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1,4-Bis(1*H*-1,2,4-triazol-1-yl)benzene

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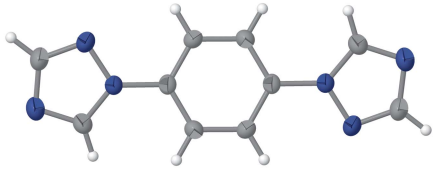
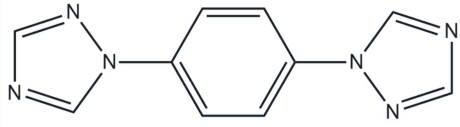
Structural data: full structural data are available from iucrdata.iucr.org

The complete molecule of the title compound, $C_{10}H_8N_6$, is generated by crystallographic inversion symmetry; the dihedral angle between the planes of the benzene and triazole rings is 16.7 (2)°. In the crystal, inversion dimers linked by pairs of weak C—H···N hydrogen bonds generate $R_2^2(6)$ loops. Weak aromatic π–π stacking interactions [centroid–centroid separation = 3.809 (1) Å] are also observed.

3D view



Chemical scheme



Structure description

Derivatives of 1,2,4-triazole exhibit a wide range of bioactivities, including anticancer activity, antitubercular activity and kinase inhibition (Kaur *et al.*, 2016; Keri *et al.*, 2015). Their copper complexes can inhibit the activity of protein tyrosine phosphatase (Lu & Zhu, 2014). Thus, we reacted 2,5-bis(1*H*-1,2,4-triazol-1-yl)terephthalic acid with $CuCl_2$ under hydrothermal conditions in an attempt to form a complex, but instead crystals of the title compound, (I), were obtained.

The molecular structure of (I) is illustrated in Fig. 1. The asymmetric unit consists of half a molecule; the complete molecule is generated by an inversion operation. The planes of the benzene and triazole rings are inclined at an angle of 16.7 (2)°. In the crystal, molecules are connected through weak C—H···N hydrogen bonds (Table 1) and π–π interactions [centroid–centroid separation = 3.809 (1) Å], leading to the formation of a supramolecular network (Fig. 2).

Synthesis and crystallization

A mixture containing $CuCl_2{\cdot}4H_2O$ (0.10 mmol, 17 mg), 2,5-bis(1*H*-1,2,4-triazol-1-yl)terephthalic acid (0.05 mmol, 15 mg), 1,10-phenanthroline (0.05 mmol, 8.5 mg), dimethylformamide (1.0 ml) and H_2O (6.0 ml) was stirred for 30 min at room temperature. The reaction mixture was sealed in a Teflon-lined stainless steel vessel and then heated to

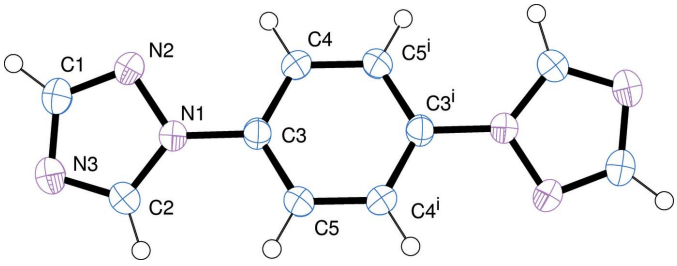


Figure 1
The molecular structure of the title compound, with displacement ellipsoids for non-H atoms drawn at the 50% probability level. [Symmetry code: (i) $2-x, 1-y, -z$.]

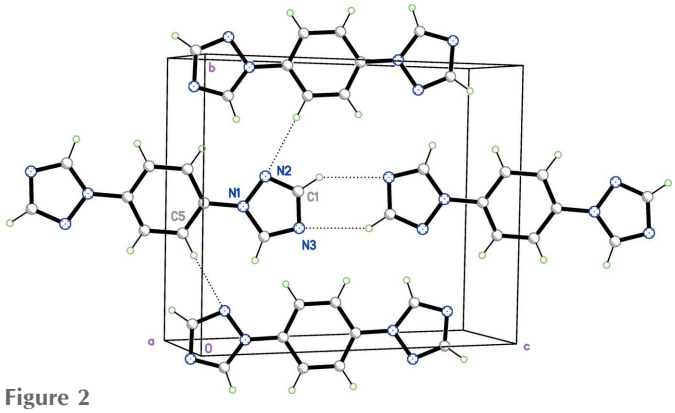


Figure 2
The C—H···N hydrogen-bonded (dotted lines) network of (I).

433 K for 3 d and then allowed to cool gradually to room temperature. Colourless blocks of the title compound were collected by filtration and washed with water.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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References

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···N3^{i}	0.93	2.55	3.3563 (19)	146
C5—H5···N2^{ii}	0.93	2.71	3.6184 (18)	165

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_8N_6$
M_r	212.22
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, b, c (Å)	3.8091 (3), 10.2616 (9), 11.9768 (11)
β (°)	96.165 (3)
V (Å^3)	465.44 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.20 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.669, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4210, 1057, 875
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.114, 1.03
No. of reflections	1057
No. of parameters	73
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.17

Computer programs: *APEX2* and *SAINT* (Bruker, 2000), *SHELXS97* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2016* (Sheldrick, 2015).

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full crystallographic data

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1,4-Bis(1*H*-1,2,4-triazol-1-yl)benzene

Crystal data

$C_{10}H_8N_6$
M_r = 212.22
Monoclinic, $P2_1/c$
a = 3.8091 (3) Å
b = 10.2616 (9) Å
c = 11.9768 (11) Å
β = 96.165 (3)°
V = 465.44 (7) Å^3
Z = 2
$F(000)$ = 220
D_x = 1.514 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2111 reflections
θ = 3.4–27.5°
μ = 0.10 mm^{-1}
T = 298 K
Block, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.669, T_{max} = 0.746
4210 measured reflections
1057 independent reflections
875 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −3→4
k = −13→13
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.114
S = 1.03
1057 reflections
73 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.1337P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.8017 (3)	0.48118 (10)	0.21842 (9)	0.0307 (3)
N2	0.7691 (4)	0.58859 (12)	0.28330 (10)	0.0451 (4)
N3	0.6288 (4)	0.40718 (13)	0.37506 (11)	0.0459 (4)
C1	0.6654 (5)	0.53760 (15)	0.37491 (13)	0.0467 (4)
H1	0.620016	0.588563	0.435947	0.056*
C2	0.7160 (4)	0.37557 (14)	0.27543 (12)	0.0417 (4)
H2	0.718064	0.290825	0.247992	0.050*
C3	0.9038 (3)	0.49129 (12)	0.10767 (11)	0.0282 (3)
C4	0.8869 (4)	0.61044 (13)	0.05306 (11)	0.0331 (3)
H4	0.811019	0.684228	0.088642	0.040*
C5	1.0163 (4)	0.38103 (13)	0.05481 (11)	0.0341 (4)
H5	1.026722	0.301276	0.091893	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0397 (7)	0.0278 (6)	0.0257 (6)	−0.0006 (5)	0.0082 (5)	−0.0003 (4)
N2	0.0729 (9)	0.0319 (7)	0.0343 (7)	−0.0005 (6)	0.0228 (6)	−0.0043 (5)
N3	0.0651 (9)	0.0412 (7)	0.0346 (7)	−0.0032 (6)	0.0199 (6)	0.0029 (5)
C1	0.0691 (11)	0.0401 (8)	0.0344 (8)	0.0005 (7)	0.0224 (7)	−0.0017 (6)
C2	0.0623 (10)	0.0307 (7)	0.0342 (7)	−0.0038 (7)	0.0153 (7)	0.0024 (6)
C3	0.0309 (7)	0.0302 (7)	0.0239 (6)	−0.0018 (5)	0.0045 (5)	−0.0004 (5)
C4	0.0439 (8)	0.0260 (7)	0.0306 (7)	0.0025 (5)	0.0099 (6)	−0.0025 (5)
C5	0.0471 (8)	0.0261 (6)	0.0301 (7)	0.0035 (6)	0.0095 (6)	0.0039 (5)

Geometric parameters (Å, º)

N1—C2	1.3397 (17)	C2—H2	0.9300
N1—N2	1.3620 (15)	C3—C4	1.3848 (18)
N1—C3	1.4255 (16)	C3—C5	1.3867 (18)
N2—C1	1.3141 (19)	C4—C5^{i}	1.3839 (17)
N3—C2	1.3133 (18)	C4—H4	0.9300
N3—C1	1.346 (2)	C5—H5	0.9300
C1—H1	0.9300		
C2—N1—N2	108.77 (11)	N1—C2—H2	124.4
C2—N1—C3	129.70 (11)	C4—C3—C5	120.38 (12)
N2—N1—C3	121.51 (10)	C4—C3—N1	120.02 (11)
C1—N2—N1	102.01 (12)	C5—C3—N1	119.60 (11)
C2—N3—C1	102.01 (12)	C5^{i}—C4—C3	119.55 (12)
N2—C1—N3	115.95 (13)	C5^{i}—C4—H4	120.2
N2—C1—H1	122.0	C3—C4—H4	120.2
N3—C1—H1	122.0	C4^{i}—C5—C3	120.07 (12)
N3—C2—N1	111.26 (13)	C4^{i}—C5—H5	120.0
N3—C2—H2	124.4	C3—C5—H5	120.0

C2—N1—N2—C1	0.02 (17)	N2—N1—C3—C4	−16.2 (2)
C3—N1—N2—C1	178.56 (13)	C2—N1—C3—C5	−17.3 (2)
N1—N2—C1—N3	0.1 (2)	N2—N1—C3—C5	164.48 (13)
C2—N3—C1—N2	−0.2 (2)	C5—C3—C4—C5^{i}	−0.1 (2)
C1—N3—C2—N1	0.19 (19)	N1—C3—C4—C5^{i}	−179.45 (12)
N2—N1—C2—N3	−0.14 (19)	C4—C3—C5—C4^{i}	0.1 (2)
C3—N1—C2—N3	−178.52 (13)	N1—C3—C5—C4^{i}	179.46 (13)
C2—N1—C3—C4	162.05 (15)		

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N3^{ii}	0.93	2.55	3.3563 (19)	146
C5—H5···N2^{iii}	0.93	2.71	3.6184 (18)	165

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