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(3,5-Dimethylpyrazol-1-yl)acetic acid

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.147
Data-to-parameter ratio = 18.8

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

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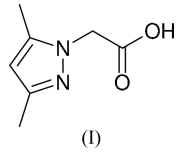
At 150 K, the title compound, $C_7H_{10}N_2O_2$, comprises one-dimensional hydrogen-bonded homochiral helical chains of molecules.

Comment

The molecular structure of the title compound, (I), is shown in Fig. 1 and selected structural parameters are listed in Table 1. The least-squares planes of the pyrazole ring and the carboxylic acid group are almost mutually perpendicular, with a dihedral angle of 87.57 (7)°, and atom N2 is close to being coplanar with the carboxylic acid group, lying only 0.0067 (15) Å out of the least-squares plane of the latter. The molecules form homochiral helical hydrogen-bonded chains parallel to the b axis (Fig. 2 and Table 2).



(I)

Experimental

The title compound, (I), was prepared according to the method of Micetich (1970).

Crystal data

$C_7H_{10}N_2O_2$
M_r = 154.17
Orthorhombic, $P2_12_12_1$
a = 4.8528 (4) Å
b = 7.0073 (6) Å
c = 23.256 (3) Å
V = 790.82 (13) Å^3
Z = 4
D_x = 1.295 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6939 reflections
θ = 3.0–34.8°
μ = 0.10 mm^{-1}
T = 150 (2) K
Lath, colourless
0.60 × 0.25 × 0.10 mm

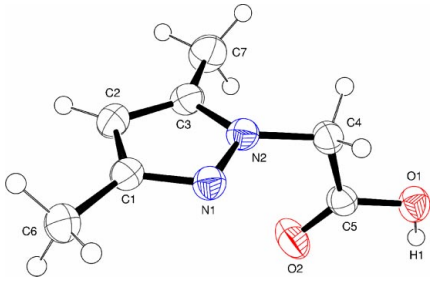


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size.

Data collection

Stoe IPDS-II area-detector diffractometer
φ and ω scans
Absorption correction: none
11979 measured reflections
2013 independent reflections
1357 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 34.8°$
$h = -7 \rightarrow 6$
$k = -11 \rightarrow 10$
$l = -37 \rightarrow 37$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.147$
$S = 1.05$
2013 reflections
107 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0896P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.088 (15)

Table 1
Selected geometric parameters (Å, °).

O1—C5	1.318 (2)	C1—C2	1.407 (3)
O2—C5	1.201 (2)	N1—C1	1.331 (2)
N1—N2	1.359 (2)	N2—C4	1.451 (2)
N2—C3	1.348 (2)	C4—C5	1.514 (3)
C2—C3	1.381 (3)		
N1—N2—C4	119.87 (14)	O2—C5—O1	124.93 (18)
N2—C4—C5	110.48 (15)		
N1—N2—C4—C5	87.48 (19)	N2—C4—C5—O2	0.7 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.95 (3)	1.79 (3)	2.723 (2)	169 (3)

Symmetry code: (i) $2 - x, y - \frac{1}{2}, \frac{1}{2} - z$.

All H atoms were initially located in a difference Fourier map. The positional and isotropic displacement parameters for the hydroxyl H atom were freely refined. The methyl H atoms were constrained to an ideal geometry, with a C—H distance of 0.98 Å, but each group was allowed to rotate freely about its X—C bond. All other C—H atoms were placed in geometrically idealized positions, with C—H distances of 0.95–0.99 Å. U_{iso}(H) values were set at $1.2U_{eq}$(C) for all C—H atoms.

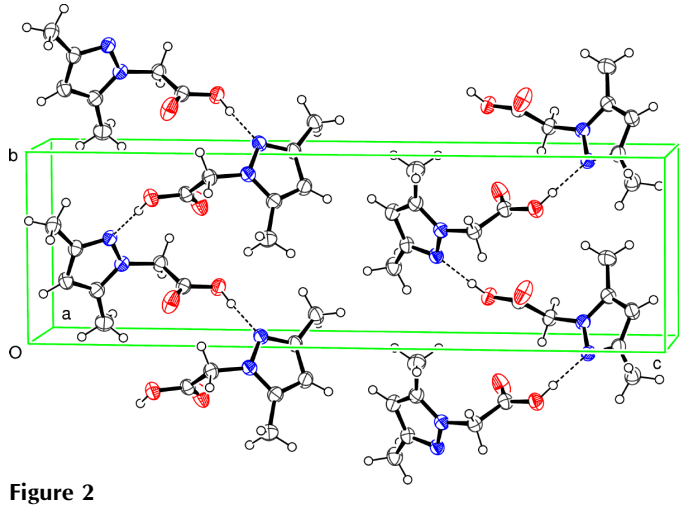


Figure 2
The packing and unit cell of (I), viewed approximately down the *a* axis. Hydrogen bonds are denoted by dashed lines.

Data collection: *X-AREA* (Stoe, 2001); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2001).

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