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5-Methyl-1,2-oxazole-3-carboxylic acid

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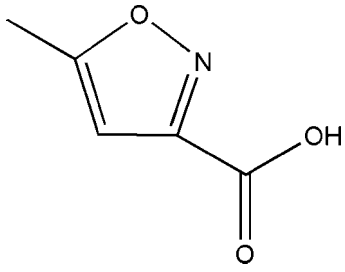
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.084; wR factor = 0.230; data-to-parameter ratio = 15.5.

In the crystal structure of the title compound, $C_5H_5NO_3$, all the non-H atoms are approximately coplanar: the carboxy O atoms deviating by 0.013 (2) and −0.075 (2) Å from the isoxazole ring plane. In the crystal, the molecules form inversion dimers linked by pairs of O—H···O hydrogen bonds and the dimers stack *via* π–π interactions [centroid–centroid distance = 3.234 (2) Å].

Related literature

The title compound is a potent inhibitor of the monoamine oxidase enzyme and multidentate ligand for transition metals, see: Birk & Weihe (2009).



Experimental

Crystal data

$C_5H_5NO_3$
M_r = 127.10
Triclinic, $P\overline{1}$
a = 4.9125 (10) Å
b = 5.6909 (11) Å
c = 10.464 (2) Å
α = 82.21 (3)°
β = 79.72 (3)°
γ = 78.96 (3)°
V = 280.96 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.975, T_{max} = 0.975
2923 measured reflections
1283 independent reflections
1052 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.230
S = 1.07
1283 reflections
83 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.98	1.68	2.650 (2)	170

Symmetry code: (i) $-x+1, -y, -z+1$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); 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: JH2316).

References

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supporting information

Acta Cryst. (2011). E**67**, o2545 [https://doi.org/10.1107/S160053681103532X]

5-Methyl-1,2-oxazole-3-carboxylic acid

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S1. Comment

5-Methylisoxazole-3-carboxylic acid is a potent inhibitor of the monoamine oxidase enzyme and excellent ligand for transition metals (Birk, *et al.*,2009) as well as other derivatives of isoxazole. As part of our interest in these compounds, we report here the crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. All the non-H atoms of the title compound are located almost in one plane, as the atoms O1 and O2 are shifted just *ca* 0.0016Å out of the isoxazole ring plane.

The title compound formed dimer *via* intermolecular O—H···O hydrogen bonds and the dimers packed *via* *π*–*π* stacking interactions (3.234 Å).(Fig. 2).

S2. Experimental

The title compound was purchased commercially. Crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

S3. Refinement

All H atoms attached to C atoms and O atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (CH) or C—H = 0.96 Å and O—H = 0.9796 Å with U_{iso}(H) = 1.2U_{eq}(CH) and U_{iso}(H) = 1.5U_{eq}(O,CH_3).

Figure 1

The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

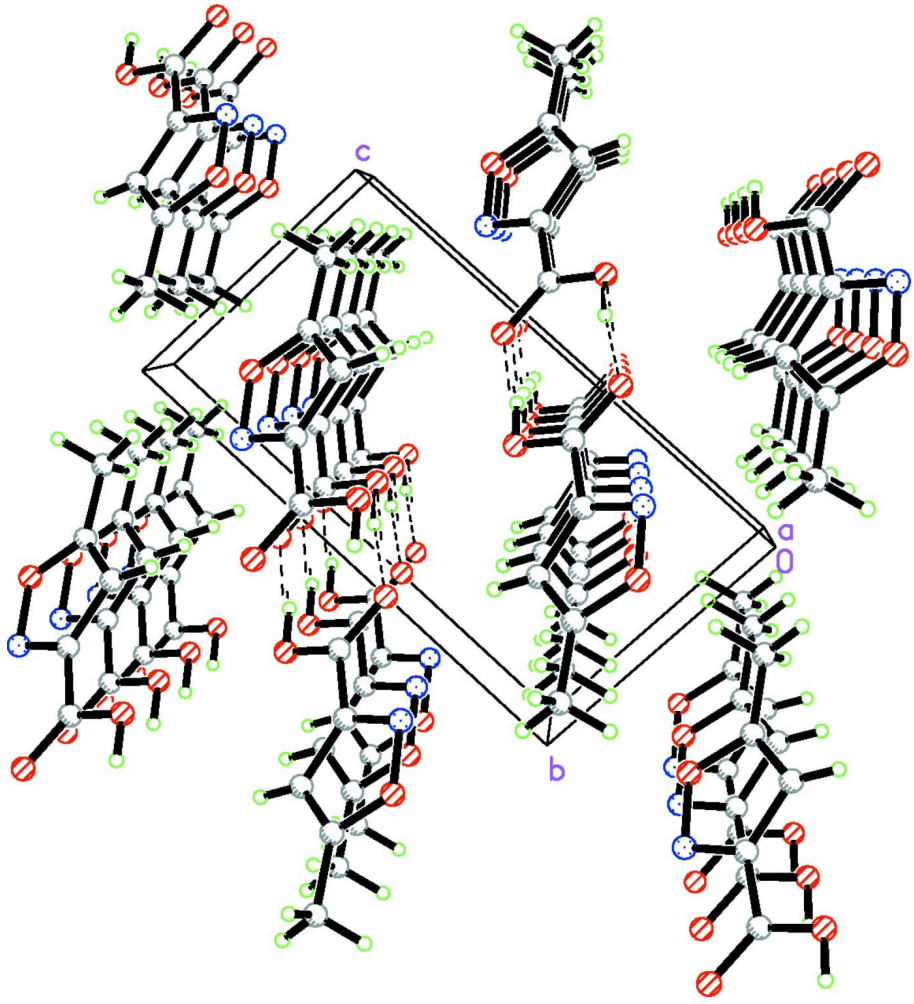

Figure 2

A packing view down the *a* axis showing the three dimensionnal network.Intermolecular hydrogen bonds are shown as dashed lines. H atoms have been omitted for the sake of clarity.

5-Methyl-1,2-oxazole-3-carboxylic acid

Crystal data

$C_5H_5NO_3$
M_r = 127.10
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 4.9125 (10) Å
b = 5.6909 (11) Å
c = 10.464 (2) Å
α = 82.21 (3)°
β = 79.72 (3)°
γ = 78.96 (3)°
V = 280.96 (10) Å^3
Z = 2
F(000) = 132
D_x = 1.502 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1283 reflections
θ = 3.7–27.5°
μ = 0.13 mm^{-1}
T = 293 K
Prism, colourless
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.975, T_{max} = 0.975
2923 measured reflections
1283 independent reflections
1052 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
θ_{max} = 27.5°, θ_{min} = 3.7°
$h = -6 \rightarrow 6$
$k = -7 \rightarrow 7$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.230
S = 1.07
1283 reflections
83 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.1395P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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.

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

	x	y	z	U_{iso}*/U_{eq}
O3	−0.2313 (3)	0.3175 (2)	0.15660 (15)	0.0539 (5)
N1	−0.0692 (4)	0.1507 (3)	0.2343 (2)	0.0530 (6)
C2	0.0502 (4)	0.2811 (3)	0.29544 (17)	0.0401 (5)
C1	0.2432 (4)	0.1560 (3)	0.38652 (18)	0.0419 (5)
C3	−0.0274 (4)	0.5290 (3)	0.26092 (19)	0.0436 (5)
H3	0.0293	0.6551	0.2915	0.052*
C4	−0.2024 (4)	0.5436 (3)	0.17357 (18)	0.0428 (5)
O1	0.2945 (3)	−0.0687 (3)	0.40024 (16)	0.0560 (5)
C5	−0.3597 (5)	0.7439 (4)	0.0956 (2)	0.0541 (6)
H5A	−0.3371	0.7068	0.0071	0.081*
H5B	−0.2886	0.8892	0.0971	0.081*
H5C	−0.5553	0.7655	0.1323	0.081*
O2	0.3450 (3)	0.2937 (2)	0.44412 (15)	0.0551 (5)
H2	0.4849 (14)	0.1977 (10)	0.4948 (5)	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0681 (10)	0.0405 (9)	0.0617 (10)	−0.0087 (7)	−0.0357 (8)	−0.0030 (7)
N1	0.0638 (11)	0.0374 (10)	0.0650 (12)	−0.0080 (8)	−0.0332 (9)	−0.0017 (8)
C2	0.0447 (10)	0.0375 (10)	0.0398 (10)	−0.0074 (7)	−0.0116 (8)	−0.0032 (8)
C1	0.0446 (10)	0.0415 (10)	0.0408 (10)	−0.0082 (8)	−0.0103 (8)	−0.0028 (8)
C3	0.0496 (11)	0.0391 (11)	0.0455 (10)	−0.0088 (8)	−0.0139 (8)	−0.0058 (8)
C4	0.0495 (10)	0.0362 (10)	0.0446 (10)	−0.0066 (8)	−0.0137 (8)	−0.0036 (7)
O1	0.0646 (10)	0.0407 (9)	0.0655 (10)	−0.0029 (7)	−0.0291 (8)	0.0015 (7)
C5	0.0625 (13)	0.0463 (12)	0.0540 (12)	−0.0031 (9)	−0.0220 (10)	0.0009 (9)
O2	0.0624 (10)	0.0517 (10)	0.0581 (10)	−0.0081 (8)	−0.0295 (8)	−0.0057 (7)

Geometric parameters (Å, º)

O3—C4	1.359 (2)	C3—C4	1.347 (3)
O3—N1	1.388 (2)	C3—H3	0.9300
N1—C2	1.317 (3)	C4—C5	1.482 (3)
C2—C3	1.404 (3)	C5—H5A	0.9600
C2—C1	1.481 (3)	C5—H5B	0.9600
C1—O1	1.249 (2)	C5—H5C	0.9600
C1—O2	1.270 (2)	O2—H2	0.9796
C4—O3—N1	109.46 (15)	C3—C4—O3	108.95 (18)
C2—N1—O3	104.75 (15)	C3—C4—C5	134.7 (2)
N1—C2—C3	112.28 (18)	O3—C4—C5	116.31 (18)
N1—C2—C1	118.65 (18)	C4—C5—H5A	109.6
C3—C2—C1	129.06 (18)	C4—C5—H5B	109.4
O1—C1—O2	125.6 (2)	H5A—C5—H5B	109.5
O1—C1—C2	119.38 (18)	C4—C5—H5C	109.5
O2—C1—C2	114.99 (17)	H5A—C5—H5C	109.5
C4—C3—C2	104.56 (17)	H5B—C5—H5C	109.5
C4—C3—H3	127.7	C1—O2—H2	109.6
C2—C3—H3	127.8		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.98	1.68	2.650 (2)	170

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.