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5-[4-(1*H*-Imidazol-1-yl)phenyl]-2*H*-tetrazole dihydrate

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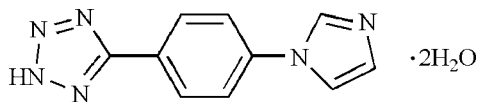
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.075; wR factor = 0.243; data-to-parameter ratio = 11.9.

In the title compound, $\text{C}_{10}\text{H}_8\text{N}_6 \cdot 2\text{H}_2\text{O}$, the central aromatic ring makes dihedral angles of 23.59 (15) and 16.99 (16)° with the terminal imidazole and tetrazole rings, respectively, which are themselves almost coplanar [dihedral angle = 6.61 (18)°]. Two H atoms of the two water molecules are half occupied. In the crystal packing, weak intermolecular $\text{O}-\text{H} \cdots \text{N}$, $\text{O}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{N}$ hydrogen bonds and $\pi-\pi$ stacking interactions [centroid-centroid distances of 3.73 (4) Å between benzene rings and 3.66 (3) Å between imidazole and tetrazole rings] are observed.

Related literature

For the biological activity of imidazole derivatives, see: Reichardt *et al.* (1992)



Experimental

Crystal data

$\text{C}_{10}\text{H}_8\text{N}_6 \cdot 2\text{H}_2\text{O}$
 $M_r = 248.26$
 Triclinic, $P\bar{1}$
 $a = 7.4300$ (7) Å
 $b = 8.2285$ (9) Å

$c = 10.2047$ (11) Å
 $\alpha = 97.011$ (1)°
 $\beta = 90.813$ (1)°
 $\gamma = 113.449$ (2)°
 $V = 566.74$ (10) Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹

$T = 298$ K
 $0.38 \times 0.17 \times 0.16$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2004)
 $T_{\min} = 0.960$, $T_{\max} = 0.983$

2913 measured reflections
 1953 independent reflections
 1199 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.075$
 $wR(F^2) = 0.243$
 $S = 1.05$
 1953 reflections

164 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.40$ e Å⁻³
 $\Delta\rho_{\min} = -0.51$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O2}-\text{H2D} \cdots \text{N2}^{\text{i}}$	0.85	2.50	3.235 (7)	146
$\text{O2}-\text{H2D} \cdots \text{N3}^{\text{i}}$	0.85	1.98	2.823 (7)	172
$\text{O2}-\text{H2C} \cdots \text{O1}^{\text{ii}}$	0.85	2.15	2.994 (9)	170
$\text{O2}-\text{H2A} \cdots \text{O1}$	0.85	1.92	2.629 (9)	141
$\text{O1}-\text{H1D} \cdots \text{O2}^{\text{ii}}$	0.85	2.55	2.994 (9)	114
$\text{O1}-\text{H1D} \cdots \text{O2}$	0.85	1.78	2.629 (9)	175
$\text{O1}-\text{H1C} \cdots \text{O1}^{\text{iii}}$	0.85	1.96	2.806 (11)	175
$\text{O1}-\text{H1A} \cdots \text{N1}$	0.85	1.99	2.790 (5)	157
$\text{N2}-\text{H2} \cdots \text{N6}^{\text{iv}}$	0.86	1.90	2.758 (5)	174

Symmetry codes: (i) $x, y + 1, z$; (ii) $-x, -y + 1, -z$; (iii) $-x + 1, -y + 1, -z$; (iv) $x, y - 1, z - 1$.

Data collection: SMART (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: 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: JH2291).

References

- Bruker (2004). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
 Reichardt, B. A., Belyavtseva, L. M. & Kulikova, O. G. (1992). *Bull. Exp. Biol. Med.* **113**, 506–508.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

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5-[4-(1*H*-Imidazol-1-yl)phenyl]-2*H*-tetrazole dihydrate

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S1. Comment

Imidazole derivatives possessing the biologically important imidazole ring, have been studied in terms of their biological activities (Reichardt *et al.*, 1992). Inspired by this, we focus on the studies of imidazole derivatives. Recently, we have obtained a new crystal structure of imidazole derivative (1-tetrazole-4-imidazole-benzene), which is crystallized by the slow evaporation of ethonal solvent at room temperature.

As shown in Fig. 1, the title molecule crystallizes as a neutral, with two terminal imidazole and tetrazole rings almost coplanar with the dihedral angle of 6.61 (18)°. They make dihedral angles of 23.59 (15)° and 16.99 (16)° with the central aromatic ring. It is noted that there are two types of π - π stacking interactions: one occurs between parallel benzene rings with centroid-centroid distances of 3.73 (4) Å; the other occurs between the imidazole and tetrazole rings with centroid-centroid distances of 3.66 (3) Å. Thus, a wide range of hydrogen bonds (O—H \cdots N, O—H \cdots O and N—H \cdots N) and π - π stacking interactions contribute to the formation of the supramolecular network.

S2. Experimental

1-tetrazole-4-imidazole-benzene (0.1 g, 0.4 mmol) was dissolved in ethonal (20 ml) and the solution was left to evaporate slowly at room temperature. After a week, colourless crystals suitable for X-ray analysis were obtained.

S3. Refinement

Carboxyl H atoms were located in a difference map but were refined as riding on the parent O atoms with O—H = 0.82 Å and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$. Carbon and nitrogen bound H atoms were placed at calculated positions and were treated as riding on the parent C or N atoms with C—H = 0.96 (methyl), 0.97 (methylene) and N—H = 0.86 Å, $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C}, \text{N})$. H atoms of the water molecule were located in a difference Fourier map and refined as riding with an O—H distance restraint of 0.84 (1) Å, with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}$. Two hydrogen atoms from two water molecules are half occupied and split into two atoms, respectively.

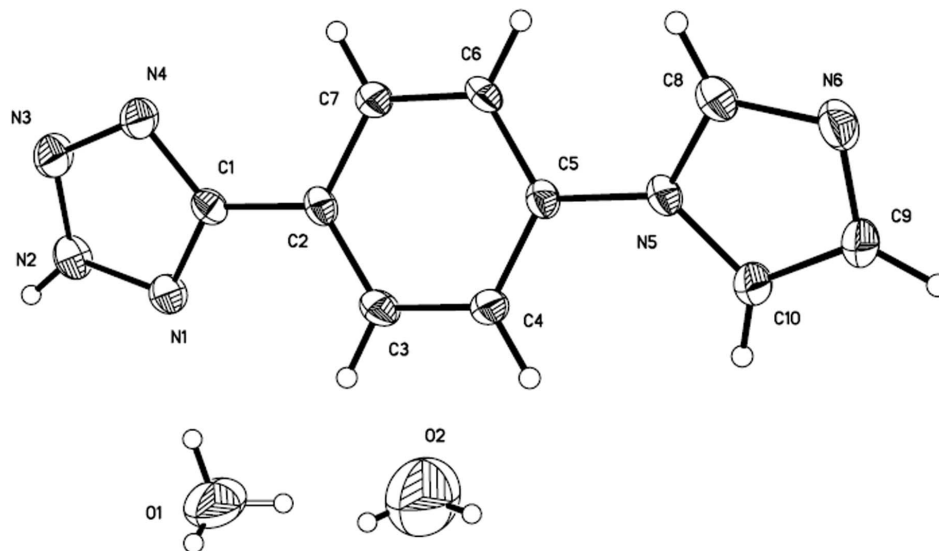


Figure 1

The structure of the title compound, showing the atomic numbering scheme with 30% probability displacement ellipsoids

5-[4-(1*H*-Imidazol-1-yl)phenyl]-2*H*-tetrazole dihydrate

Crystal data

$C_{10}H_8N_6 \cdot 2H_2O$

$M_r = 248.26$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.4300$ (7) Å

$b = 8.2285$ (9) Å

$c = 10.2047$ (11) Å

$\alpha = 97.011$ (1)°

$\beta = 90.813$ (1)°

$\gamma = 113.449$ (2)°

$V = 566.74$ (10) Å³

$Z = 2$

$F(000) = 260$

$D_x = 1.455$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1702 reflections

$\theta = 2.5$ – 25.9 °

$\mu = 0.11$ mm⁻¹

$T = 298$ K

Block, colorless

$0.38 \times 0.17 \times 0.16$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2004)

$T_{\min} = 0.960$, $T_{\max} = 0.983$

2913 measured reflections

1953 independent reflections

1199 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 3.2$ °

$h = -8 \rightarrow 8$

$k = -9 \rightarrow 9$

$l = -11 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.075$

$wR(F^2) = 0.243$

$S = 1.05$

1953 reflections

164 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-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.1194P)^2 + 0.5477P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.40 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.13 (2)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
N1	0.2591 (5)	0.1994 (4)	0.1928 (3)	0.0420 (9)	
N2	0.2495 (6)	0.0363 (4)	0.1481 (3)	0.0483 (10)	
H2	0.2561	-0.0008	0.0665	0.058*	
N3	0.2288 (6)	-0.0589 (5)	0.2440 (3)	0.0499 (10)	
N4	0.2239 (6)	0.0414 (4)	0.3577 (3)	0.0457 (10)	
N5	0.2568 (4)	0.7806 (4)	0.6934 (3)	0.0329 (8)	
N6	0.2612 (5)	0.9372 (4)	0.8813 (3)	0.0447 (10)	
O1	0.2945 (8)	0.4108 (6)	-0.0073 (4)	0.1116 (18)	
H1A	0.2650	0.3229	0.0363	0.134*	
H1C	0.4182	0.4705	-0.0013	0.134*	0.50
H1D	0.2401	0.4795	0.0231	0.134*	0.50
O2	0.1048 (12)	0.6070 (9)	0.0820 (6)	0.183 (3)	
H2A	0.2078	0.5941	0.0576	0.220*	0.50
H2C	-0.0111	0.5894	0.0548	0.220*	0.50
H2D	0.1533	0.7067	0.1322	0.220*	
C1	0.2426 (5)	0.1985 (5)	0.3235 (3)	0.0320 (9)	
C2	0.2436 (5)	0.3498 (5)	0.4159 (3)	0.0304 (9)	
C3	0.3121 (6)	0.5229 (5)	0.3835 (3)	0.0377 (10)	
H3	0.3556	0.5438	0.2997	0.045*	
C4	0.3163 (6)	0.6638 (5)	0.4737 (4)	0.0367 (10)	
H4A	0.3632	0.7788	0.4508	0.044*	
C5	0.2507 (5)	0.6338 (5)	0.5985 (3)	0.0296 (9)	
C6	0.1766 (6)	0.4619 (5)	0.6316 (3)	0.0372 (10)	
H6	0.1290	0.4413	0.7144	0.045*	
C7	0.1736 (6)	0.3217 (5)	0.5418 (3)	0.0374 (10)	
H7	0.1245	0.2067	0.5648	0.045*	
C8	0.2597 (6)	0.7830 (6)	0.8248 (4)	0.0416 (11)	
H8	0.2604	0.6911	0.8692	0.050*	
C9	0.2610 (6)	1.0379 (5)	0.7849 (4)	0.0436 (11)	
H9	0.2632	1.1526	0.7977	0.052*	

C10	0.2571 (6)	0.9415 (5)	0.6680 (4)	0.0424 (11)
H10	0.2550	0.9768	0.5850	0.051*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.059 (2)	0.0374 (19)	0.0299 (17)	0.0204 (17)	0.0075 (15)	-0.0007 (14)
N2	0.075 (3)	0.044 (2)	0.0252 (17)	0.027 (2)	0.0086 (16)	-0.0097 (15)
N3	0.077 (3)	0.043 (2)	0.0345 (18)	0.032 (2)	0.0062 (17)	-0.0028 (16)
N4	0.070 (3)	0.0366 (19)	0.0340 (18)	0.0267 (18)	0.0090 (16)	0.0007 (15)
N5	0.0396 (19)	0.0335 (18)	0.0248 (16)	0.0156 (15)	0.0047 (13)	-0.0015 (13)
N6	0.053 (2)	0.045 (2)	0.0346 (18)	0.0218 (18)	0.0061 (15)	-0.0048 (16)
O1	0.194 (5)	0.088 (3)	0.069 (3)	0.067 (3)	0.034 (3)	0.033 (2)
O2	0.248 (9)	0.142 (6)	0.156 (6)	0.078 (6)	0.023 (6)	0.004 (5)
C1	0.035 (2)	0.036 (2)	0.0244 (18)	0.0141 (17)	0.0037 (15)	0.0017 (16)
C2	0.032 (2)	0.036 (2)	0.0239 (18)	0.0159 (17)	0.0013 (14)	-0.0017 (15)
C3	0.049 (3)	0.041 (2)	0.0230 (18)	0.0178 (19)	0.0084 (16)	0.0051 (16)
C4	0.050 (3)	0.028 (2)	0.031 (2)	0.0137 (18)	0.0091 (17)	0.0055 (16)
C5	0.033 (2)	0.031 (2)	0.0250 (18)	0.0151 (17)	0.0019 (14)	-0.0005 (15)
C6	0.050 (3)	0.039 (2)	0.0242 (18)	0.019 (2)	0.0149 (16)	0.0045 (16)
C7	0.052 (3)	0.032 (2)	0.0300 (19)	0.0187 (19)	0.0100 (17)	0.0056 (16)
C8	0.054 (3)	0.043 (2)	0.0271 (19)	0.020 (2)	0.0049 (17)	-0.0005 (17)
C9	0.057 (3)	0.036 (2)	0.040 (2)	0.023 (2)	0.0051 (19)	-0.0023 (18)
C10	0.061 (3)	0.036 (2)	0.033 (2)	0.023 (2)	0.0077 (18)	0.0022 (17)

Geometric parameters (Å, °)

N1—N2	1.337 (5)	O2—H2D	0.8501
N1—C1	1.341 (5)	C1—C2	1.465 (5)
N2—N3	1.300 (5)	C2—C3	1.393 (5)
N2—H2	0.8600	C2—C7	1.403 (5)
N3—N4	1.350 (5)	C3—C4	1.379 (5)
N4—C1	1.335 (5)	C3—H3	0.9300
N5—C8	1.338 (5)	C4—C5	1.386 (5)
N5—C10	1.379 (5)	C4—H4A	0.9300
N5—C5	1.438 (5)	C5—C6	1.385 (5)
N6—C8	1.324 (5)	C6—C7	1.375 (5)
N6—C9	1.362 (5)	C6—H6	0.9300
O1—H1A	0.8500	C7—H7	0.9300
O1—H1C	0.8500	C8—H8	0.9300
O1—H1D	0.8499	C9—C10	1.343 (5)
O2—H2A	0.8500	C9—H9	0.9300
O2—H2C	0.8500	C10—H10	0.9300
N2—N1—C1	104.1 (3)	C4—C3—H3	119.5
N3—N2—N1	111.2 (3)	C2—C3—H3	119.5
N3—N2—H2	124.4	C3—C4—C5	119.9 (3)
N1—N2—H2	124.4	C3—C4—H4A	120.1

N2—N3—N4	108.3 (3)	C5—C4—H4A	120.1
C1—N4—N3	105.4 (3)	C6—C5—C4	120.0 (3)
C8—N5—C10	107.3 (3)	C6—C5—N5	119.9 (3)
C8—N5—C5	125.3 (3)	C4—C5—N5	120.1 (3)
C10—N5—C5	127.4 (3)	C7—C6—C5	120.0 (3)
C8—N6—C9	108.6 (3)	C7—C6—H6	120.0
H1A—O1—H1C	110.2	C5—C6—H6	120.0
H1A—O1—H1D	110.2	C6—C7—C2	120.9 (4)
H1C—O1—H1D	108.5	C6—C7—H7	119.6
H2A—O2—H2C	142.7	C2—C7—H7	119.6
H2A—O2—H2D	101.7	N6—C8—N5	109.1 (3)
H2C—O2—H2D	108.1	N6—C8—H8	125.5
N4—C1—N1	111.1 (3)	N5—C8—H8	125.5
N4—C1—C2	124.6 (3)	C10—C9—N6	107.5 (4)
N1—C1—C2	124.3 (3)	C10—C9—H9	126.2
C3—C2—C7	118.1 (3)	N6—C9—H9	126.2
C3—C2—C1	122.3 (3)	C9—C10—N5	107.5 (3)
C7—C2—C1	119.6 (3)	C9—C10—H10	126.2
C4—C3—C2	121.0 (3)	N5—C10—H10	126.2
C1—N1—N2—N3	-0.1 (5)	C8—N5—C5—C6	23.6 (6)
N1—N2—N3—N4	0.1 (5)	C10—N5—C5—C6	-155.1 (4)
N2—N3—N4—C1	0.0 (5)	C8—N5—C5—C4	-157.2 (4)
N3—N4—C1—N1	-0.1 (5)	C10—N5—C5—C4	24.1 (6)
N3—N4—C1—C2	179.5 (4)	C4—C5—C6—C7	1.9 (6)
N2—N1—C1—N4	0.1 (4)	N5—C5—C6—C7	-178.9 (3)
N2—N1—C1—C2	-179.5 (3)	C5—C6—C7—C2	-0.4 (6)
N4—C1—C2—C3	163.4 (4)	C3—C2—C7—C6	-1.4 (6)
N1—C1—C2—C3	-17.1 (6)	C1—C2—C7—C6	178.6 (4)
N4—C1—C2—C7	-16.6 (6)	C9—N6—C8—N5	-0.5 (5)
N1—C1—C2—C7	162.9 (4)	C10—N5—C8—N6	0.2 (5)
C7—C2—C3—C4	1.8 (6)	C5—N5—C8—N6	-178.7 (3)
C1—C2—C3—C4	-178.2 (3)	C8—N6—C9—C10	0.7 (5)
C2—C3—C4—C5	-0.4 (6)	N6—C9—C10—N5	-0.6 (5)
C3—C4—C5—C6	-1.5 (6)	C8—N5—C10—C9	0.3 (5)
C3—C4—C5—N5	179.3 (3)	C5—N5—C10—C9	179.1 (4)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2D \cdots N2 ⁱ	0.85	2.50	3.235 (7)	146
O2—H2D \cdots N3 ⁱ	0.85	1.98	2.823 (7)	172
O2—H2C \cdots O1 ⁱⁱ	0.85	2.15	2.994 (9)	170
O2—H2A \cdots O1	0.85	1.92	2.629 (9)	141
O1—H1D \cdots O2 ⁱⁱ	0.85	2.55	2.994 (9)	114
O1—H1D \cdots O2	0.85	1.78	2.629 (9)	175
O1—H1C \cdots O1 ⁱⁱⁱ	0.85	1.96	2.806 (11)	175

O1—H1A···N1	0.85	1.99	2.790 (5)	157
N2—H2···N6 ^{iv}	0.86	1.90	2.758 (5)	174

Symmetry codes: (i) $x, y+1, z$; (ii) $-x, -y+1, -z$; (iii) $-x+1, -y+1, -z$; (iv) $x, y-1, z-1$.