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5-(1*H*-Tetrazol-5-yl)-1*H*-indole monohydrate

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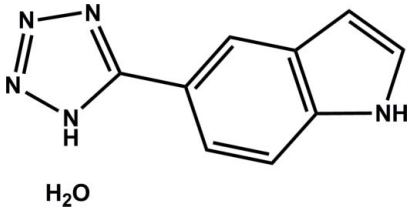
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.105; data-to-parameter ratio = 8.5.

In the title compound, $C_9H_7N_5\cdot H_2O$, the interplanar angles between the benzene and tetrazole rings and between the benzene and imidazole rings are 8.71 (3) and 1.32 (2)°, respectively. In the crystal, strong N—H···N hydrogen bonds link the organic 5-(1*H*-tetrazol-5-yl)-1*H*-indole molecules into chains extended along the *b* axis. The chains are further interconnected into layers parallel to (100) *via* strong O—H···N and N—H···O hydrogen bonds. Furthermore, the layers are interconnected *via* strong O—H···N hydrogen bonds. Moreover, cohesion between the layers is provided by the π–π interactions between the imidazole, tetrazole and benzene rings with centroid–centroid distances of 3.766 (2), 3.832 (2) and 3.733 (2) Å.

Related literature

For applications of tetrazole derivatives, see: Jin *et al.* (1994); Fu *et al.* (2009). For their use in the synthesis of metal-organic frameworks, see: Brewis *et al.* (2003). For related structures, see: Zhao *et al.* (2008); Fu *et al.* (2009). For the classification of hydrogen bonds, see: Desiraju & Steiner (1999).



Experimental

Crystal data

$C_9H_7N_5\cdot H_2O$
M_r = 203.21
Orthorhombic, $P2_12_12_1$
a = 6.8978 (14) Å
b = 9.953 (2) Å
c = 13.713 (3) Å
V = 941.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.89, T_{max} = 0.95
9741 measured reflections
1258 independent reflections
971 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.105
S = 1.06
1258 reflections
148 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N3^{i}	0.87 (3)	2.18 (3)	3.042 (3)	171 (3)
O1*W*—H1*WA*···N2^{ii}	0.80 (2)	2.08 (2)	2.869 (3)	173 (3)
O1*W*—H1*WB*···N4^{iii}	0.79 (2)	2.33 (2)	3.098 (3)	164 (3)
N5—H5···O1*W*	0.91 (3)	1.85 (3)	2.757 (3)	173 (3)

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

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2235).

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5-(1*H*-Tetrazol-5-yl)-1*H*-indole monohydrate

Xing-Wei Cai, Hong-Fei Lu and Zhen Zhou

S1. Comment

The tetrazole functional derivatives have found a wide range of applications in coordination chemistry as ligands (Fu *et al.*, 2009), in medicinal chemistry as metabolically stable surrogates for the carboxylic acid group (Fu *et al.*, 2009) and in materials science as highly energetical materials for production of tetrazole explosives (Jin *et al.*, 1994). For the varying ability of the tetrazoles to coordinate metal ions, a large number of novel metal-organic frameworks have been synthesized (Brewis *et al.*, 2003). As extension of these works, we report here the crystal structure of the title compound, 5-(1*H*-tetrazol-5-yl)-1*H*-indole hydrate.

The interplanar angles between the benzene and the tetrazole and the benzene and imidazole rings equal to 8.71 (3)° and 1.32 (2)°, respectively. The geometric parameters of the tetrazole ring are comparable to those in the related molecules (Zhao *et al.*, 2008; Fu *et al.*, 2009).

The molecular packing is stabilized by strong intermolecular N—H···O, N—H···N and O—H···N hydrogen bonds (the classification of the hydrogen bonds is according to Desiraju & Steiner, 1999). The H-bonds link the molecules into a three-dimensional network (Fig. 2 and Tab. 1). In a more detail, N1-H1···N3 connects the molecules into chains extended along the *b*-axis. These chains are interconnected by the hydrogen bonds O1W—H1WA···N2 and N5—H5···O1W, forming thus layers parallel to (1 0 0) - see Fig. 2 and Tab. 1. The hydrogen bond O1W—H1WB···N4 interconnects the layers.

The layers are also connected by the π-electron ring··· π-electron ring interactions. The centroid—centroid distances are *Cg*1—*Cg*2 (1 + *x*, *y*, *z*) = 3.766 (2) Å; *Cg*1—*Cg*2 (1/2 + *x*, 3/2 - *y*, 1 - *z*) = 3.832 (2)Å and *Cg*3—*Cg*3 (1/2 + *x*, 3/2 - *y* or -1/2 + *x*, 3/2 - *y*, 1 - *z*) = 3.733 (2) Å , where *Cg*1, *Cg*2 and *Cg*3 are the centroids referring to the imidazole, tetrazole and the benzene rings, respectively.

S2. Experimental

5-(1*H*-tetrazol-5-yl)-1*H*-indole was obtained commercially from Alfa Aesar. Colourless block-shaped crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol/water (2:1 *v*/*v*) solution.

S3. Refinement

All the H atoms were discernible in the difference electron density maps. All the H atoms attached to the C atoms were situated into the idealized positions and treated as riding with C–H = 0.93 Å with U_{iso}(H)=1.2U_{eq}(C). The positional parameters of the H atoms involved in the hydrogen bonds were refined either freely (N1, N5) or as restrained (Ow). The restraints regarded the distances between the water oxygens and the water hydrogens (0.82 (2)Å) while the H1WA—O1w—H1WB angle was set to 105(1.5)°. The constraints regarding the displacement parameters of the amine and water hydrogens: U_{iso}(H)=1.2U_{eq}(N); U_{iso}(H)=1.5U_{eq}(Ow). Since there has been no significant anomalous scatterer in the structure, 889 Friedel pairs have been merged.

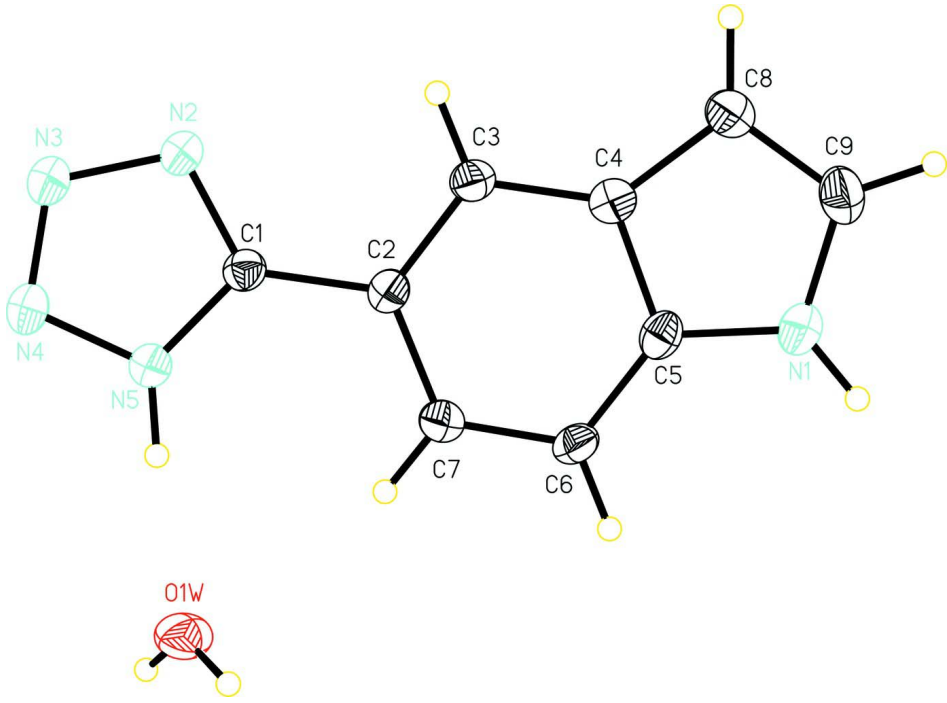

Figure 1

A view of the title molecules with the atomic numbering scheme. The displacement ellipsoids were drawn at the 30% probability level.

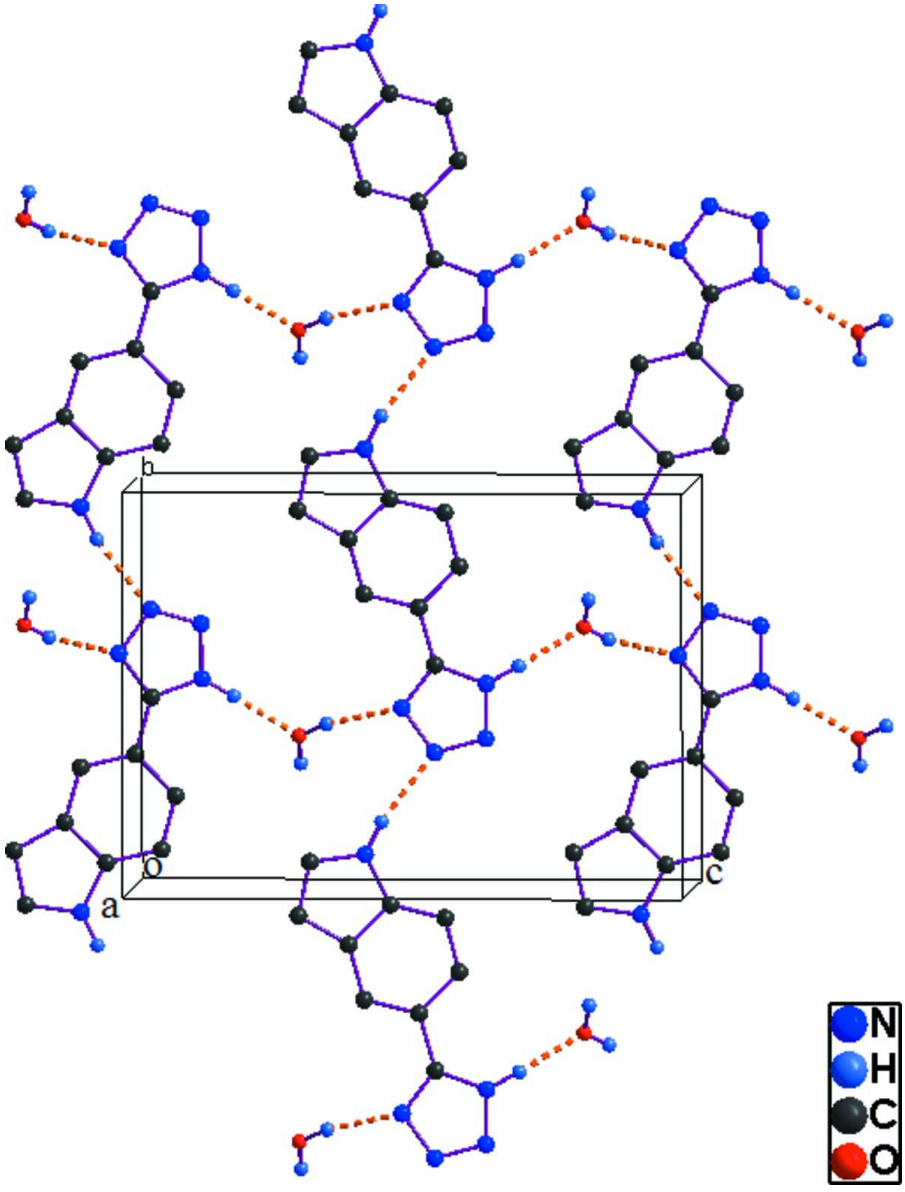

Figure 2

One layer with the atoms with the fractional coordinates of the constituting atoms $x < 0.5$. The H atoms not involved in the hydrogen bonding (dashed lines) have been omitted for clarity.

5-(1*H*-Tetrazol-5-yl)-1*H*-indole monohydrate

Crystal data

$C_9H_7N_5·H_2O$
$M_r = 203.21$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.8978$ (14) Å
$b = 9.953$ (2) Å
$c = 13.713$ (3) Å
$V = 941.4$ (3) Å^3
$Z = 4$
$F(000) = 424$
$D_x = 1.434$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1258 reflections
$\theta = 3.3$–$27.5°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.89, T_{max} = 0.95
9741 measured reflections
1258 independent reflections
971 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −8→8
k = −12→12
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.105
S = 1.06
1258 reflections
148 parameters
3 restraints
24 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 0.0295P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Special details

Experimental. The distance between the sample and the detector is 55 mm.

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}
N1	0.1423 (4)	1.0672 (2)	0.40317 (17)	0.0433 (6)
H1	0.144 (5)	1.145 (3)	0.433 (2)	0.052*
N5	0.1331 (4)	0.4891 (2)	0.61965 (15)	0.0371 (5)
H5	0.120 (4)	0.532 (3)	0.6781 (19)	0.045*
C2	0.1601 (4)	0.6777 (2)	0.49991 (17)	0.0296 (6)
C3	0.1565 (4)	0.7101 (2)	0.40154 (17)	0.0339 (6)
H3	0.1578	0.6428	0.3545	0.041*
C7	0.1607 (4)	0.7798 (3)	0.57174 (18)	0.0357 (6)
H7	0.1637	0.7561	0.6373	0.043*
N4	0.1313 (4)	0.3538 (2)	0.61809 (16)	0.0456 (6)
C5	0.1512 (4)	0.9450 (2)	0.44822 (18)	0.0339 (6)
N3	0.1556 (4)	0.3203 (2)	0.52735 (17)	0.0471 (6)
C8	0.1406 (5)	0.9156 (3)	0.28329 (19)	0.0441 (7)
H8	0.1375	0.8770	0.2215	0.053*

C1	0.1569 (4)	0.5364 (2)	0.52883 (18)	0.0308 (6)
C4	0.1510 (4)	0.8459 (2)	0.37392 (18)	0.0334 (6)
C6	0.1569 (4)	0.9126 (2)	0.54653 (18)	0.0362 (6)
H6	0.1582	0.9794	0.5940	0.043*
C9	0.1359 (5)	1.0484 (3)	0.3040 (2)	0.0471 (7)
H9	0.1294	1.1169	0.2579	0.056*
N2	0.1706 (4)	0.4307 (2)	0.47002 (16)	0.0421 (6)
O1W	0.1242 (4)	0.6288 (2)	0.79322 (13)	0.0541 (6)
H1WA	0.183 (4)	0.606 (3)	0.8404 (19)	0.081*
H1WB	0.045 (4)	0.683 (3)	0.806 (2)	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0523 (14)	0.0299 (11)	0.0477 (14)	−0.0015 (15)	0.0014 (13)	−0.0001 (10)
N5	0.0484 (14)	0.0301 (11)	0.0328 (12)	−0.0004 (11)	0.0015 (13)	−0.0005 (10)
C2	0.0271 (13)	0.0275 (12)	0.0344 (13)	−0.0007 (13)	0.0031 (13)	−0.0015 (9)
C3	0.0377 (14)	0.0327 (13)	0.0312 (13)	−0.0018 (14)	−0.0009 (13)	−0.0034 (11)
C7	0.0409 (15)	0.0368 (14)	0.0292 (12)	−0.0006 (15)	0.0005 (13)	−0.0012 (11)
N4	0.0628 (15)	0.0275 (12)	0.0466 (14)	0.0006 (13)	0.0021 (15)	0.0031 (10)
C5	0.0290 (12)	0.0279 (12)	0.0447 (15)	0.0000 (14)	0.0015 (12)	−0.0013 (11)
N3	0.0662 (16)	0.0301 (12)	0.0450 (14)	−0.0044 (14)	0.0075 (15)	−0.0014 (10)
C8	0.0552 (18)	0.0421 (17)	0.0349 (15)	−0.0046 (16)	−0.0009 (15)	0.0029 (12)
C1	0.0299 (13)	0.0295 (13)	0.0331 (13)	−0.0031 (13)	0.0006 (13)	−0.0035 (11)
C4	0.0289 (12)	0.0355 (14)	0.0359 (14)	−0.0013 (13)	0.0009 (14)	−0.0039 (11)
C6	0.0449 (15)	0.0298 (14)	0.0338 (14)	0.0019 (14)	−0.0015 (14)	−0.0079 (10)
C9	0.0540 (18)	0.0397 (15)	0.0475 (17)	0.0002 (18)	0.0029 (16)	0.0124 (13)
N2	0.0601 (16)	0.0291 (11)	0.0370 (12)	−0.0023 (13)	0.0048 (12)	−0.0025 (10)
O1W	0.0737 (17)	0.0559 (14)	0.0327 (10)	0.0169 (13)	−0.0053 (11)	−0.0024 (10)

Geometric parameters (Å, º)

N1—C5	1.366 (3)	N4—N3	1.299 (3)
N1—C9	1.373 (3)	C5—C6	1.387 (4)
N1—H1	0.87 (3)	C5—C4	1.418 (3)
N5—C1	1.341 (3)	N3—N2	1.354 (3)
N5—N4	1.347 (3)	C8—C9	1.353 (4)
N5—H5	0.91 (3)	C8—C4	1.425 (4)
C2—C3	1.387 (3)	C8—H8	0.9300
C2—C7	1.415 (3)	C1—N2	1.329 (3)
C2—C1	1.462 (3)	C6—H6	0.9300
C3—C4	1.403 (3)	C9—H9	0.9300
C3—H3	0.9300	O1W—H1WA	0.797 (17)
C7—C6	1.367 (3)	O1W—H1WB	0.792 (17)
C7—H7	0.9300		
C5—N1—C9	109.1 (2)	N4—N3—N2	111.0 (2)
C5—N1—H1	125.4 (19)	C9—C8—C4	107.1 (2)

C9—N1—H1	125.5 (19)	C9—C8—H8	126.5
C1—N5—N4	109.7 (2)	C4—C8—H8	126.5
C1—N5—H5	131.5 (18)	N2—C1—N5	107.1 (2)
N4—N5—H5	118.9 (18)	N2—C1—C2	126.6 (2)
C3—C2—C7	120.7 (2)	N5—C1—C2	126.2 (2)
C3—C2—C1	119.2 (2)	C3—C4—C5	118.4 (2)
C7—C2—C1	120.1 (2)	C3—C4—C8	134.8 (2)
C2—C3—C4	119.1 (2)	C5—C4—C8	106.7 (2)
C2—C3—H3	120.4	C7—C6—C5	118.1 (2)
C4—C3—H3	120.4	C7—C6—H6	120.9
C6—C7—C2	121.2 (2)	C5—C6—H6	120.9
C6—C7—H7	119.4	C8—C9—N1	109.9 (2)
C2—C7—H7	119.4	C8—C9—H9	125.1
N3—N4—N5	105.7 (2)	N1—C9—H9	125.1
N1—C5—C6	130.4 (2)	C1—N2—N3	106.5 (2)
N1—C5—C4	107.1 (2)	H1WA—O1W—H1WB	111 (2)
C6—C5—C4	122.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.87 (3)	2.18 (3)	3.042 (3)	171 (3)
O1*W*—H1*WA*···N2^{ii}	0.80 (2)	2.08 (2)	2.869 (3)	173 (3)
O1*W*—H1*WB*···N4^{iii}	0.79 (2)	2.33 (2)	3.098 (3)	164 (3)
N5—H5···O1*W*	0.91 (3)	1.85 (3)	2.757 (3)	173 (3)

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