—H9	127.4
N2—C1—C2	111.97 (19)	N3—C10—C9	106.1 (2)
N2—C1—C4	119.0 (2)	N3—C10—C13	118.9 (2)
C2—C1—C4	129.1 (2)	C9—C10—C13	135.0 (2)
C3—C2—C1	104.9 (2)	O5—C11—O6	124.5 (2)
C3—C2—H2	127.5	O5—C11—C8	124.3 (2)
C1—C2—H2	127.5	O6—C11—C8	111.2 (2)
N1—C3—C2	106.34 (19)	O6—C12—H12A	109.5
N1—C3—C6	120.33 (19)	O6—C12—H12B	109.5
C2—C3—C6	133.3 (2)	H12A—C12—H12B	109.5
O1—C4—O2	123.5 (2)	O6—C12—H12C	109.5
O1—C4—C1	126.9 (2)	H12A—C12—H12C	109.5
O2—C4—C1	109.6 (2)	H12B—C12—H12C	109.5
O2—C5—H5A	109.5	O7—C13—O8	124.7 (2)
O2—C5—H5B	109.5	O7—C13—C10	123.4 (2)
H5A—C5—H5B	109.5	O8—C13—C10	112.0 (2)
O2—C5—H5C	109.5	O8—C14—H14A	109.5
H5A—C5—H5C	109.5	O8—C14—H14B	109.5
H5B—C5—H5C	109.5	H14A—C14—H14B	109.5
O3—C6—O4	123.8 (2)	O8—C14—H14C	109.5
O3—C6—C3	124.7 (2)	H14A—C14—H14C	109.5
O4—C6—C3	111.58 (19)	H14B—C14—H14C	109.5

C3—N1—N2—C1	0.0	C2—C3—C6—O4	0.0
C10—N3—N4—C8	0.0	N3—N4—C8—C9	0.0
N1—N2—C1—C2	0.0	N3—N4—C8—C11	180.0
N1—N2—C1—C4	180.0	N4—C8—C9—C10	0.0
N2—C1—C2—C3	0.0	C11—C8—C9—C10	180.0
C4—C1—C2—C3	180.0	N4—N3—C10—C9	0.0
N2—N1—C3—C2	0.0	N4—N3—C10—C13	180.0
N2—N1—C3—C6	180.0	C8—C9—C10—N3	0.0
C1—C2—C3—N1	0.0	C8—C9—C10—C13	180.0
C1—C2—C3—C6	180.0	C12—O6—C11—O5	0.0
C5—O2—C4—O1	0.0	C12—O6—C11—C8	180.0
C5—O2—C4—C1	180.0	N4—C8—C11—O5	180.0
N2—C1—C4—O1	0.000 (1)	C9—C8—C11—O5	0.0
C2—C1—C4—O1	180.0	N4—C8—C11—O6	0.0
N2—C1—C4—O2	180.0	C9—C8—C11—O6	180.0
C2—C1—C4—O2	0.0	C14—O8—C13—O7	0.0
C7—O4—C6—O3	0.0	C14—O8—C13—C10	180.0
C7—O4—C6—C3	180.0	N3—C10—C13—O7	0.0
N1—C3—C6—O3	0.0	C9—C10—C13—O7	180.0
C2—C3—C6—O3	180.0	N3—C10—C13—O8	180.0
N1—C3—C6—O4	180.0	C9—C10—C13—O8	0.0

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O3	0.86	2.13	2.796 (2)	134
N1—H1···N4	0.86	2.06	2.919 (2)	176
C2—H2···O5^{i}	0.93	2.55	3.467 (3)	167
C7—H7A···O8^{i}	0.96	2.54	3.431 (3)	155
C5—H5C···O1^{ii}	0.96	2.56	3.243 (3)	128
C14—H14C···O7^{iii}	0.96	2.56	3.424 (3)	150

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*+1/2, −*y*+1/2, −*z*+3/2; (iii) *x*−1/2, −*y*+1/2, −*z*+1/2.

Fig. 1

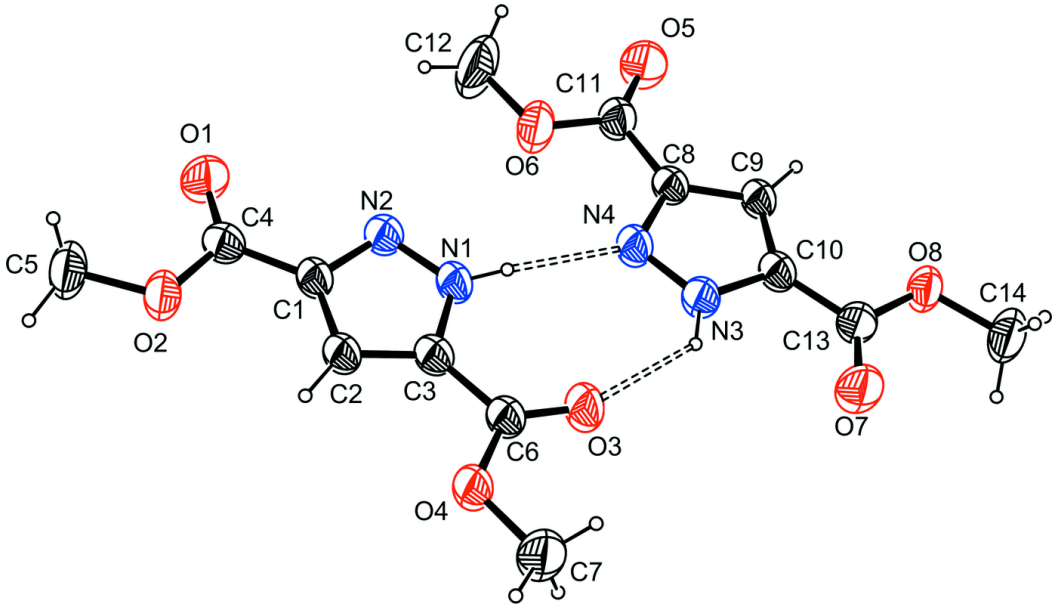
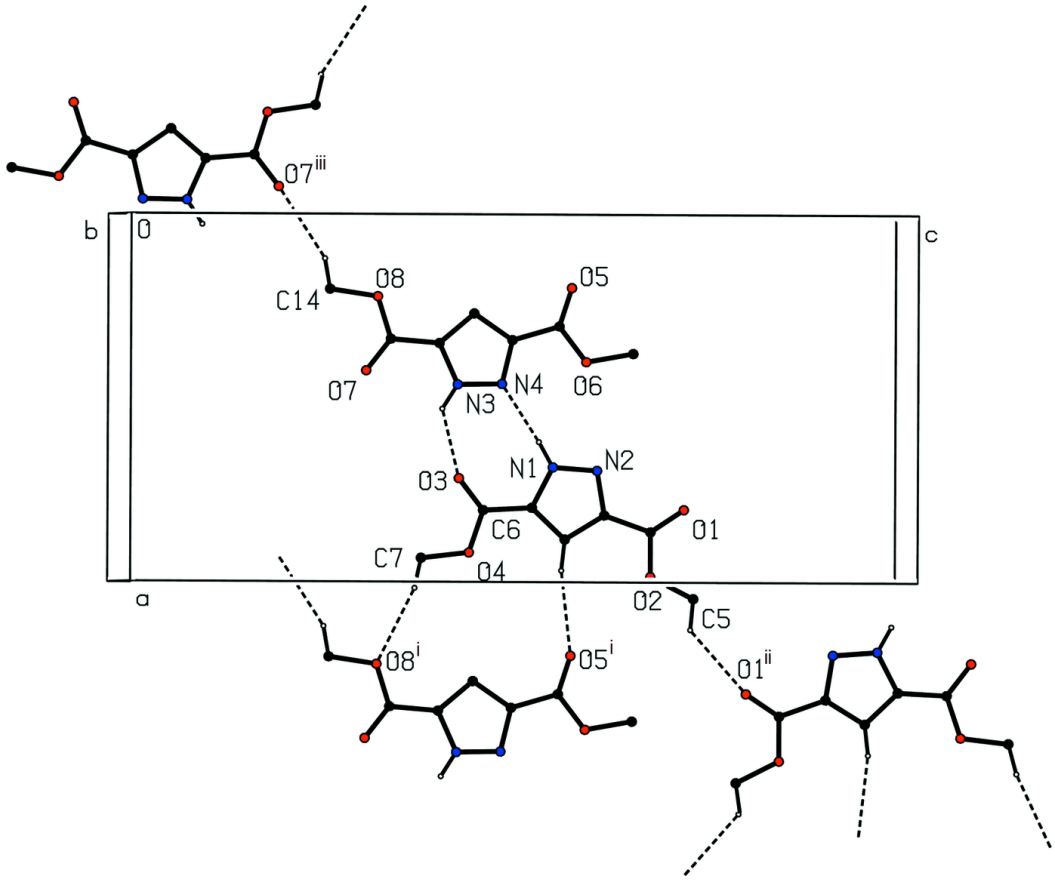

C12
O5
C11
O1
O6
C8
C9
N2
C4
N4
N1
C10
O8
C5
C1
N3
C14
O2
C13
C2
C3
O7
C6
O3
O4
C7

Fig. 2


O7iii
b
0
c
C14
O8
O5
O7
N4
O6
N3
O3
N1
N2
C6
O1
C7
O4
a
O2
C5
O8i
O5i
O1ii