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4-(1*H*-Tetrazol-5-yl)benzene-1,3-diol

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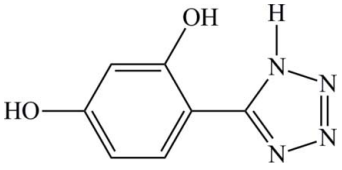
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.057; wR factor = 0.168; data-to-parameter ratio = 19.8.

In the title compound, $C_7H_6N_4O_2$, rings are almost coplanar, the dihedral angle between them being 8.45 (13)°. An intramolecular N—H···O hydrogen bond occurs. In the crystal, the molecules are linked by O—H···N and N—H···O hydrogen bonds into a three-dimensional network.

Related literature

For the structure of 4-(5-tetrazolyl)-1,3-benzenediol sesquihydrate, see: Gallardo *et al.* (1995). For the synthesis, see: Meyer *et al.* (1998).



Experimental

Crystal data

$C_7H_6N_4O_2$
M_r = 178.16
Orthorhombic, *Pccn*
a = 16.109 (2) Å
b = 7.2931 (11) Å
c = 12.8708 (17) Å
V = 1512.2 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 296 K
0.10 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.96, T_{max} = 0.98
20096 measured reflections
2452 independent reflections
1273 reflections with $I > 2\sigma(I)$
R_{int} = 0.110

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.168
S = 1.05
2452 reflections
124 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N4^{i}	0.82	1.94	2.759 (3)	173
O2—H2···N3^{ii}	0.82	2.00	2.817 (3)	173
N1—H101···O1	0.89 (3)	2.22 (3)	2.701 (3)	113 (2)
N1—H101···O2^{iii}	0.89 (3)	2.40 (3)	3.034 (3)	129 (2)
C3—H3···N2^{ii}	0.93	2.57	3.439 (3)	155

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2096).

References

Bruker (2006). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Gallardo, H., Meyer, E. & Vencato, I. (1995). *Acta Cryst.* C**51**, 2430–2432.
Meyer, E., Zucco, C. & Gallardo, H. (1998). *J. Mater. Chem.*, **8**, 1351–1354.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2013). E**69**, o380 [doi:10.1107/S160053681300411X]

4-(1*H*-Tetrazol-5-yl)benzene-1,3-diol

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S1. Comment

The similar structure of the title compound with two tetrazolylbenzenediol molecules per asymmetric unit together with three water molecules was reported in the literature (Gallardo *et al.*, 1995). In this compound, the two tetrazolylbenzendiol are linked through a hydrogen-bonded network to water molecules, forming layers extending along the face of the unit cell (Gallardo *et al.*, 1995). Herein, we report the related X-ray structure of the title compound (I) with eight tetrazolylbenzenediol molecules in unit cell and only one molecule in the asymmetric unit without any solvents. The title compound (I) could be isolated in more than 80% yield *via* the previously reported method (Meyer *et al.*, 1998). Like the structure of related compound (Gallardo *et al.*, 1995), the phenyl ring and the tetrazole ring of each molecule in the asymmetric unit are coplanar (Fig. 1), with the dihedral angle between the benzene and tetrazole rings of 8.45 (13)°. They are connected by a network of intermolecular hydrogen bonds (Fig. 2).

S2. Experimental

The title compound could be synthesized by the previously reported method (Meyer *et al.*, 1998). Crystal of the title compound suitable for X-ray analysis were grown in ethanol by slow evaporation.

S3. Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.93, O—H = 0.82 and N—H = 0.89 with U_{iso}(H) = 1.2Ueq(C), U_{iso}(H) = 1.5Ueq(O) and U_{iso}(H) = 1.4Ueq(N).

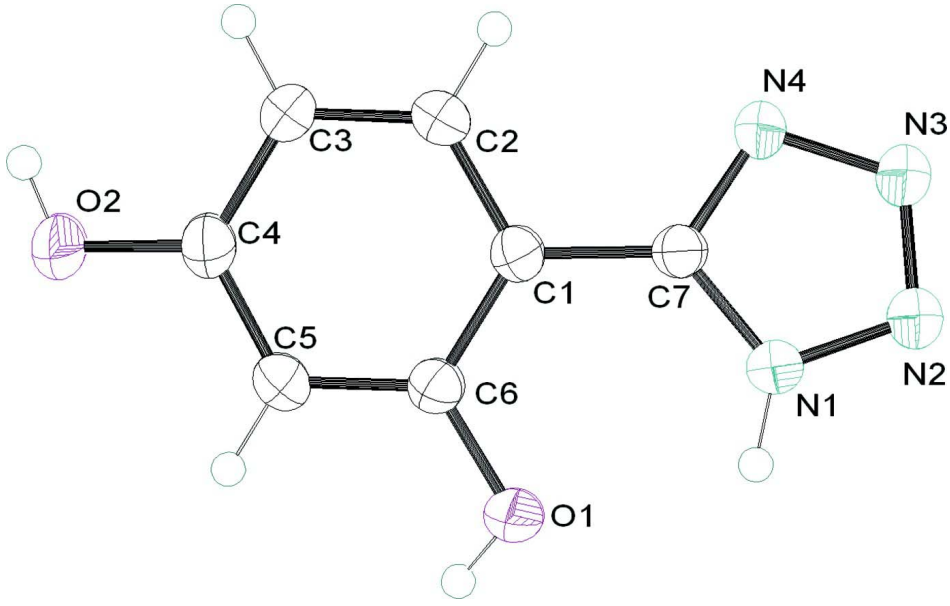

Figure 1

Molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

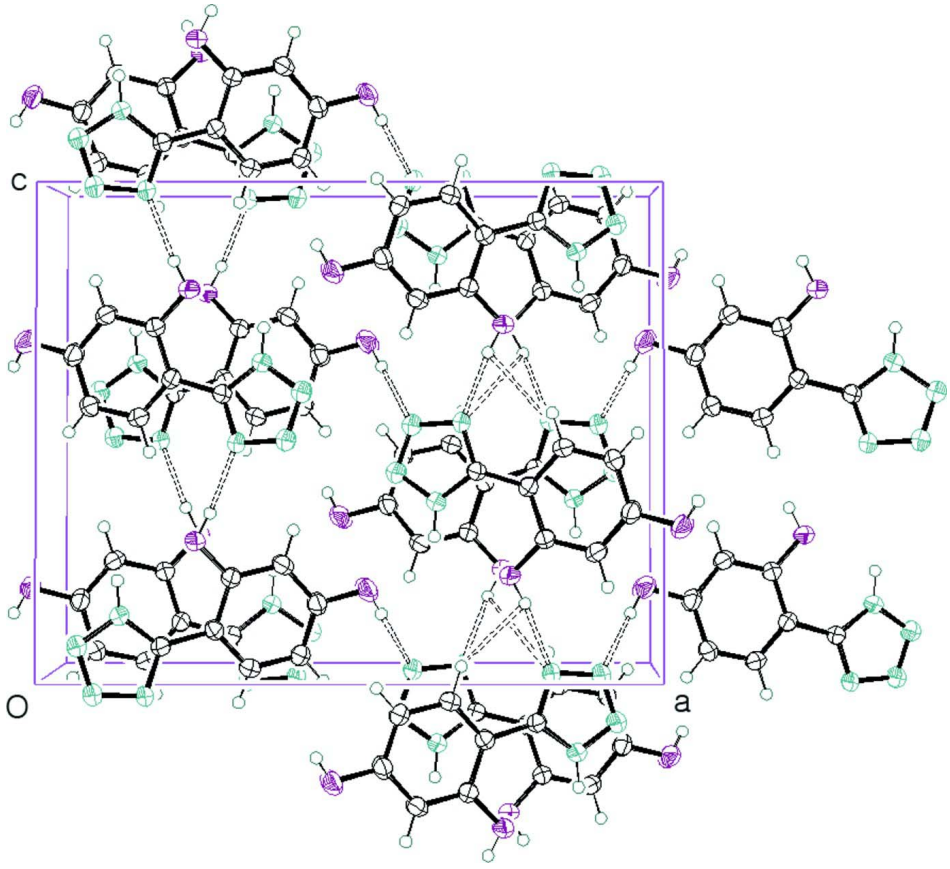

Figure 2

Hydrogen bonding network viewed along the *b*-axis.

4-(1*H*-Tetrazol-5-yl)benzene-1,3-diol

Crystal data

$C_7H_6N_4O_2$
$M_r = 178.16$
Orthorhombic, *Pccn*
$a = 16.109$ (2) Å
$b = 7.2931$ (11) Å
$c = 12.8708$ (17) Å
$V = 1512.2$ (4) Å^3
$Z = 8$
$F(000) = 736$
$D_x = 1.565$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3776 reflections
$\theta = 3.1$–$27.9°$
$\mu = 0.12$ mm^{-1}
$T = 296$ K
Block, white
0.10 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
$T_{min} = 0.96$, $T_{max} = 0.98$
20096 measured reflections
2452 independent reflections
1273 reflections with $I > 2\sigma(I)$
$R_{int} = 0.110$
$\theta_{max} = 31.3°$, $\theta_{min} = 2.5°$
$h = -23\rightarrow23$
$k = -10\rightarrow9$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.168$
$S = 1.05$
2452 reflections
124 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
$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 1.9684P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-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}
N1	0.86210 (12)	1.0811 (3)	0.86101 (16)	0.0332 (5)

H101	0.8653 (17)	1.079 (4)	0.792 (2)	0.047 (9)*
N2	0.92672 (12)	1.1375 (3)	0.91859 (16)	0.0387 (5)
N3	0.90167 (12)	1.1289 (3)	1.01390 (16)	0.0384 (5)
N4	0.82224 (11)	1.0674 (3)	1.01992 (15)	0.0322 (5)
O1	0.74465 (11)	1.0193 (3)	0.71535 (12)	0.0424 (5)
H1	0.7208	1.0311	0.6595	0.064*
O2	0.47535 (11)	0.8148 (3)	0.81787 (15)	0.0546 (6)
H2	0.4521	0.7686	0.8681	0.082*
C1	0.71543 (13)	0.9735 (3)	0.89292 (17)	0.0275 (5)
C2	0.66041 (14)	0.9179 (4)	0.97055 (18)	0.0329 (6)
H2A	0.6780	0.9178	1.0394	0.040*
C3	0.58072 (14)	0.8633 (4)	0.94770 (18)	0.0350 (6)
H3	0.5449	0.8270	1.0005	0.042*
C4	0.55424 (14)	0.8628 (4)	0.84451 (19)	0.0349 (6)
C5	0.60837 (15)	0.9128 (4)	0.76517 (19)	0.0355 (6)
H5	0.5909	0.9091	0.6963	0.043*
C6	0.68889 (14)	0.9686 (3)	0.78936 (17)	0.0292 (5)
C7	0.79789 (13)	1.0372 (3)	0.92276 (17)	0.0266 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0273 (9)	0.0474 (14)	0.0249 (10)	−0.0028 (9)	0.0009 (8)	0.0013 (9)
N2	0.0284 (10)	0.0561 (15)	0.0318 (11)	−0.0080 (10)	−0.0014 (8)	−0.0014 (10)
N3	0.0274 (10)	0.0547 (15)	0.0330 (11)	−0.0071 (10)	−0.0011 (8)	−0.0014 (10)
N4	0.0229 (9)	0.0453 (13)	0.0284 (10)	−0.0029 (9)	−0.0009 (7)	−0.0006 (9)
O1	0.0314 (8)	0.0715 (14)	0.0243 (8)	−0.0072 (9)	−0.0010 (7)	0.0069 (9)
O2	0.0359 (10)	0.0896 (18)	0.0382 (11)	−0.0275 (11)	−0.0102 (8)	0.0150 (11)
C1	0.0251 (10)	0.0299 (13)	0.0276 (11)	0.0006 (9)	−0.0018 (8)	0.0014 (10)
C2	0.0319 (11)	0.0427 (15)	0.0242 (11)	−0.0024 (11)	−0.0030 (9)	0.0018 (10)
C3	0.0280 (11)	0.0471 (16)	0.0300 (12)	−0.0090 (11)	0.0019 (9)	0.0032 (11)
C4	0.0279 (11)	0.0407 (16)	0.0359 (13)	−0.0057 (11)	−0.0046 (9)	0.0027 (11)
C5	0.0332 (11)	0.0466 (16)	0.0266 (12)	−0.0067 (11)	−0.0057 (9)	0.0038 (11)
C6	0.0270 (10)	0.0339 (13)	0.0268 (11)	0.0003 (10)	−0.0004 (9)	0.0031 (10)
C7	0.0254 (10)	0.0299 (13)	0.0245 (11)	0.0017 (9)	0.0006 (8)	0.0013 (9)

Geometric parameters (Å, º)

N1—N2	1.342 (3)	C1—C2	1.396 (3)
N1—C7	1.343 (3)	C1—C6	1.400 (3)
N1—H101	0.89 (3)	C1—C7	1.459 (3)
N2—N3	1.293 (3)	C2—C3	1.376 (3)
N3—N4	1.358 (3)	C2—H2A	0.9300
N4—C7	1.329 (3)	C3—C4	1.395 (3)
O1—C6	1.360 (3)	C3—H3	0.9300
O1—H1	0.8200	C4—C5	1.391 (3)
O2—C4	1.362 (3)	C5—C6	1.395 (3)
O2—H2	0.8200	C5—H5	0.9300

N2—N1—C7	110.1 (2)	C2—C3—H3	120.4
N2—N1—H101	120.8 (18)	C4—C3—H3	120.4
C7—N1—H101	129.1 (18)	O2—C4—C5	117.9 (2)
N3—N2—N1	105.49 (19)	O2—C4—C3	121.7 (2)
N2—N3—N4	111.35 (19)	C5—C4—C3	120.4 (2)
C7—N4—N3	106.20 (18)	C4—C5—C6	119.7 (2)
C6—O1—H1	109.5	C4—C5—H5	120.2
C4—O2—H2	109.5	C6—C5—H5	120.2
C2—C1—C6	118.7 (2)	O1—C6—C5	122.5 (2)
C2—C1—C7	118.8 (2)	O1—C6—C1	117.3 (2)
C6—C1—C7	122.5 (2)	C5—C6—C1	120.3 (2)
C3—C2—C1	121.6 (2)	N4—C7—N1	106.87 (19)
C3—C2—H2A	119.2	N4—C7—C1	124.7 (2)
C1—C2—H2A	119.2	N1—C7—C1	128.4 (2)
C2—C3—C4	119.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N4^{i}	0.82	1.94	2.759 (3)	173
O2—H2···N3^{ii}	0.82	2.00	2.817 (3)	173
N1—H101···O1	0.89 (3)	2.22 (3)	2.701 (3)	113 (2)
N1—H101···O2^{iii}	0.89 (3)	2.40 (3)	3.034 (3)	129 (2)
C3—H3···N2^{ii}	0.93	2.57	3.439 (3)	155

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