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3-(1*H*-Tetrazol-5-yl)benzoic acid

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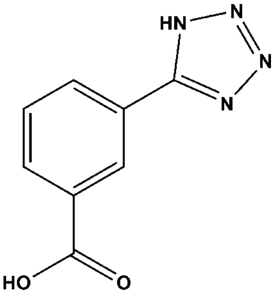
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.106; data-to-parameter ratio = 11.6.

The title compound, $C_8H_6N_4O_2$, is a difunctional compound with a carboxylate and a tetrazole residue. In the crystal structure, molecules are linked into two-dimensional sheets by intermolecular N—H⋯O and O—H⋯N hydrogen bonds.

Related literature

For the applications of tetrazoles, see: Chen & Tong (2007); Demko & Sharpless (2001). For related structures, see: Rizk *et al.* (2005).



Experimental

Crystal data

$C_8H_6N_4O_2$	V = 812.5 (3) Å^3
M_r = 190.17	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 5.2501 (10) Å	μ = 0.12 mm^{-1}
b = 16.805 (3) Å	T = 293 (2) K
c = 9.3290 (18) Å	0.45 × 0.14 × 0.13 mm
β = 99.188 (3)°	

Data collection

Bruker SMART APEX CCD diffractometer	5991 measured reflections
Absorption correction: multi-scan *SADABS* (Sheldrick, 2000)	1583 independent reflections
T_{min} = 0.949, T_{max} = 0.985	1425 reflections with $I > 2\sigma(I)$
	R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.106	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
S = 1.07	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
1583 reflections	
136 parameters	

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O2—H2B⋯N4^{i}	0.93 (2)	1.76 (2)	2.6664 (15)	164 (2)
N1—H1A⋯O1^{ii}	0.94 (2)	1.77 (2)	2.7118 (16)	179.1 (19)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: BT2829).

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supplementary materials

Acta Cryst. (2009). E**65**, o89 [**doi:10.1107/S1600536808041482**]

3-(1*H*-Tetrazol-5-yl)benzoic acid

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Comment

Tetrazoles have been extensively investigated in organic synthetic chemistry for several decades due to the fact that they have wide ranging applications in pharmaceuticals, especially explosives, photography, information recording systems, agriculture, and as precursors to a variety of heterocycles (Chen *et al.* 2007; Demko *et al.* 2001). They have also been used as a type of important multidentate ligands in coordination chemistry. Here, we report the crystal structure of a new tetrazole, 3-(1*H*-tetrazol-5-yl)benzoic acid.

The title compound, $C_8H_6N_4O_2$, is a difunctional compound with carboxylate and tetrazole groups. The C=O distance of the carboxylate is 1.216 (2) Å, which is much shorter than the C—O distance of 1.311 (2) Å. In the tetrazole group, the N=N distance is 1.288 (2) Å, and the N—N distances are 1.343 (2) and 1.358 (2) Å, respectively. The C—N distance is 1.333 (2) Å, being close to the C=N distance of 1.325 (2) Å, which is considered to have part double-bond character. In the crystalline state, the molecules are linked to two-dimensional hydrogen-bonding networks by intermolecular N—H···O and O—H···N hydrogen bonds. The N···O distance is 2.712 (2) Å, and the O···N distance is 2.666 (2) Å.

Experimental

A mixture of 3-cyanobenzoic acid (0.147 g, 1.0 mmol), $Cd(NO_3)_2.6H_2O$ (0.345 g, 1 mmol) and water (8 ml) was was heated in a 15-ml Teflon-lined autoclave at 160 ° for 3 days, followed by slow cooling (5 ° h-1) to room temperature. The resulting mixture was washed with water and collected. Then, the obtained solids were put into 20 ml water, and 10% Na_2S aqueous solution was droped to the suspension liquid until that no precipitation appeared. The solution was filtered and the filtrate was acidified with 50% HCl solution until the pH value was 1.0. White products were filtered, washed with water, then dried and collected in 76.2% yield (0.145 g) based on 3-cyanobenzoic acid. Colorless block shaped crystals were collected from the filtrate after the second filtration.

Refinement

H atoms bonded to N and O atoms were located in a difference map and were freely refined. Other H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å and with $U_{iso}(H)$ = 1.2.

Figures

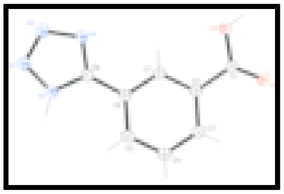

Fig. 1. Structure of the title compound with 30% displacement ellipsoids.

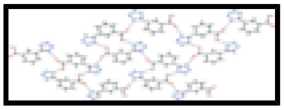

Fig. 2. The two-dimensional hydrogen bonding network of the title compound.

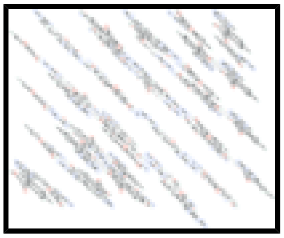

Fig. 3. Packing of the title compound with view onto the *ac* plane.

(I)

Crystal data

$C_8H_6N_4O_2$	F_{000} = 392
M_r = 190.17	D_x = 1.555 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 785 reflections
a = 5.2501 (10) Å	θ = 2.4–28.0º
b = 16.805 (3) Å	μ = 0.12 mm^{-1}
c = 9.3290 (18) Å	T = 293 (2) K
β = 99.188 (3)º	Block, colorless
V = 812.5 (3) Å^3	0.45 × 0.14 × 0.13 mm
Z = 4	

Data collection

Bruker APX CCD diffractometer	1583 independent reflections
Radiation source: fine-focus sealed tube	1425 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.018
T = 293(2) K	θ_{max} = 26.0º
phi and ω scan	θ_{min} = 2.4º
Absorption correction: multi-scan SADABS (Sheldrick, 2000)	h = −6→6
T_{min} = 0.949, T_{max} = 0.985	k = −20→20
5991 measured reflections	l = −11→11

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.1634P]$ where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2)$ = 0.106	$(\Delta/\sigma)_{\max} < 0.001$
S = 1.07	$\Delta\rho_{\max}$ = 0.19 e Å^{-3}
1583 reflections	$\Delta\rho_{\min}$ = −0.24 e Å^{-3}
136 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.018 (3)
Secondary atom site location: difference Fourier map	

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	$U_{\rm iso}$*/$U_{\rm eq}$
O1	0.0644 (2)	0.36005 (6)	0.68049 (12)	0.0471 (3)
O2	0.3759 (2)	0.42002 (6)	0.58687 (13)	0.0496 (3)
H2B	0.410 (4)	0.3707 (14)	0.550 (2)	0.082 (7)*
C1	0.1794 (3)	0.42040 (8)	0.65768 (15)	0.0358 (3)
C2	0.1127 (3)	0.50146 (7)	0.70380 (15)	0.0349 (3)
C3	−0.0705 (3)	0.51184 (8)	0.79498 (16)	0.0403 (4)
H3A	−0.1499	0.4680	0.8296	0.048*
C4	−0.1332 (3)	0.58797 (9)	0.83368 (16)	0.0439 (4)
H4A	−0.2539	0.5950	0.8955	0.053*
C5	−0.0189 (3)	0.65372 (8)	0.78180 (16)	0.0392 (3)
H5A	−0.0640	0.7046	0.8081	0.047*
C6	0.1642 (3)	0.64386 (7)	0.68994 (14)	0.0338 (3)
C7	0.2301 (2)	0.56732 (8)	0.65297 (14)	0.0356 (3)
H7A	0.3544	0.5602	0.5934	0.043*
C8	0.2910 (3)	0.71171 (7)	0.63149 (14)	0.0338 (3)
N1	0.2597 (2)	0.78846 (7)	0.66034 (13)	0.0402 (3)
N2	0.4101 (3)	0.83282 (7)	0.58804 (14)	0.0453 (3)
N3	0.5310 (3)	0.78398 (7)	0.51637 (14)	0.0445 (3)
N4	0.4608 (2)	0.70804 (7)	0.54077 (13)	0.0394 (3)
H1A	0.147 (4)	0.8129 (12)	0.716 (2)	0.067 (5)*

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

O1	0.0573 (7)	0.0296 (5)	0.0618 (7)	−0.0056 (4)	0.0317 (5)	0.0017 (4)
O2	0.0616 (7)	0.0266 (5)	0.0718 (7)	−0.0021 (4)	0.0446 (6)	−0.0037 (5)
C1	0.0416 (7)	0.0290 (7)	0.0408 (7)	−0.0007 (5)	0.0188 (6)	0.0037 (5)
C2	0.0379 (7)	0.0299 (7)	0.0400 (7)	0.0007 (5)	0.0158 (6)	0.0010 (5)
C3	0.0448 (8)	0.0328 (7)	0.0485 (8)	−0.0023 (6)	0.0231 (6)	0.0013 (6)
C4	0.0468 (8)	0.0408 (8)	0.0510 (8)	0.0015 (6)	0.0285 (7)	−0.0021 (6)
C5	0.0434 (8)	0.0305 (7)	0.0474 (8)	0.0036 (5)	0.0188 (6)	−0.0048 (6)
C6	0.0374 (7)	0.0285 (7)	0.0380 (7)	−0.0004 (5)	0.0133 (5)	−0.0002 (5)
C7	0.0394 (7)	0.0311 (7)	0.0406 (7)	0.0002 (5)	0.0195 (6)	0.0003 (5)
C8	0.0383 (7)	0.0266 (6)	0.0388 (7)	0.0026 (5)	0.0131 (5)	−0.0021 (5)
N1	0.0498 (7)	0.0263 (6)	0.0496 (7)	0.0012 (5)	0.0238 (6)	−0.0017 (5)
N2	0.0564 (8)	0.0290 (6)	0.0559 (8)	−0.0022 (5)	0.0257 (6)	0.0001 (5)
N3	0.0537 (7)	0.0293 (6)	0.0562 (8)	−0.0026 (5)	0.0260 (6)	0.0005 (5)
N4	0.0470 (7)	0.0263 (6)	0.0504 (7)	−0.0010 (5)	0.0247 (5)	−0.0010 (5)

Geometric parameters (Å, °)

O1—C1	1.2163 (16)	C5—H5A	0.9300
O2—C1	1.3112 (16)	C6—C7	1.3898 (18)
O2—H2B	0.93 (2)	C6—C8	1.4684 (18)
C1—C2	1.4871 (18)	C7—H7A	0.9300
C2—C7	1.3868 (18)	C8—N4	1.3254 (17)
C2—C3	1.3927 (19)	C8—N1	1.3331 (17)
C3—C4	1.3833 (19)	N1—N2	1.3430 (16)
C3—H3A	0.9300	N1—H1A	0.94 (2)
C4—C5	1.381 (2)	N2—N3	1.2882 (17)
C4—H4A	0.9300	N3—N4	1.3576 (16)
C5—C6	1.3961 (18)		
C1—O2—H2B	114.1 (14)	C7—C6—C5	119.03 (12)
O1—C1—O2	122.47 (12)	C7—C6—C8	118.74 (11)
O1—C1—C2	124.52 (12)	C5—C6—C8	122.22 (12)
O2—C1—C2	113.01 (11)	C2—C7—C6	120.79 (12)
C7—C2—C3	119.79 (12)	C2—C7—H7A	119.6
C7—C2—C1	119.61 (11)	C6—C7—H7A	119.6
C3—C2—C1	120.59 (11)	N4—C8—N1	106.91 (11)
C4—C3—C2	119.44 (12)	N4—C8—C6	126.31 (11)
C4—C3—H3A	120.3	N1—C8—C6	126.77 (12)
C2—C3—H3A	120.3	C8—N1—N2	109.54 (11)
C5—C4—C3	120.91 (12)	C8—N1—H1A	129.9 (12)
C5—C4—H4A	119.5	N2—N1—H1A	120.5 (12)
C3—C4—H4A	119.5	N3—N2—N1	106.56 (11)
C4—C5—C6	120.02 (12)	N2—N3—N4	110.02 (11)
C4—C5—H5A	120.0	C8—N4—N3	106.96 (10)
C6—C5—H5A	120.0		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2B···N4^{i}	0.93 (2)	1.76 (2)	2.6664 (15)	164 (2)

N1—H1A···O1^{ii}	0.94 (2)	1.77 (2)	2.7118 (16)	179.1 (19)

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

Fig. 1

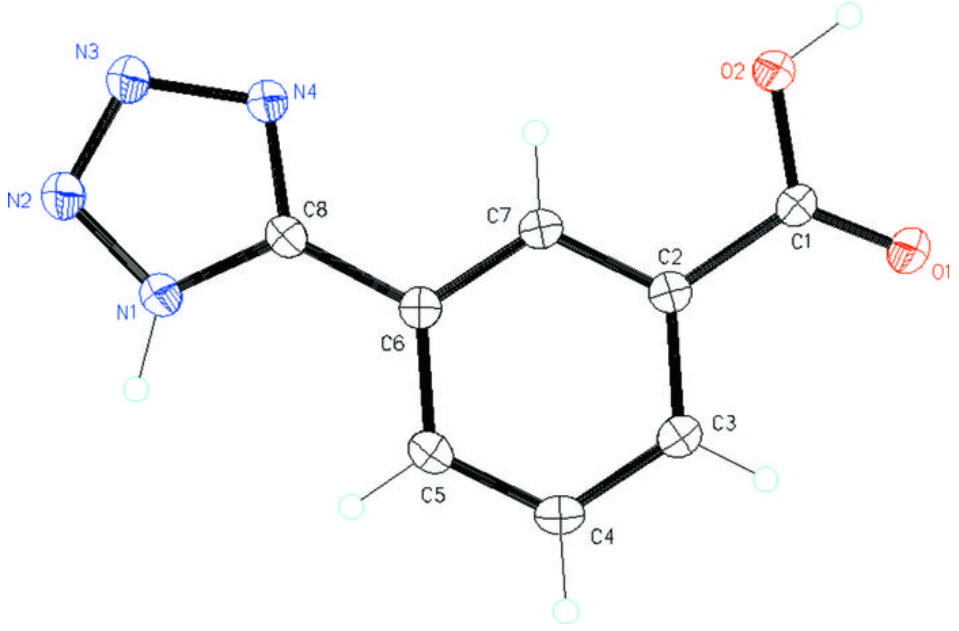

Fig. 2

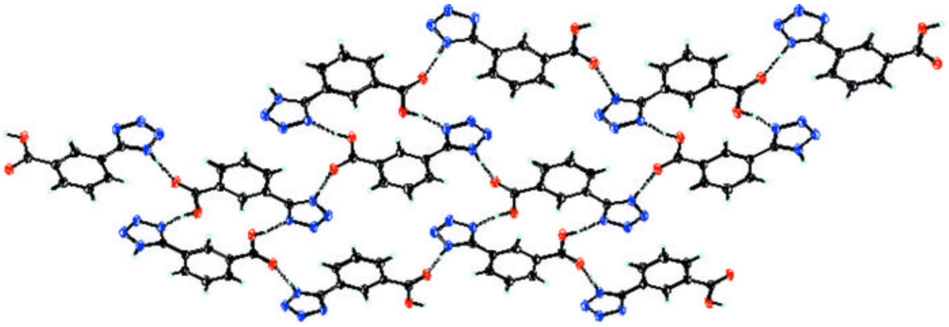

Fig. 3