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2-Cyano-*N*′-[1-(2-hydroxyphenyl)ethylidene]acetohydrazide monohydrate

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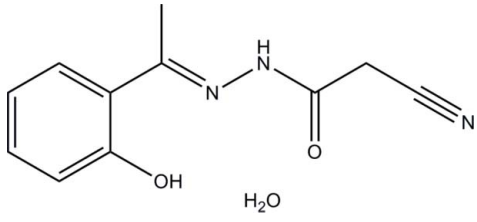
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.070; wR factor = 0.147; data-to-parameter ratio = 15.2.

The title compound, $C_{11}H_{11}N_3O_2\cdot H_2O$, was obtained by the reaction of 2-acetylphenol with cyanoacetohydrazide in methanol. The asymmetric unit contains two hydrazone molecules and two water molecules of crystallization. There is an intramolecular O—H···N hydrogen bond in each hydrazone molecule. The crystal structure is stabilized by intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds.

Related literature

For the structures of hydrazones, see: Wang *et al.* (2011); Hashemian *et al.* (2011); Singh & Singh (2010); Ahmad *et al.* (2010). For compounds we have reported on recently, see: Li & Ni (2011); Li & Chen (2011).



Experimental

Crystal data

$C_{11}H_{11}N_3O_2\cdot H_2O$
M_r = 235.24
Monoclinic, $P2_1/n$
a = 17.387 (3) Å
b = 7.576 (2) Å
c = 17.855 (3) Å
β = 90.962 (2)°
V = 2351.7 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.20 × 0.18 × 0.17 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.981, T_{max} = 0.983
14877 measured reflections
4994 independent reflections
2551 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.147
S = 1.02
4994 reflections
329 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6B···N6^{i}	0.84 (1)	2.17 (2)	2.975 (4)	159 (3)
O5—H5B···O3^{ii}	0.85 (1)	2.43 (2)	3.120 (4)	140 (3)
O6—H6A···O4^{iii}	0.85 (1)	2.06 (1)	2.900 (3)	173 (3)
O5—H5A···O2	0.85 (1)	1.93 (1)	2.777 (3)	174 (3)
N5—H5···O5^{iv}	0.90 (1)	1.93 (1)	2.820 (3)	171 (3)
N2—H2···O6^{v}	0.90 (1)	2.03 (1)	2.905 (3)	162 (3)
O3—H3A···N4	0.82	1.82	2.534 (3)	145
O1—H1···N1	0.82	1.81	2.528 (3)	145

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2036).

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supporting information

Acta Cryst. (2011). E**67**, o3001 [doi:10.1107/S1600536811042565]

2-Cyano-*N*′-[1-(2-hydroxyphenyl)ethylidene]acetohydrazide monohydrate

Hongbo Li, Peng Chen and Zhonglu You

S1. Comment

Recently, a great number of hydrazones derived from the reaction of salicylaldehyde and its derivatives with benzohydrazides have been reported (Wang *et al.*, 2011; Hashemian *et al.*, 2011; Singh & Singh, 2010; Ahmad *et al.*, 2010). As a continuation of our work on the hydrazones derived from cyanoacetohydrazide (Li & Ni, 2011; Li & Chen, 2011), in this paper, the title new hydrazone compound, (I), is reported.

The asymmetric unit of the compound contains two hydrazone molecules and two water molecules of crystallization, Fig. 1. There is an intramolecular O—H···N hydrogen bond (Table 1) in the hydrazone molecule. The non-hydrogen atoms of the hydrazone molecules are approximately coplanar, with mean deviations from the least-squares planes of 0.107 (3) Å for molecule A and 0.100 (3) Å for molecule B. The crystal structure is stabilized by intermolecular N—H···O, O—H···O, and O—H···N hydrogen bonds (Table 2, and Fig. 2).

S2. Experimental

The title compound was obtained by the reaction of equimolar quantities (1.0 mmol each) of 2-acetylphenol with cyanoacetohydrazide in methanol. Single crystals suitable for X-ray diffraction were obtained by the slow evaporation of the solution containing the compound in open air.

S3. Refinement

The water H atoms and the amino H atoms were located from a difference Fourier map and refined isotropically, with O—H, H···H, and N—H distances restrained to 0.85 (1), 1.37 (2), and 0.90 (1) Å, respectively. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2 (1.5 for methyl group) times U_{eq}(C).

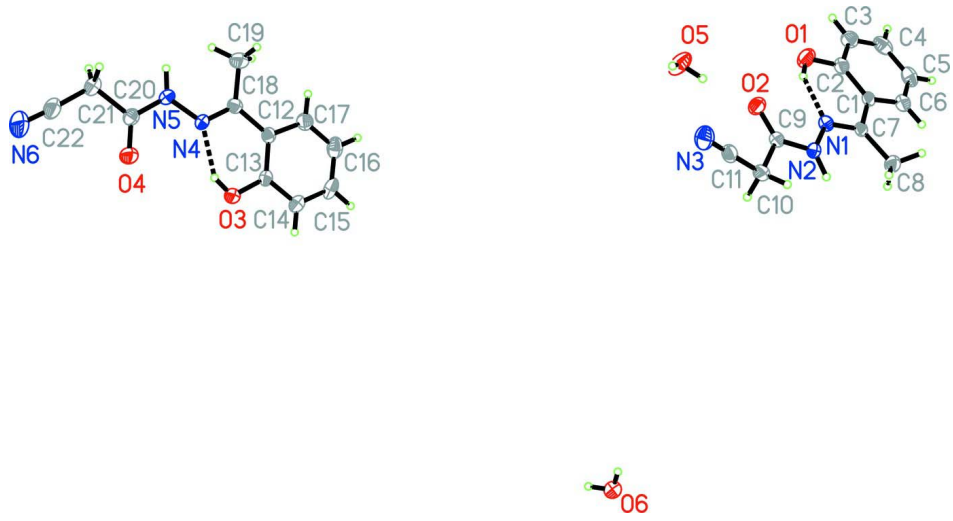

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms. Intramolecular O—H···N hydrogen bonds are shown as dashed lines.

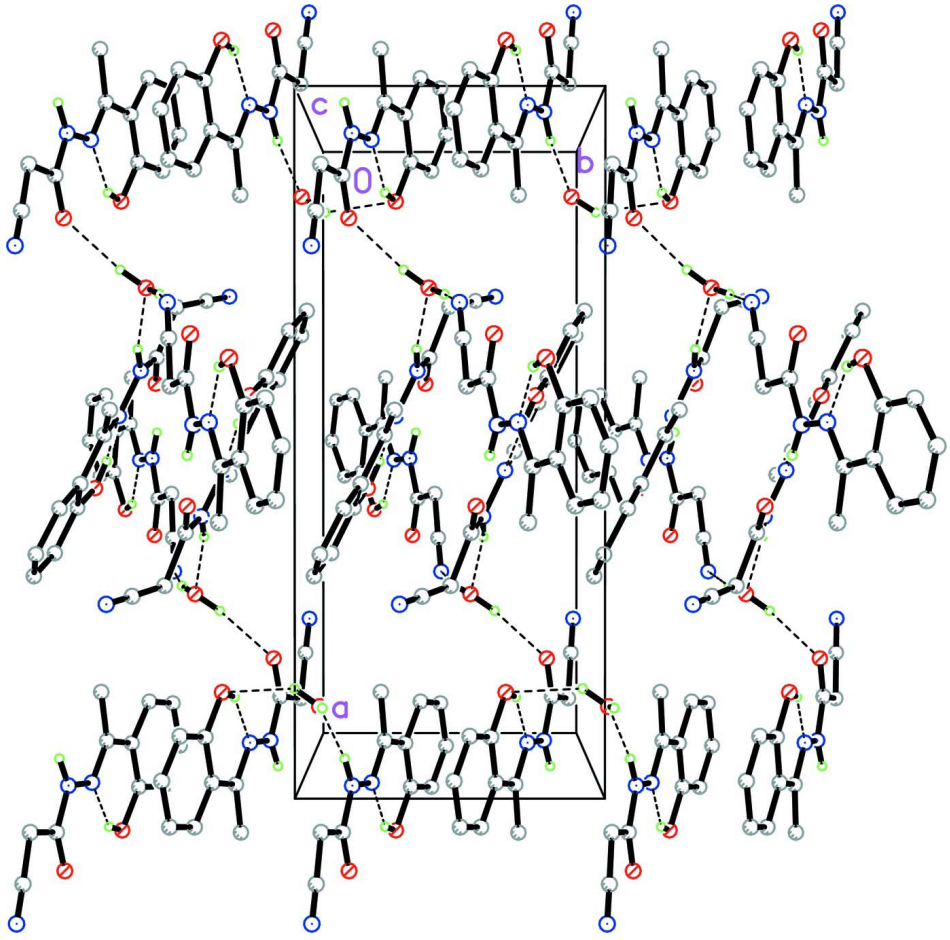

Figure 2

The packing of (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

2-Cyano-*N*′-[1-(2-hydroxyphenyl)ethylidene]acetohydrazide monohydrate

Crystal data

$C_{11}H_{11}N_3O_2·H_2O$
M_r = 235.24
Monoclinic, $P2_1/n$
a = 17.387 (3) Å
b = 7.576 (2) Å
c = 17.855 (3) Å
β = 90.962 (2)°
V = 2351.7 (8) Å^3
Z = 8
$F(000)$ = 992
D_x = 1.329 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2383 reflections
θ = 2.3–24.5°
μ = 0.10 mm^{-1}
T = 298 K
Block, colorless
0.20 × 0.18 × 0.17 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.981, T_{max} = 0.983
14877 measured reflections
4994 independent reflections

2551 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.3°$
$h = -22 \rightarrow 22$
$k = -9 \rightarrow 9$
$l = -22 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.147$
$S = 1.02$
4994 reflections
329 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.2161P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.04236 (11)	0.8041 (3)	0.03832 (12)	0.0382 (5)
N2	0.11383 (11)	0.8825 (3)	0.04497 (12)	0.0384 (6)
N3	0.23967 (15)	1.1713 (4)	0.24440 (16)	0.0695 (8)
N4	0.52913 (12)	0.2797 (3)	1.02064 (12)	0.0413 (6)
N5	0.52601 (12)	0.3436 (3)	1.09279 (13)	0.0448 (6)
N6	0.7097 (2)	0.4674 (6)	1.28277 (19)	0.1359 (17)
O1	−0.07228 (11)	0.6992 (3)	0.11129 (11)	0.0655 (6)
H1	−0.0294	0.7422	0.1060	0.098*
O2	0.09556 (10)	0.9093 (3)	0.16978 (10)	0.0584 (6)
O3	0.61680 (9)	0.1973 (3)	0.91423 (10)	0.0626 (6)
H3A	0.6061	0.2342	0.9560	0.094*
O4	0.65614 (10)	0.3548 (3)	1.10066 (11)	0.0614 (6)
O5	0.10243 (14)	0.9509 (4)	0.32426 (12)	0.0823 (8)
O6	0.76091 (12)	0.0749 (3)	0.05910 (11)	0.0669 (7)
C1	−0.06363 (13)	0.6818 (3)	−0.02411 (15)	0.0364 (6)
C2	−0.10201 (15)	0.6524 (4)	0.04338 (17)	0.0452 (7)
C3	−0.17375 (16)	0.5708 (4)	0.04299 (19)	0.0577 (8)
H3	−0.1992	0.5539	0.0878	0.069*
C4	−0.20720 (16)	0.5150 (4)	−0.0231 (2)	0.0608 (9)
H4	−0.2546	0.4582	−0.0225	0.073*
C5	−0.17115 (17)	0.5424 (4)	−0.0898 (2)	0.0580 (9)

H5C	−0.1940	0.5052	−0.1346	0.070*
C6	−0.10039 (15)	0.6262 (4)	−0.08989 (16)	0.0480 (8)
H6	−0.0766	0.6460	−0.1354	0.058*
C7	0.01282 (13)	0.7672 (3)	−0.02630 (15)	0.0345 (6)
C8	0.05050 (15)	0.8057 (4)	−0.09932 (15)	0.0515 (8)
H8A	0.0888	0.8957	−0.0921	0.077*
H8B	0.0125	0.8457	−0.1350	0.077*
H8C	0.0744	0.7004	−0.1177	0.077*
C9	0.13657 (14)	0.9254 (4)	0.11518 (17)	0.0406 (7)
C10	0.21757 (14)	0.9977 (4)	0.12086 (16)	0.0496 (8)
H10A	0.2539	0.9009	0.1186	0.060*
H10B	0.2267	1.0749	0.0786	0.060*
C11	0.23035 (14)	1.0954 (4)	0.19022 (18)	0.0471 (8)
C12	0.47824 (13)	0.1629 (3)	0.90922 (15)	0.0389 (7)
C13	0.55132 (15)	0.1436 (4)	0.87800 (15)	0.0465 (8)
C14	0.55919 (17)	0.0688 (4)	0.80791 (17)	0.0619 (9)
H14	0.6080	0.0552	0.7882	0.074*
C15	0.4960 (2)	0.0143 (4)	0.76702 (17)	0.0643 (9)
H15	0.5023	−0.0372	0.7202	0.077*
C16	0.42393 (19)	0.0356 (4)	0.79496 (19)	0.0624 (9)
H16	0.3810	0.0012	0.7669	0.075*
C17	0.41539 (16)	0.1081 (4)	0.86462 (18)	0.0536 (8)
H17	0.3660	0.1215	0.8831	0.064*
C18	0.46728 (14)	0.2340 (3)	0.98523 (15)	0.0400 (7)
C19	0.38820 (15)	0.2469 (5)	1.01681 (17)	0.0688 (10)
H19A	0.3919	0.2576	1.0703	0.103*
H19B	0.3595	0.1427	1.0040	0.103*
H19C	0.3625	0.3487	0.9964	0.103*
C20	0.59330 (16)	0.3755 (4)	1.12859 (15)	0.0443 (7)
C21	0.58370 (16)	0.4428 (4)	1.20823 (15)	0.0546 (8)
H21A	0.5595	0.5582	1.2065	0.066*
H21B	0.5499	0.3637	1.2348	0.066*
C22	0.6557 (2)	0.4559 (5)	1.24854 (19)	0.0759 (11)
H2	0.1463 (13)	0.880 (4)	0.0059 (11)	0.080*
H5	0.4823 (10)	0.368 (4)	1.1171 (15)	0.080*
H5A	0.1041 (17)	0.937 (4)	0.2772 (6)	0.080*
H6A	0.7337 (16)	0.163 (3)	0.0707 (15)	0.080*
H5B	0.1286 (16)	1.039 (3)	0.3379 (15)	0.080*
H6B	0.7723 (17)	0.019 (3)	0.0987 (11)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0374 (12)	0.0357 (14)	0.0415 (15)	0.0014 (10)	−0.0027 (10)	0.0008 (12)
N2	0.0390 (12)	0.0451 (15)	0.0310 (15)	0.0014 (10)	−0.0022 (10)	−0.0015 (12)
N3	0.0771 (19)	0.074 (2)	0.057 (2)	−0.0111 (15)	−0.0134 (15)	−0.0057 (17)
N4	0.0430 (13)	0.0508 (15)	0.0303 (14)	0.0010 (11)	0.0024 (10)	0.0005 (12)
N5	0.0449 (14)	0.0549 (16)	0.0348 (15)	0.0034 (12)	0.0067 (11)	−0.0013 (13)

N6	0.092 (3)	0.233 (5)	0.082 (3)	−0.017 (3)	−0.021 (2)	−0.051 (3)
O1	0.0614 (13)	0.0916 (18)	0.0436 (14)	−0.0126 (12)	0.0070 (10)	0.0058 (12)
O2	0.0450 (11)	0.0912 (17)	0.0389 (13)	−0.0068 (10)	0.0018 (9)	−0.0022 (11)
O3	0.0386 (10)	0.1050 (18)	0.0441 (13)	0.0030 (11)	0.0005 (9)	−0.0131 (13)
O4	0.0458 (11)	0.0855 (17)	0.0530 (14)	−0.0069 (11)	0.0077 (9)	−0.0082 (12)
O5	0.0884 (17)	0.108 (2)	0.0508 (15)	−0.0382 (14)	0.0206 (13)	−0.0045 (15)
O6	0.0567 (13)	0.090 (2)	0.0542 (15)	0.0036 (11)	0.0051 (11)	0.0093 (13)
C1	0.0382 (14)	0.0330 (16)	0.0378 (17)	0.0080 (12)	−0.0024 (12)	0.0038 (14)
C2	0.0454 (15)	0.0450 (19)	0.045 (2)	0.0040 (14)	−0.0027 (14)	0.0052 (16)
C3	0.0477 (17)	0.060 (2)	0.065 (2)	−0.0003 (15)	0.0080 (16)	0.0150 (19)
C4	0.0408 (16)	0.049 (2)	0.092 (3)	−0.0020 (14)	−0.0071 (18)	0.009 (2)
C5	0.0531 (18)	0.053 (2)	0.067 (2)	−0.0006 (15)	−0.0208 (17)	−0.0009 (18)
C6	0.0485 (16)	0.0470 (19)	0.048 (2)	0.0045 (14)	−0.0059 (14)	0.0026 (15)
C7	0.0385 (14)	0.0317 (16)	0.0334 (17)	0.0075 (11)	−0.0017 (12)	0.0033 (13)
C8	0.0453 (15)	0.067 (2)	0.0417 (19)	−0.0043 (14)	−0.0018 (13)	0.0024 (16)
C9	0.0366 (14)	0.0436 (18)	0.0415 (19)	0.0054 (12)	−0.0011 (13)	0.0041 (15)
C10	0.0384 (15)	0.066 (2)	0.045 (2)	0.0052 (14)	−0.0032 (13)	−0.0046 (16)
C11	0.0392 (15)	0.055 (2)	0.047 (2)	−0.0027 (13)	−0.0065 (14)	0.0077 (17)
C12	0.0426 (15)	0.0383 (17)	0.0357 (17)	−0.0015 (12)	−0.0007 (12)	0.0086 (14)
C13	0.0465 (16)	0.060 (2)	0.0327 (18)	0.0011 (14)	−0.0028 (13)	0.0050 (16)
C14	0.0600 (19)	0.087 (3)	0.038 (2)	0.0016 (17)	0.0045 (15)	−0.0049 (19)
C15	0.090 (3)	0.070 (2)	0.033 (2)	−0.0125 (19)	−0.0023 (18)	0.0001 (17)
C16	0.071 (2)	0.064 (2)	0.052 (2)	−0.0215 (18)	−0.0126 (17)	0.0075 (19)
C17	0.0477 (17)	0.061 (2)	0.052 (2)	−0.0074 (15)	−0.0003 (15)	0.0073 (18)
C18	0.0392 (15)	0.0393 (18)	0.0414 (18)	0.0016 (12)	0.0012 (13)	0.0083 (14)
C19	0.0436 (17)	0.098 (3)	0.065 (2)	−0.0001 (17)	0.0098 (15)	−0.010 (2)
C20	0.0498 (17)	0.0450 (19)	0.0383 (18)	−0.0031 (14)	0.0052 (14)	0.0070 (15)
C21	0.0664 (19)	0.057 (2)	0.0404 (19)	−0.0009 (16)	0.0021 (15)	−0.0048 (16)
C22	0.074 (2)	0.105 (3)	0.049 (2)	−0.012 (2)	0.0000 (19)	−0.021 (2)

Geometric parameters (Å, º)

N1—C7	1.286 (3)	C5—H5C	0.9300
N1—N2	1.381 (3)	C6—H6	0.9300
N2—C9	1.348 (3)	C7—C8	1.498 (3)
N2—H2	0.904 (10)	C8—H8A	0.9600
N3—C11	1.135 (3)	C8—H8B	0.9600
N4—C18	1.286 (3)	C8—H8C	0.9600
N4—N5	1.378 (3)	C9—C10	1.513 (3)
N5—C20	1.346 (3)	C10—C11	1.457 (4)
N5—H5	0.901 (10)	C10—H10A	0.9700
N6—C22	1.115 (4)	C10—H10B	0.9700
O1—C2	1.357 (3)	C12—C13	1.404 (3)
O1—H1	0.8200	C12—C17	1.404 (4)
O2—C9	1.224 (3)	C12—C18	1.476 (3)
O3—C13	1.362 (3)	C13—C14	1.383 (4)
O3—H3A	0.8200	C14—C15	1.372 (4)
O4—C20	1.219 (3)	C14—H14	0.9300

O5—H5A	0.848 (10)	C15—C16	1.367 (4)
O5—H5B	0.845 (10)	C15—H15	0.9300
O6—H6A	0.848 (10)	C16—C17	1.370 (4)
O6—H6B	0.843 (10)	C16—H16	0.9300
C1—C6	1.393 (3)	C17—H17	0.9300
C1—C2	1.405 (4)	C18—C19	1.498 (3)
C1—C7	1.480 (3)	C19—H19A	0.9600
C2—C3	1.392 (4)	C19—H19B	0.9600
C3—C4	1.373 (4)	C19—H19C	0.9600
C3—H3	0.9300	C20—C21	1.523 (4)
C4—C5	1.372 (4)	C21—C22	1.437 (4)
C4—H4	0.9300	C21—H21A	0.9700
C5—C6	1.384 (4)	C21—H21B	0.9700

C7—N1—N2	121.1 (2)	C11—C10—H10A	109.3
C9—N2—N1	115.7 (2)	C9—C10—H10A	109.3
C9—N2—H2	123.0 (19)	C11—C10—H10B	109.3
N1—N2—H2	119.9 (19)	C9—C10—H10B	109.3
C18—N4—N5	120.6 (2)	H10A—C10—H10B	107.9
C20—N5—N4	117.4 (2)	N3—C11—C10	179.4 (3)
C20—N5—H5	117.9 (19)	C13—C12—C17	116.4 (3)
N4—N5—H5	124.7 (19)	C13—C12—C18	122.3 (2)
C2—O1—H1	109.5	C17—C12—C18	121.2 (2)
C13—O3—H3A	109.5	O3—C13—C14	117.2 (2)
H5A—O5—H5B	111 (2)	O3—C13—C12	122.4 (3)
H6A—O6—H6B	108 (2)	C14—C13—C12	120.4 (3)
C6—C1—C2	117.2 (2)	C15—C14—C13	121.0 (3)
C6—C1—C7	120.6 (2)	C15—C14—H14	119.5
C2—C1—C7	122.1 (2)	C13—C14—H14	119.5
O1—C2—C3	116.6 (3)	C16—C15—C14	120.1 (3)
O1—C2—C1	123.1 (2)	C16—C15—H15	120.0
C3—C2—C1	120.3 (3)	C14—C15—H15	120.0
C4—C3—C2	120.5 (3)	C15—C16—C17	119.5 (3)
C4—C3—H3	119.7	C15—C16—H16	120.2
C2—C3—H3	119.7	C17—C16—H16	120.2
C5—C4—C3	120.5 (3)	C16—C17—C12	122.6 (3)
C5—C4—H4	119.8	C16—C17—H17	118.7
C3—C4—H4	119.8	C12—C17—H17	118.7
C4—C5—C6	119.3 (3)	N4—C18—C12	115.5 (2)
C4—C5—H5C	120.4	N4—C18—C19	124.2 (3)
C6—C5—H5C	120.4	C12—C18—C19	120.2 (2)
C5—C6—C1	122.2 (3)	C18—C19—H19A	109.5
C5—C6—H6	118.9	C18—C19—H19B	109.5
C1—C6—H6	118.9	H19A—C19—H19B	109.5
N1—C7—C1	114.6 (2)	C18—C19—H19C	109.5
N1—C7—C8	124.4 (2)	H19A—C19—H19C	109.5
C1—C7—C8	121.0 (2)	H19B—C19—H19C	109.5
C7—C8—H8A	109.5	O4—C20—N5	124.1 (3)

C7—C8—H8B	109.5	O4—C20—C21	122.6 (3)
H8A—C8—H8B	109.5	N5—C20—C21	113.3 (2)
C7—C8—H8C	109.5	C22—C21—C20	112.5 (3)
H8A—C8—H8C	109.5	C22—C21—H21A	109.1
H8B—C8—H8C	109.5	C20—C21—H21A	109.1
O2—C9—N2	123.5 (2)	C22—C21—H21B	109.1
O2—C9—C10	122.5 (3)	C20—C21—H21B	109.1
N2—C9—C10	114.1 (2)	H21A—C21—H21B	107.8
C11—C10—C9	111.7 (2)	N6—C22—C21	176.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*B*···N6^{i}	0.84 (1)	2.17 (2)	2.975 (4)	159 (3)
O5—H5*B*···O3^{ii}	0.85 (1)	2.43 (2)	3.120 (4)	140 (3)
O6—H6*A*···O4^{iii}	0.85 (1)	2.06 (1)	2.900 (3)	173 (3)
O5—H5*A*···O2	0.85 (1)	1.93 (1)	2.777 (3)	174 (3)
N5—H5···O5^{iv}	0.90 (1)	1.93 (1)	2.820 (3)	171 (3)
N2—H2···O6^{v}	0.90 (1)	2.03 (1)	2.905 (3)	162 (3)
O3—H3*A*···N4	0.82	1.82	2.534 (3)	145
O1—H1···N1	0.82	1.81	2.528 (3)	145

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