Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

2-(4*H*-1,2,4-Triazol-4-yl)phenol

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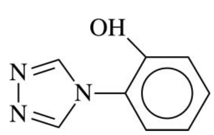
Received 2 August 2010; accepted 7 August 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.067; wR factor = 0.237; data-to-parameter ratio = 13.3.

In the title compound, $C_8H_7N_3O$, the dihedral angle between the benzene and triazole rings is 41.74 (12)°.

Related literature

For the use of substituted 1,2,4-triazoles as ligands, see: Ouellette *et al.* (2006); Zhang *et al.* (2005); Zhou *et al.* (2007, 2008). For related structures, see: Wiley & Hart (1953); Bartlett & Humphrey (1967); Li *et al.* (2004); Zhu *et al.* (2000); Xu *et al.* (2004).



Experimental

Crystal data

$C_8H_7N_3O$
M_r = 161.17
Monoclinic, $P2_1/n$
a = 7.273 (3) Å
b = 14.265 (4) Å
c = 7.720 (3) Å
β = 90.93 (3)°
V = 800.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.42 × 0.37 × 0.35 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (Sphere in *CrystalClear*; Rigaku, 2002)
T_{min} = 0.815, T_{max} = 1.000
5037 measured reflections
1460 independent reflections
863 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.237
S = 1.09
1460 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We gratefully acknowledge financial support from the Natural Science Foundation of the Education Department of Anhui Province (KJ2010B203, KJ2010B205) and the Science Foundation of Shandong Province (ZR2009BM041).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2195).

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supporting information

Acta Cryst. (2010). E**66**, o2318 [https://doi.org/10.1107/S1600536810031739]

2-(4*H*-1,2,4-Triazol-4-yl)phenol

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S1. Comment

Many compounds with uncommon properties have been widely investigated by using substituted 1,2,4-triazoles ligands, resulting from their rich coordination fashions and broad potential applications in various fields (Ouellette *et al.* (2006); Zhang *et al.* (2005); Zhou *et al.* (2007); Zhou *et al.* (2008)). Substituted 1,2,4-triazoles can be synthesized from different amines and diformylhydrazine. The triazole ring, having strong -donor and weak-acceptor properties, potentially has two different coordination modes through three nitrogen-donor atoms coordinating to metal ions. Recently, we have prepared some new substituted 1,2,4-triazole derivatives and their transition-metal complexes, and we report here the crystal structure analysis of 2-(1*H*-1,2,4-Triazol-4-yl)phenol, (I).

S2. Experimental

The title compound was prepared by reacting diformylhydrazine (0.6 mmol, 0.053 g) and *o*-aminophenol (0.6 mmol, 0.065 g) in a Telon-lined stainless steel autoclave in a furnace at 443 K for 2 d. The reaction vessel was then cooled to 293 K. The product was isolated and washed with hot water and hot ethanol and black crystals suitable for X-ray diffraction studies were obtained. The crystals are air-stable. Yield based on *o*-aminophenol: 0.062 g, 64%. Elemental analysis (%) for C8H7N3O, found (calculated): C 59.70 (59.61), H 4.25 (4.38), N 26.06 (26.08).

S3. Refinement

Hydrogen atoms were allowed to ride on their respective parent atoms with C—H distances of 0.93 Å, and were included in the refinement with isotropic displacement parameters U_{iso}(H) = 1.2U_{eq}(C).

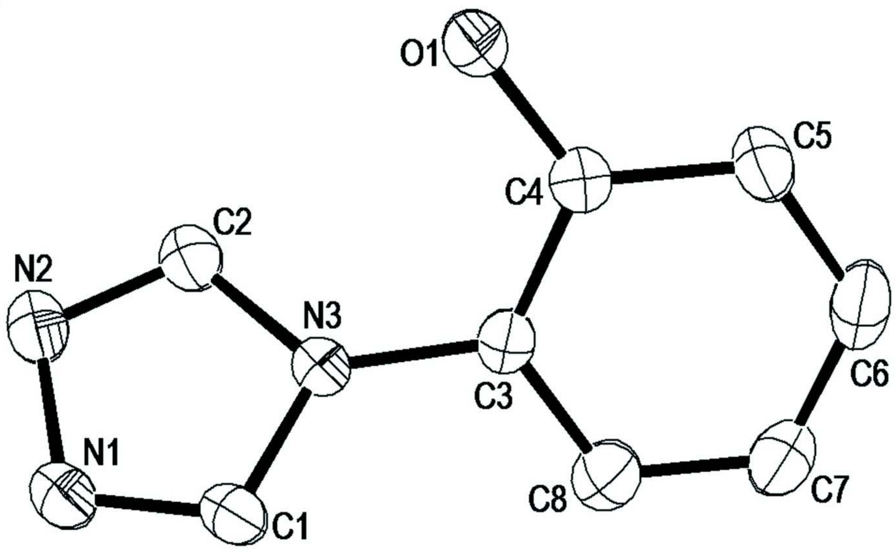

Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

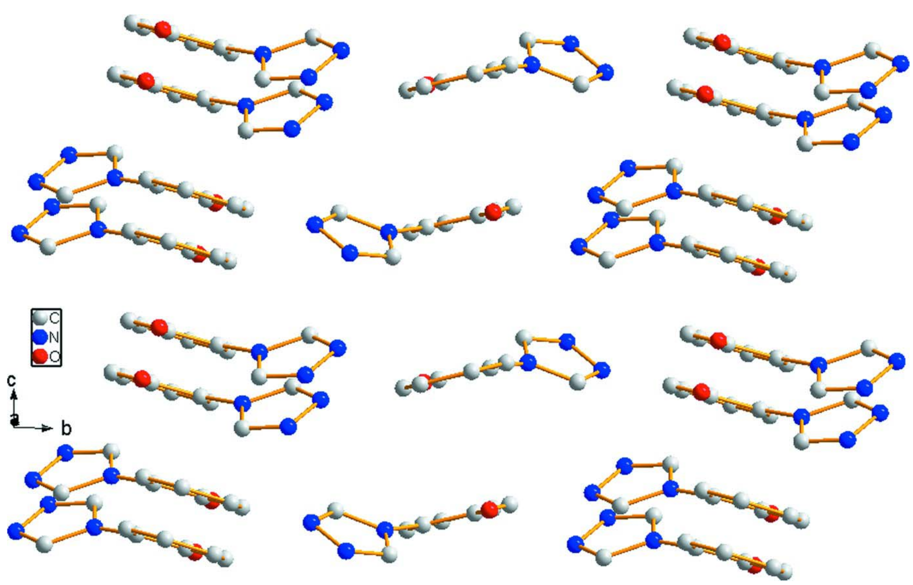

Figure 2

View of the 3-D structure of the title compound.

2-(4*H*-1,2,4-Triazol-4-yl)phenol

Crystal data

$C_8H_7N_3O$
M_r = 161.17
Monoclinic, $P2_1/n$
a = 7.273 (3) Å
b = 14.265 (4) Å
c = 7.720 (3) Å
β = 90.93 (3)°
V = 800.8 (5) Å^3
Z = 4
F(000) = 336
D_x = 1.337 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1048 reflections
θ = 2.6–27.4°

μ = 0.09 mm^{-1}
T = 293 K

Block, black
0.42 × 0.37 × 0.35 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: rotating-anode generator
Graphite monochromator
ω scans
Absorption correction: multi-scan (Sphere in *CrystalClear*; Rigaku, 2002)
T_{min} = 0.815, T_{max} = 1.000

5037 measured reflections
1460 independent reflections
863 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 25.4°, θ_{min} = 3.0°
$h = -8 \rightarrow 8$
$k = -16 \rightarrow 17$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.237
S = 1.09
1460 reflections
110 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
$w = 1/[\sigma^2(F_o^2) + (0.144P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.08 (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}
C1	0.5881 (5)	0.7175 (2)	0.7593 (5)	0.0559 (10)
H1A	0.5053	0.7418	0.8381	0.067*
C2	0.7294 (5)	0.6248 (2)	0.5912 (4)	0.0510 (10)
H2A	0.7633	0.5718	0.5293	0.061*
C3	0.4535 (4)	0.5571 (2)	0.7425 (4)	0.0423 (8)
C4	0.5137 (4)	0.4665 (2)	0.7748 (4)	0.0448 (9)
C5	0.3858 (5)	0.4004 (2)	0.8286 (4)	0.0542 (10)
H5A	0.4233	0.3394	0.8527	0.065*
C6	0.2034 (5)	0.4252 (3)	0.8463 (5)	0.0651 (11)
H6A	0.1194	0.3807	0.8837	0.078*
C7	0.1443 (5)	0.5148 (3)	0.8091 (5)	0.0633 (11)
H7A	0.0210	0.5308	0.8200	0.076*

C8	0.2698 (5)	0.5804 (3)	0.7557 (5)	0.0582 (10)
H8A	0.2309	0.6408	0.7284	0.070*
N1	0.7219 (4)	0.76432 (19)	0.6942 (4)	0.0632 (10)
N2	0.8157 (4)	0.70426 (19)	0.5852 (4)	0.0618 (10)
N3	0.5836 (3)	0.62837 (17)	0.6985 (3)	0.0443 (8)
O1	0.6918 (3)	0.44556 (15)	0.7550 (3)	0.0582 (8)
H1B	0.7472	0.4923	0.7229	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.068 (2)	0.0332 (18)	0.068 (2)	0.0041 (15)	0.0238 (18)	0.0022 (16)
C2	0.057 (2)	0.0414 (18)	0.0553 (19)	−0.0010 (15)	0.0129 (17)	0.0025 (15)
C3	0.0378 (18)	0.0426 (17)	0.0466 (17)	−0.0030 (14)	0.0046 (13)	0.0028 (14)
C4	0.0428 (19)	0.0414 (19)	0.0504 (17)	−0.0018 (14)	0.0042 (14)	0.0001 (14)
C5	0.060 (2)	0.0429 (19)	0.060 (2)	−0.0089 (15)	0.0074 (18)	0.0071 (16)
C6	0.058 (2)	0.075 (3)	0.063 (2)	−0.024 (2)	0.0154 (18)	−0.005 (2)
C7	0.047 (2)	0.070 (3)	0.072 (2)	−0.0036 (18)	0.0121 (18)	−0.001 (2)
C8	0.050 (2)	0.058 (2)	0.067 (2)	0.0034 (16)	0.0065 (17)	0.0065 (17)
N1	0.073 (2)	0.0368 (16)	0.081 (2)	−0.0025 (14)	0.0284 (17)	−0.0018 (15)
N2	0.065 (2)	0.0458 (17)	0.076 (2)	−0.0100 (14)	0.0222 (16)	−0.0004 (14)
N3	0.0449 (16)	0.0329 (15)	0.0553 (16)	0.0000 (11)	0.0117 (12)	0.0012 (11)
O1	0.0451 (15)	0.0400 (13)	0.0897 (19)	0.0004 (10)	0.0081 (12)	0.0087 (12)

Geometric parameters (Å, º)

C1—N1	1.289 (4)	C4—C5	1.393 (4)
C1—N3	1.356 (4)	C5—C6	1.382 (5)
C1—H1A	0.9300	C5—H5A	0.9300
C2—N2	1.297 (4)	C6—C7	1.378 (6)
C2—N3	1.357 (4)	C6—H6A	0.9300
C2—H2A	0.9300	C7—C8	1.375 (5)
C3—C8	1.382 (4)	C7—H7A	0.9300
C3—C4	1.385 (5)	C8—H8A	0.9300
C3—N3	1.433 (4)	N1—N2	1.388 (4)
C4—O1	1.340 (4)	O1—H1B	0.8200
N1—C1—N3	111.4 (3)	C7—C6—C5	120.9 (3)
N1—C1—H1A	124.3	C7—C6—H6A	119.5
N3—C1—H1A	124.3	C5—C6—H6A	119.5
N2—C2—N3	111.9 (3)	C8—C7—C6	119.2 (3)
N2—C2—H2A	124.1	C8—C7—H7A	120.4
N3—C2—H2A	124.1	C6—C7—H7A	120.4
C8—C3—C4	120.9 (3)	C7—C8—C3	120.4 (4)
C8—C3—N3	119.3 (3)	C7—C8—H8A	119.8
C4—C3—N3	119.8 (3)	C3—C8—H8A	119.8
O1—C4—C3	119.4 (3)	C1—N1—N2	107.4 (3)
O1—C4—C5	122.3 (3)	C2—N2—N1	105.9 (3)

C3—C4—C5	118.4 (3)	C1—N3—C2	103.4 (2)
C6—C5—C4	120.2 (3)	C1—N3—C3	126.6 (3)
C6—C5—H5A	119.9	C2—N3—C3	130.0 (3)
C4—C5—H5A	119.9	C4—O1—H1B	109.5