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1*H*-Benzotriazole–4-hydroxybenzoic acid (1/1)

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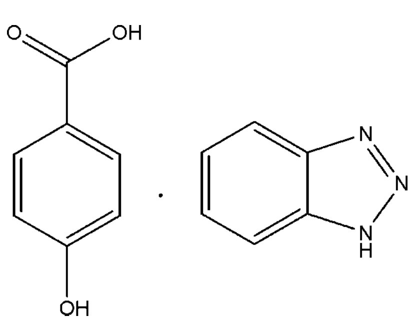
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.074; data-to-parameter ratio = 12.6.

The asymmetric unit of the title compound, $C_6H_5N_3\cdot C_7H_6O_3$, comprises independent benzotriazole and 4-hydroxybenzoic acid molecules. The dihedral angle between the benzene ring and the benzotriazole ring system is 15.18 (7)°. The mean plane of the carboxyl group is twisted at an angle of 18.55 (1)° with respect to the benzene ring. The crystal structure is stabilized by weak intermolecular N—H⋯N, O—H⋯N, O—H⋯O and C—H⋯O interactions, forming a three-dimensional network.

Related literature

For biological activities of benzotriazole derivates, see: Dubey *et al.* (2011); Gaikwad, *et al.* (2012). For reported structures, see: Sieroń (2007); Sudhahar *et al.*(2013); Yang *et al.* (2010).



Experimental

Crystal data

$C_6H_5N_3\cdot C_7H_6O_3$
M_r = 257.25
Orthorhombic, $Pna2_1$
a = 17.3634 (13) Å
b = 11.4669 (9) Å
c = 6.0818 (4) Å
V = 1210.91 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.976
6611 measured reflections
2195 independent reflections
1925 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.074
S = 1.04
2195 reflections
174 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯N2^{i}	0.86	2.20	2.982 (2)	152
O2—H2A⋯N3^{ii}	0.82	1.87	2.6817 (19)	169
O3—H3A⋯O1^{iii}	0.82	1.88	2.6912 (17)	171
C13—H13⋯O3^{iv}	0.93	2.49	3.373 (2)	159

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors thanks SAIF, IIT, Madras, for data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2200).

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supporting information

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1*H*-Benzotriazole–4-hydroxybenzoic acid (1/1)

A. Thirunavukkarasu, A. Silambarasan, G. Chakkaravarthi, R. Mohankumar and P. R. Umarani

S1. Comment

Benzotriazole derivates exhibit numerous essential bioactivitities, especially in antitubercular and antimicrobial (Dubey *et al.*, 2011; Gaikwad *et al.*, 2012) activities. We herewith report the crystal structure of the title compound (I) (Fig.1). The geometric parameters are comparable with reported structures (Sieroń , 2007; Sudhahar *et al.*, 2013; Yang *et al.*, 2010).

The benzene ring (C1-C6) is planar, with the maximum deviation of 0.010 (2) Å. The dihedral angle between the benzene ring and benzotriazole ring system is 15.18 (7)°. The mean plane of carboxyl group is twisted at an angle of 18.55 (1)° with the benzene ring. The crystal structure is stabilized by weak intermolecular N—H···N, O—H···N, O—H···O, C—H···O (Table 1 & Fig. 2) interactions to form a three dimensional network.

S2. Experimental

Benzotriazole ($C_6H_5N_3$, 1.1913 g) and p-hydroxy benzoic acid ($C_7H_6O_3$, 1.3812 g) were mixed in equimolar ratio in methanol and the prepared solution was allowed for slow evaporation at room temperature. Good quality crystals suitable for X-ray intensity data collection were collected in a period of 10 days.

S3. Refinement

H atoms were positioned geometrically and refined using riding model with C-H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for CH, N-H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for NH, O-H = 0.82 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for OH.

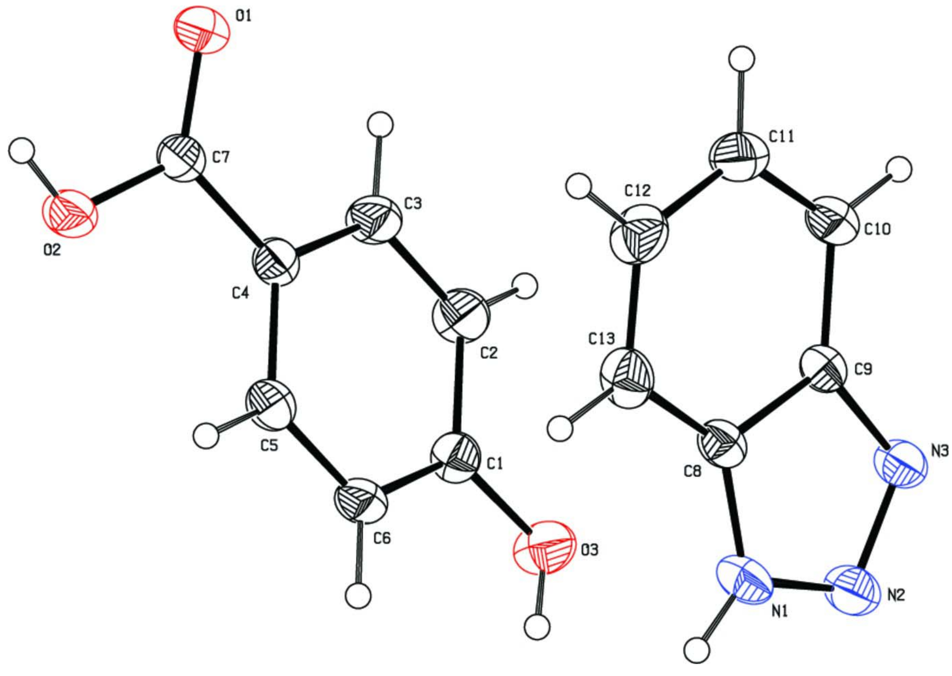

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

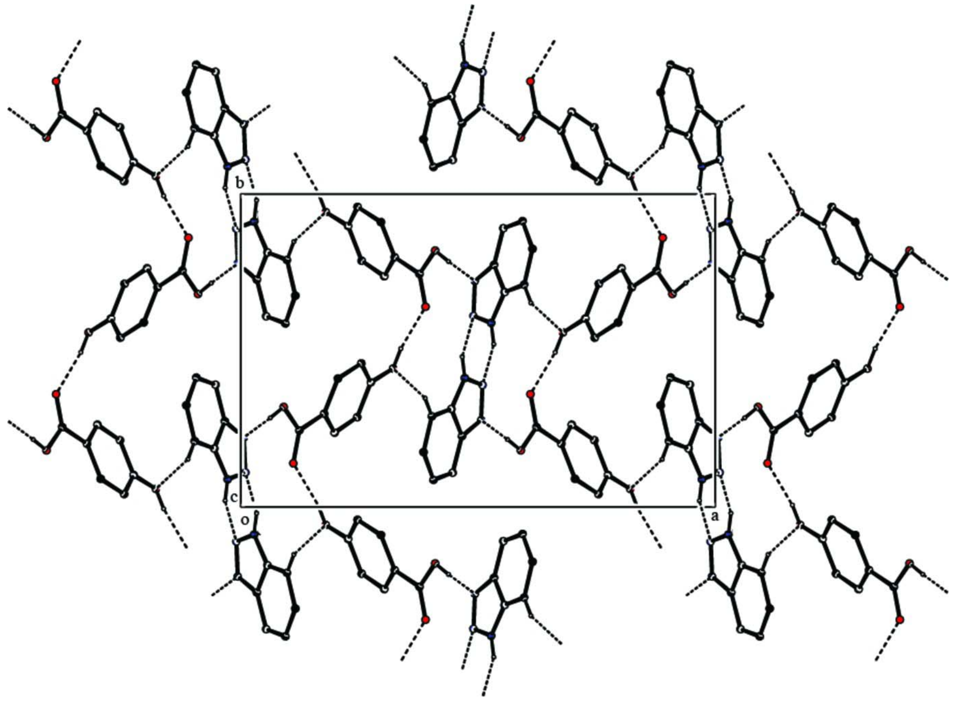

Figure 2

The packing of (I), viewed down *c* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

1*H*-Benzotriazole–4-hydroxybenzoic acid (1/1)

Crystal data

$C_6H_5N_3 \cdot C_7H_6O_3$
$M_r = 257.25$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 17.3634$ (13) Å
$b = 11.4669$ (9) Å
$c = 6.0818$ (4) Å
$V = 1210.91$ (15) Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.411$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2578 reflections
$\theta = 2.1–25.2°$
$\mu = 0.10$ mm^{-1}
$T = 295$ K
Block, colourless
0.30 × 0.26 × 0.24 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.970$, $T_{max} = 0.976$
6611 measured reflections
2195 independent reflections
1925 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 26.8°$, $\theta_{min} = 2.1°$
$h = -20 \rightarrow 22$
$k = -13 \rightarrow 14$
$l = -7 \rightarrow 4$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.074$
$S = 1.04$
2195 reflections
174 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
$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 0.0577P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.11$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.025 (2)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C7	0.37669 (8)	0.74471 (13)	0.7594 (3)	0.0363 (4)
C4	0.32444 (9)	0.79794 (14)	0.5984 (3)	0.0353 (4)
C3	0.30244 (10)	0.73727 (15)	0.4112 (3)	0.0457 (4)

H3	0.3204	0.6617	0.3895	0.055*
C2	0.25482 (10)	0.78675 (16)	0.2581 (3)	0.0492 (5)
H2	0.2416	0.7452	0.1323	0.059*
C1	0.22618 (9)	0.89793 (15)	0.2887 (3)	0.0385 (4)
C6	0.24605 (9)	0.95891 (15)	0.4762 (3)	0.0417 (4)
H6	0.2261	1.0331	0.4997	0.050*
C5	0.29535 (10)	0.91033 (14)	0.6286 (3)	0.0419 (4)
H5	0.3093	0.9528	0.7527	0.050*
N2	−0.00946 (8)	0.88952 (13)	0.2498 (3)	0.0477 (4)
C9	0.03383 (9)	0.72630 (14)	0.3824 (3)	0.0345 (4)
C8	0.05616 (10)	0.81341 (14)	0.5280 (3)	0.0366 (4)
C13	0.09730 (10)	0.78968 (17)	0.7199 (3)	0.0485 (5)
H13	0.1117	0.8480	0.8178	0.058*
C12	0.11490 (10)	0.67520 (17)	0.7544 (4)	0.0539 (5)
H12	0.1419	0.6551	0.8809	0.065*
C11	0.09398 (12)	0.58653 (16)	0.6071 (3)	0.0521 (5)
H11	0.1083	0.5101	0.6375	0.062*
C10	0.05347 (10)	0.60939 (14)	0.4216 (3)	0.0459 (4)
H10	0.0393	0.5504	0.3248	0.055*
N3	−0.00650 (8)	0.77773 (12)	0.2146 (2)	0.0418 (3)
N1	0.02792 (8)	0.91193 (12)	0.4377 (3)	0.0456 (4)
H1	0.0332	0.9803	0.4935	0.055*
O1	0.38942 (6)	0.63969 (10)	0.7712 (2)	0.0472 (3)
O2	0.40973 (7)	0.81933 (10)	0.8925 (2)	0.0504 (3)
H2A	0.4380	0.7843	0.9779	0.076*
O3	0.17907 (8)	0.94246 (11)	0.13231 (19)	0.0531 (4)
H3A	0.1627	1.0060	0.1729	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C7	0.0366 (8)	0.0325 (9)	0.0398 (9)	−0.0021 (6)	0.0031 (7)	−0.0020 (9)
C4	0.0346 (8)	0.0338 (8)	0.0376 (9)	−0.0022 (6)	0.0022 (7)	−0.0032 (7)
C3	0.0509 (10)	0.0377 (9)	0.0485 (11)	0.0083 (7)	−0.0051 (9)	−0.0119 (10)
C2	0.0575 (10)	0.0467 (10)	0.0434 (11)	0.0084 (8)	−0.0093 (10)	−0.0186 (9)
C1	0.0391 (8)	0.0405 (9)	0.0359 (9)	0.0005 (7)	−0.0001 (7)	−0.0029 (8)
C6	0.0480 (9)	0.0303 (8)	0.0468 (10)	0.0029 (7)	−0.0041 (8)	−0.0082 (7)
C5	0.0463 (9)	0.0375 (9)	0.0418 (10)	−0.0014 (7)	−0.0062 (8)	−0.0101 (8)
N2	0.0591 (9)	0.0351 (8)	0.0488 (9)	−0.0029 (6)	−0.0070 (8)	0.0017 (7)
C9	0.0379 (8)	0.0318 (8)	0.0336 (9)	−0.0030 (6)	−0.0001 (7)	−0.0033 (7)
C8	0.0397 (9)	0.0324 (9)	0.0376 (9)	−0.0030 (7)	0.0033 (7)	−0.0053 (7)
C13	0.0527 (10)	0.0538 (12)	0.0391 (10)	−0.0031 (8)	−0.0053 (8)	−0.0128 (10)
C12	0.0563 (11)	0.0610 (12)	0.0445 (11)	0.0052 (9)	−0.0124 (10)	0.0009 (11)
C11	0.0582 (11)	0.0405 (11)	0.0574 (12)	0.0063 (8)	−0.0091 (10)	0.0023 (10)
C10	0.0524 (10)	0.0326 (9)	0.0528 (12)	−0.0006 (7)	−0.0056 (10)	−0.0074 (9)
N3	0.0519 (8)	0.0330 (8)	0.0406 (8)	−0.0022 (6)	−0.0058 (7)	−0.0004 (7)
N1	0.0587 (9)	0.0295 (7)	0.0486 (9)	−0.0043 (6)	−0.0009 (8)	−0.0086 (7)
O1	0.0533 (7)	0.0323 (7)	0.0560 (8)	0.0004 (5)	−0.0065 (6)	−0.0008 (7)

O2	0.0630 (7)	0.0339 (7)	0.0542 (8)	0.0015 (5)	−0.0221 (7)	−0.0036 (6)
O3	0.0654 (8)	0.0509 (8)	0.0430 (7)	0.0145 (6)	−0.0147 (6)	−0.0089 (6)

Geometric parameters (Å, º)

C7—O1	1.2265 (18)	C9—N3	1.371 (2)
C7—O2	1.3102 (19)	C9—C8	1.390 (2)
C7—C4	1.468 (2)	C9—C10	1.404 (2)
C4—C3	1.388 (2)	C8—N1	1.348 (2)
C4—C5	1.396 (2)	C8—C13	1.395 (3)
C3—C2	1.369 (2)	C13—C12	1.364 (3)
C3—H3	0.9300	C13—H13	0.9300
C2—C1	1.381 (2)	C12—C11	1.403 (3)
C2—H2	0.9300	C12—H12	0.9300
C1—O3	1.3545 (19)	C11—C10	1.355 (3)
C1—C6	1.381 (2)	C11—H11	0.9300
C6—C5	1.380 (2)	C10—H10	0.9300
C6—H6	0.9300	N1—H1	0.8600
C5—H5	0.9300	O2—H2A	0.8200
N2—N3	1.3008 (19)	O3—H3A	0.8200
N2—N1	1.339 (2)		
O1—C7—O2	121.74 (15)	N3—C9—C10	131.39 (15)
O1—C7—C4	123.97 (15)	C8—C9—C10	120.69 (16)
O2—C7—C4	114.28 (13)	N1—C8—C9	103.95 (15)
C3—C4—C5	118.12 (15)	N1—C8—C13	133.65 (17)
C3—C4—C7	120.59 (15)	C9—C8—C13	122.39 (16)
C5—C4—C7	121.30 (15)	C12—C13—C8	115.53 (17)
C2—C3—C4	121.11 (16)	C12—C13—H13	122.2
C2—C3—H3	119.4	C8—C13—H13	122.2
C4—C3—H3	119.4	C13—C12—C11	122.75 (19)
C3—C2—C1	120.55 (16)	C13—C12—H12	118.6
C3—C2—H2	119.7	C11—C12—H12	118.6
C1—C2—H2	119.7	C10—C11—C12	121.73 (17)
O3—C1—C2	118.07 (15)	C10—C11—H11	119.1
O3—C1—C6	122.67 (15)	C12—C11—H11	119.1
C2—C1—C6	119.26 (16)	C11—C10—C9	116.89 (16)
C5—C6—C1	120.36 (15)	C11—C10—H10	121.6
C5—C6—H6	119.8	C9—C10—H10	121.6
C1—C6—H6	119.8	N2—N3—C9	108.75 (14)
C6—C5—C4	120.56 (15)	N2—N1—C8	111.29 (14)
C6—C5—H5	119.7	N2—N1—H1	124.4
C4—C5—H5	119.7	C8—N1—H1	124.4
N3—N2—N1	108.09 (14)	C7—O2—H2A	109.5
N3—C9—C8	107.91 (14)	C1—O3—H3A	109.5
O1—C7—C4—C3	−18.0 (2)	N3—C9—C8—C13	178.84 (16)
O2—C7—C4—C3	161.82 (15)	C10—C9—C8—C13	−1.3 (3)

O1—C7—C4—C5	161.86 (16)	N1—C8—C13—C12	179.32 (19)
O2—C7—C4—C5	−18.3 (2)	C9—C8—C13—C12	0.6 (3)
C5—C4—C3—C2	1.3 (3)	C8—C13—C12—C11	0.6 (3)
C7—C4—C3—C2	−178.86 (17)	C13—C12—C11—C10	−1.2 (3)
C4—C3—C2—C1	−1.3 (3)	C12—C11—C10—C9	0.5 (3)
C3—C2—C1—O3	−179.75 (16)	N3—C9—C10—C11	−179.47 (17)
C3—C2—C1—C6	−0.1 (3)	C8—C9—C10—C11	0.6 (2)
O3—C1—C6—C5	−178.87 (16)	N1—N2—N3—C9	−0.20 (18)
C2—C1—C6—C5	1.5 (3)	C8—C9—N3—N2	0.25 (18)
C1—C6—C5—C4	−1.5 (3)	C10—C9—N3—N2	−179.65 (18)
C3—C4—C5—C6	0.1 (2)	N3—N2—N1—C8	0.09 (19)
C7—C4—C5—C6	−179.74 (16)	C9—C8—N1—N2	0.06 (18)
N3—C9—C8—N1	−0.18 (17)	C13—C8—N1—N2	−178.79 (18)
C10—C9—C8—N1	179.72 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.86	2.20	2.982 (2)	152
O2—H2*A*···N3^{ii}	0.82	1.87	2.6817 (19)	169
O3—H3*A*···O1^{iii}	0.82	1.88	2.6912 (17)	171
C13—H13···O3^{iv}	0.93	2.49	3.373 (2)	159

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