Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Lin Cheng,[a]* Ya-Wen Zhang,[a] Jian-Quan Wang[a] and Gong Zhang[b]

[a]Department of Chemistry and Chemical Engineering, Southeast University, Nanjing, 211189, People's Republic of China, and [b]Department of Chemistry and Chemical Engineering, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing, 211189, People's Republic of China
Correspondence e-mail: cep02chl@yahoo.com.cn

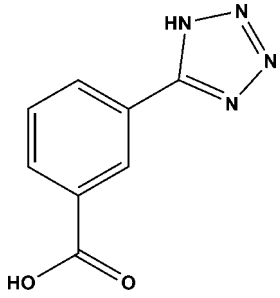
Received 8 December 2008; accepted 8 December 2008

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

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

Data collection

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

Refinement

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

The authors thank the Program for Young Excellent Talents in Southeast University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2829).

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supporting information

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

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

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S1. 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.

S2. 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.

S3. 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.

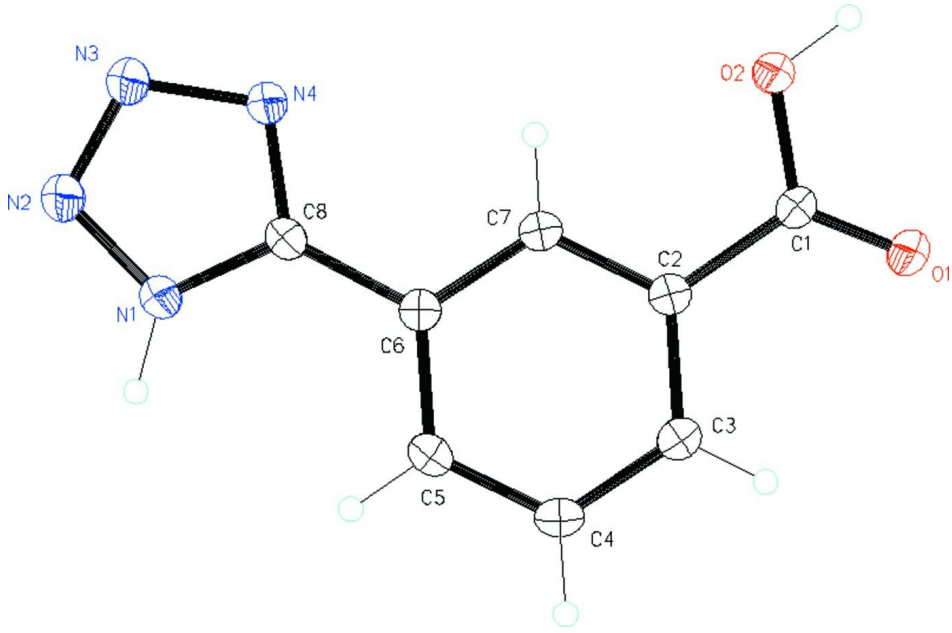

Figure 1

Structure of the title compound with 30% displacement ellipsoids.

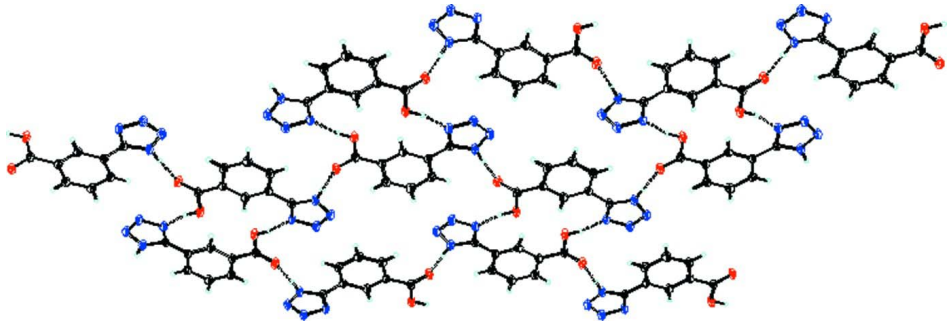

Figure 2

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

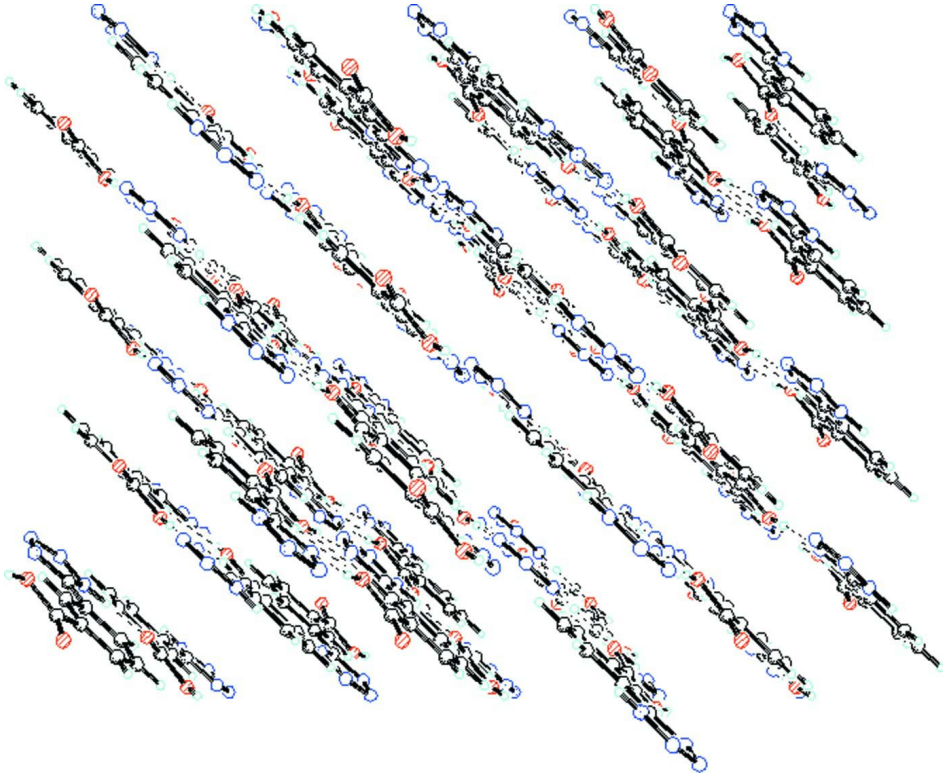

Figure 3

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

(I)

Crystal data

$C_8H_6N_4O_2$
$M_r = 190.17$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.2501\ (10)$ Å
$b = 16.805\ (3)$ Å
$c = 9.3290\ (18)$ Å
$\beta = 99.188\ (3)°$
$V = 812.5\ (3)$ Å^3
$Z = 4$

$F(000) = 392$
$D_x = 1.555$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 785 reflections
$\theta = 2.4–28.0°$
$\mu = 0.12$ mm^{-1}
$T = 293$ K
Block, colorless
0.45 × 0.14 × 0.13 mm

Data collection

Bruker APX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scan
Absorption correction: multi-scan *SADABS* (Sheldrick, 2000)
$T_{min} = 0.949$, $T_{max} = 0.985$

5991 measured reflections
1583 independent reflections
1425 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.4°$
$h = -6\rightarrow6$
$k = -20\rightarrow20$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.106$
$S = 1.07$
1583 reflections
136 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.1634P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.018 (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}
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 (Å²)

	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, º)

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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*B*···N4^{i}	0.93 (2)	1.76 (2)	2.6664 (15)	164 (2)
N1—H1*A*···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.