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(*E*)-*N*′-[(Furan-2-yl)methylene]-2-hydroxy-2,2-diphenylacetohydrazide monohydrate

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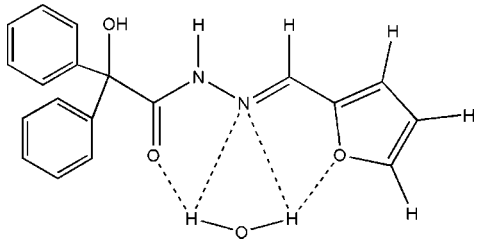
Key indicators: single-crystal X-ray study; T = 213 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.123; data-to-parameter ratio = 11.1.

In the structure of the title compound, $C_{19}H_{16}N_2O_3\cdot H_2O$, the configuration with respect to the C=N double bond is *trans*. The molecules form layers parallel to the *ac* plane, linked to each other by water molecules and OH groups, which are extended along the *b* axis involving the NH groups of adjacent molecules *via* N—H···OH_2 interactions, thus resulting in sheets of molecules. In addition, there are edge-to-face and offset face-to-face interactions between phenyl rings of adjacent molecules along both the *a* and *b* axes [C···C distances in the range 3.9–4.1 Å]. The extremely strong hydrogen bonds and phenyl–phenyl interactions contribute greatly to stabilizing the three-dimensional network.

Related literature

For general background, see: Sun *et al.* (2006); Gup & Kirkan (2005); Ganjali *et al.* (2006); Getautis *et al.* (2006); Kuriakose *et al.* (2007); Owen & Wenbin (2002); Tobin (1990). For related literature, see: Allen *et al.* (1987); Yathirajan *et al.* (2007); Mathew *et al.* (2007); Sun *et al.* (2007); Dance (1996).



Experimental

Crystal data

$C_{19}H_{16}N_2O_3\cdot H_2O$
M_r = 338.35
Monoclinic, $P2_1/c$
a = 10.6339 (17) Å
b = 10.857 (2) Å
c = 14.5207 (12) Å
β = 91.819 (10)°
V = 1675.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 213 (2) K
0.55 × 0.50 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (*HELENA*; Spek, 1996)
T_{min} = 0.937, T_{max} = 0.985
3847 measured reflections
3293 independent reflections
1981 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
3 standard reflections
every 400 reflections
intensity decay: 3.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.123
S = 1.01
3293 reflections
298 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O4^{i}	0.89 (2)	2.40 (2)	3.248 (3)	159 (2)
O3—H3A···O4^{ii}	0.92 (3)	1.94 (3)	2.776 (2)	151 (3)
O4—H4″···O2	0.86 (5)	2.11 (5)	2.937 (3)	161 (4)
O4—H4″···N1	0.86 (5)	2.38 (5)	2.929 (3)	122 (4)
O4—H4′···O1	0.97 (5)	2.07 (5)	3.003 (3)	163 (4)
O4—H4′···N1	0.97 (5)	2.56 (5)	2.929 (3)	103 (4)
N2—H2A···O3	0.89 (2)	2.09 (2)	2.521 (3)	109 (2)

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

Data collection: *CAD-4* (Enraf–Nonius, 1994); cell refinement: *SET4* and *CELDIM* (Enraf–Nonius, 1994); data reduction: *HELENA* (Spek, 1996) and *PLATON* (Spek, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *PLATON*; software used to prepare material for publication: *XCIF* in *SHELXTL* (Sheldrick, 1997*b*).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2031).

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supplementary materials

Acta Cryst. (2007). E**63**, o4078-o4079 [**doi:10.1107/S1600536807044443**]

(*E*)-*N*'-[(Furan-2-yl)methylene]-2-hydroxy-2,2-diphenylacetohydrazide monohydrate

M. A. Khanfar, K. A. Abu-Safieh, R. Al-Far, B. F. Ali and C. Maichle-Moessmer

Comment

Schiff base hydrazones derived from the condensation of aromatic carbaldehydes and hydrazides are of interest owing to their biological activities and applications (Sun *et al.*, 2006; Gup & Kirkan, 2005; Ganjali *et al.*, 2006; Getautis *et al.*, 2006). They have been also used as multidentate ligands for complexation with metal ions (Kuriakose *et al.*, 2007). On the other hand, research in the field of supramolecular complexes containing metal ions and aroylhdrazones is of a considerable interest due to their possible applications as molecule-based metals and magnets, optical and thermal switches, and probes for DNA structurs (Owen & Wenbin, 2002; Tobin, 1990). The crystal structure of the title compound is reported here.

The asymmetric unit of the title compound comprises an organic moiety and a water of solvation (Fig. 1). Bond distances and angles, are within normal ranges (Allen *et al.*, 1987), and in accordance with those reported for similar compounds (Yathirajan *et al.*, 2007; Mathew *et al.*, 2007; Sun *et al.*, 2007). The existance of organic moiety in the title compound in the expected keto form is evident from the C6—O2 bond length, and the C5=N1 bond length confirms the double bond character. The C6–N2 bond length is typical for an intermediate between a single and a double bond, suggesting some degree of delocalization in the hydrazide.

The molecules are packed efficiently in a layer motif running parallel to the *c* axis, Fig. 2. In this arrangement, the molecules are linked to each other by water molecules that involve in multihydrogen bonding with the organic moiety. Its two H atoms engage each in binding to one O and one N atoms simultyaneouly (Fig. 1) as O—H···N, O—H···O and O—H···O, forming a double bifurcated hydrogen bonds. The water molecules further interact with the OH groups from the next organic molecule parallel to *c* axis (Fig. 2). These hydrogen bonds are extremely strong (Table 1) as is evident by relatively short D···A distances and D—H···A angles. There is a strong intramolecular interaction N2—H2A···O3 in the structure. In addition to the hydrogen bonding, molecules within layers exhibit *via* phenyl···phenyl (Ph···Ph) interactions (Dance 1996) in an edge-to-face **ef** motif (C—H···π; C12—H12···C17, C18 (*x*, 1/2 − *y*, 1/2 + *z*) of the order of 2.969 and 2.978 Å, respectively). The Ph···Ph interactions, using the diphenyl groups, between each layer and the adjacent one parallel to the *a* axis also exist comprising both offset-to-face (**off**) and edge-to-face (**ef**) motifs (C···C distances in the range 3.9 − 4.1 Å), Fig. 2.

Ph···Ph interactions together with the extremely strong hydrogen bonds contribute greatly in stabilization of a three-dimensional network.

Experimental

For the preparation of the title compound, a mixture of 2-hydroxy-2,2-diphenylacetohydrazide (240 mg, 1 mmol) and furan-2-carbaldehyde (110 mg, 1.1 mmol) dissolved in propanol (25 ml), was refluxed with stirring for 3 h. The resulting mixture was filtered off and allowed to stand undisturbed at room temperature. The title compound crystallized out during few days as colourless plates. Crystals were filtered off, washed with 20 ml cold methanol then 10 ml diethylether, and dried under vacuum (yield: 89%). Solid; mp 451–452 K; Spectroscopic analysis: IR (KBr, ν cm^{-1}): 3280; νNH, 1667; νC=O,

1625; νC=N; ^{1}H NMR (300 MHz, DMSO, δ, p.p.m.): 3.50 (s, OH); 9.9 (s, CONH); 9.30 (s,CH=); 7.10 − 7.40 (m, ArH); 7.70–7.90 (m, *R*); EIMS: m/*z* = 320 (*M*+).

Refinement

All H atoms were located in the difference map and refined independently with isotropic thermal displacement coefficients.

Figures

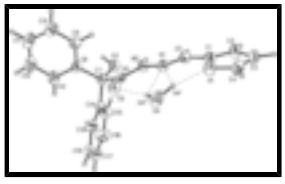

Fig. 1. The structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

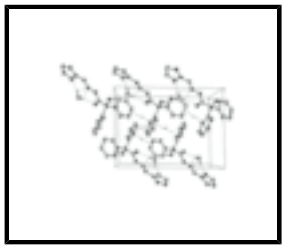

Fig. 2. Packing diagram of the title compound showing the layers of molecules; hydrogen atoms not involved in hydrogen bonding were omitted for clarity. Hydrogen bonds and Ph···Ph interactions are shown with dashed and solid lines, respectively.

(*E*)—*N*'-[(furan-2-yl)methylene]-2-hydroxy-2,2- diphenylacetohydrazide monohydrate

Crystal data

$C_{19}H_{16}N_2O_3·H_2O$	F_{000} = 712
M_r = 338.35	D_x = 1.341 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
a = 10.6339 (17) Å	θ = 2.1–27.4º
b = 10.857 (2) Å	μ = 0.10 mm^{-1}
c = 14.5207 (12) Å	*T* = 213 (2) K
β = 91.819 (10)º	Plate, colorless
V = 1675.6 (4) Å^3	0.55 × 0.50 × 0.20 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.054
Radiation source: fine-focus sealed tube	θ_{max} = 26.1º
Monochromator: graphite	θ_{min} = 3.1º
T = 293(2) K	*h* = −1→13
ω scans	*k* = 0→13
Absorption correction: ψ scan	*l* = −17→17

(program; reference?)

T_{min} = 0.937, T_{max} = 0.985

3847 measured reflections

3293 independent reflections

1981 reflections with $I > 2\sigma(I)$

3 standard reflections

every 400 reflections

intensity decay: 3.0%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.123$

$S = 1.01$

3293 reflections

298 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.0604P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.17$ e Å^{-3}

$\Delta\rho_{min} = -0.20$ e Å^{-3}

Extinction correction: none

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 $F^2 > 2$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	1.1720 (2)	0.2889 (2)	0.13010 (15)	0.0332 (5)
O1	1.14268 (15)	0.18466 (15)	0.07977 (11)	0.0413 (4)
C4	1.2148 (3)	0.1898 (3)	0.00285 (17)	0.0436 (6)
H4	1.201 (2)	0.116 (3)	−0.0400 (18)	0.058 (8)*
C3	1.2863 (3)	0.2907 (3)	0.00473 (17)	0.0444 (6)
H3	1.346 (2)	0.316 (2)	−0.0402 (19)	0.058 (8)*
C2	1.2589 (2)	0.3555 (3)	0.08660 (18)	0.0413 (6)
H2	1.288 (2)	0.432 (3)	0.1031 (18)	0.053 (8)*
C5	1.1047 (2)	0.3121 (2)	0.21232 (16)	0.0346 (5)
H5	1.124 (2)	0.390 (2)	0.2423 (15)	0.038 (6)*
N1	1.02022 (17)	0.23747 (18)	0.23979 (12)	0.0347 (5)
N2	0.95604 (18)	0.2774 (2)	0.31553 (13)	0.0341 (5)
H2A	0.978 (2)	0.347 (2)	0.3437 (16)	0.037 (7)*

O2	0.81756 (15)	0.11956 (15)	0.30338 (11)	0.0408 (4)
C6	0.8530 (2)	0.2155 (2)	0.34018 (14)	0.0311 (5)
C7	0.7808 (2)	0.2756 (2)	0.41943 (15)	0.0330 (5)
O3	0.85302 (15)	0.38056 (15)	0.44913 (12)	0.0368 (4)
H3A	0.851 (3)	0.390 (3)	0.512 (2)	0.084 (11)*
C8	0.7711 (2)	0.1843 (2)	0.49953 (14)	0.0336 (5)
C9	0.8780 (3)	0.1208 (2)	0.52946 (17)	0.0413 (6)
H9	0.955 (2)	0.130 (2)	0.4964 (17)	0.049 (7)*
C10	0.8751 (3)	0.0443 (2)	0.60630 (17)	0.0472 (7)
H10	0.953 (3)	−0.001 (3)	0.6239 (18)	0.055 (8)*
C11	0.7665 (3)	0.0320 (3)	0.65384 (18)	0.0526 (8)
H11	0.762 (2)	−0.023 (2)	0.708 (2)	0.061 (8)*
C12	0.6610 (3)	0.0944 (3)	0.6250 (2)	0.0588 (8)
H12	0.584 (3)	0.088 (3)	0.652 (2)	0.070 (9)*
C13	0.6619 (3)	0.1708 (3)	0.54799 (18)	0.0480 (7)
H13	0.586 (2)	0.213 (2)	0.5267 (18)	0.053 (8)*
C14	0.6519 (2)	0.3186 (2)	0.38027 (14)	0.0331 (5)
C19	0.5693 (2)	0.2389 (3)	0.33438 (17)	0.0425 (6)
H19	0.593 (2)	0.155 (3)	0.3246 (18)	0.048 (8)*
C18	0.4533 (3)	0.2802 (3)	0.30040 (19)	0.0504 (7)
H18	0.400 (3)	0.226 (2)	0.2699 (18)	0.054 (8)*
C17	0.4181 (3)	0.4014 (3)	0.31322 (19)	0.0520 (8)
H17	0.340 (3)	0.429 (3)	0.2918 (18)	0.059 (8)*
C16	0.4982 (3)	0.4808 (3)	0.3585 (2)	0.0538 (7)
H16	0.474 (3)	0.568 (3)	0.3693 (19)	0.063 (8)*
C15	0.6151 (3)	0.4395 (3)	0.39158 (18)	0.0456 (7)
H15	0.669 (3)	0.496 (2)	0.4232 (19)	0.055 (8)*
O4	0.9139 (2)	0.03785 (18)	0.12617 (13)	0.0501 (5)
H4"	0.892 (4)	0.079 (4)	0.174 (3)	0.137 (18)*
H4'	0.997 (4)	0.071 (4)	0.116 (3)	0.123 (15)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0347 (13)	0.0348 (13)	0.0300 (12)	0.0010 (11)	0.0006 (10)	−0.0048 (11)
O1	0.0487 (10)	0.0379 (9)	0.0380 (9)	−0.0019 (8)	0.0098 (8)	−0.0047 (8)
C4	0.0563 (16)	0.0442 (15)	0.0309 (13)	0.0065 (14)	0.0097 (12)	−0.0021 (12)
C3	0.0478 (15)	0.0518 (17)	0.0343 (13)	0.0051 (14)	0.0122 (12)	0.0069 (13)
C2	0.0453 (16)	0.0393 (15)	0.0398 (15)	−0.0069 (12)	0.0072 (12)	−0.0003 (12)
C5	0.0348 (13)	0.0373 (14)	0.0318 (12)	−0.0024 (12)	0.0018 (10)	−0.0052 (11)
N1	0.0372 (11)	0.0400 (11)	0.0270 (10)	0.0027 (9)	0.0053 (8)	−0.0032 (9)
N2	0.0386 (11)	0.0366 (11)	0.0276 (10)	−0.0036 (10)	0.0070 (8)	−0.0069 (9)
O2	0.0500 (10)	0.0373 (10)	0.0357 (9)	−0.0073 (8)	0.0091 (8)	−0.0073 (8)
C6	0.0359 (13)	0.0333 (13)	0.0241 (11)	−0.0002 (11)	−0.0002 (9)	0.0003 (10)
C7	0.0370 (13)	0.0336 (13)	0.0284 (12)	−0.0031 (11)	0.0011 (10)	−0.0039 (10)
O3	0.0439 (10)	0.0381 (9)	0.0285 (9)	−0.0079 (8)	0.0031 (8)	−0.0063 (8)
C8	0.0405 (13)	0.0373 (13)	0.0230 (11)	−0.0031 (11)	0.0017 (10)	−0.0040 (10)
C9	0.0421 (15)	0.0484 (16)	0.0332 (13)	−0.0046 (13)	−0.0023 (12)	−0.0016 (12)

C10	0.0601 (18)	0.0457 (16)	0.0353 (14)	−0.0015 (15)	−0.0073 (13)	0.0006 (12)
C11	0.081 (2)	0.0479 (17)	0.0291 (14)	−0.0066 (16)	0.0059 (14)	0.0025 (13)
C12	0.065 (2)	0.069 (2)	0.0439 (17)	−0.0013 (17)	0.0223 (15)	0.0081 (15)
C13	0.0477 (16)	0.0589 (18)	0.0380 (14)	0.0064 (14)	0.0117 (13)	0.0048 (13)
C14	0.0365 (12)	0.0414 (14)	0.0216 (11)	−0.0010 (11)	0.0056 (10)	0.0013 (10)
C19	0.0415 (15)	0.0479 (17)	0.0380 (14)	−0.0075 (13)	−0.0017 (11)	0.0000 (12)
C18	0.0396 (15)	0.069 (2)	0.0418 (15)	−0.0119 (15)	−0.0047 (12)	0.0025 (15)
C17	0.0400 (16)	0.077 (2)	0.0396 (15)	0.0099 (16)	0.0021 (13)	0.0074 (15)
C16	0.0537 (18)	0.057 (2)	0.0507 (16)	0.0158 (15)	0.0037 (14)	−0.0042 (15)
C15	0.0490 (16)	0.0456 (16)	0.0421 (14)	0.0016 (14)	−0.0013 (13)	−0.0090 (13)
O4	0.0717 (14)	0.0477 (12)	0.0309 (10)	−0.0153 (10)	0.0000 (9)	−0.0013 (9)

Geometric parameters (Å, °)

C1—C2	1.347 (3)	C9—C10	1.392 (4)
C1—O1	1.377 (3)	C9—H9	0.97 (3)
C1—C5	1.434 (3)	C10—C11	1.370 (4)
O1—C4	1.376 (3)	C10—H10	0.99 (3)
C4—C3	1.333 (4)	C11—C12	1.365 (4)
C4—H4	1.02 (3)	C11—H11	0.98 (3)
C3—C2	1.420 (4)	C12—C13	1.393 (4)
C3—H3	0.96 (3)	C12—H12	0.92 (3)
C2—H2	0.91 (3)	C13—H13	0.97 (3)
C5—N1	1.282 (3)	C14—C15	1.381 (3)
C5—H5	0.97 (2)	C14—C19	1.389 (3)
N1—N2	1.382 (3)	C19—C18	1.388 (4)
N2—C6	1.343 (3)	C19—H19	0.95 (3)
N2—H2A	0.89 (2)	C18—C17	1.381 (4)
O2—C6	1.225 (3)	C18—H18	0.92 (3)
C6—C7	1.548 (3)	C17—C16	1.366 (4)
C7—O3	1.433 (3)	C17—H17	0.93 (3)
C7—C8	1.534 (3)	C16—C15	1.392 (4)
C7—C14	1.539 (3)	C16—H16	1.00 (3)
O3—H3A	0.92 (3)	C15—H15	0.94 (3)
C8—C13	1.384 (3)	O4—H4"	0.86 (5)
C8—C9	1.388 (3)	O4—H4'	0.97 (5)
C2—C1—O1	109.8 (2)	C8—C9—H9	119.6 (15)
C2—C1—C5	131.6 (2)	C10—C9—H9	119.8 (15)
O1—C1—C5	118.4 (2)	C11—C10—C9	120.2 (3)
C4—O1—C1	105.93 (19)	C11—C10—H10	122.2 (15)
C3—C4—O1	110.4 (2)	C9—C10—H10	117.7 (16)
C3—C4—H4	136.8 (15)	C12—C11—C10	119.6 (3)
O1—C4—H4	112.8 (15)	C12—C11—H11	118.8 (16)
C4—C3—C2	107.0 (2)	C10—C11—H11	121.5 (16)
C4—C3—H3	127.2 (16)	C11—C12—C13	121.0 (3)
C2—C3—H3	125.8 (16)	C11—C12—H12	124.2 (19)
C1—C2—C3	106.8 (2)	C13—C12—H12	114.7 (19)
C1—C2—H2	126.6 (17)	C8—C13—C12	119.9 (3)
C3—C2—H2	126.3 (17)	C8—C13—H13	119.2 (16)

N1—C5—C1	121.4 (2)	C12—C13—H13	120.9 (16)
N1—C5—H5	123.4 (14)	C15—C14—C19	118.2 (2)
C1—C5—H5	115.0 (14)	C15—C14—C7	119.8 (2)
C5—N1—N2	114.69 (19)	C19—C14—C7	122.0 (2)
C6—N2—N1	118.8 (2)	C18—C19—C14	120.7 (3)
C6—N2—H2A	120.6 (16)	C18—C19—H19	119.2 (16)
N1—N2—H2A	120.3 (16)	C14—C19—H19	120.1 (16)
O2—C6—N2	123.5 (2)	C17—C18—C19	120.1 (3)
O2—C6—C7	122.0 (2)	C17—C18—H18	120.7 (17)
N2—C6—C7	114.5 (2)	C19—C18—H18	119.2 (17)
O3—C7—C8	109.50 (17)	C16—C17—C18	119.9 (3)
O3—C7—C14	109.42 (18)	C16—C17—H17	119.7 (17)
C8—C7—C14	113.30 (18)	C18—C17—H17	120.4 (17)
O3—C7—C6	106.54 (18)	C17—C16—C15	120.0 (3)
C8—C7—C6	109.77 (18)	C17—C16—H16	120.9 (16)
C14—C7—C6	108.08 (17)	C15—C16—H16	119.2 (16)
C7—O3—H3A	111 (2)	C14—C15—C16	121.2 (3)
C13—C8—C9	118.7 (2)	C14—C15—H15	120.0 (16)
C13—C8—C7	122.1 (2)	C16—C15—H15	118.8 (16)
C9—C8—C7	119.0 (2)	H4"—O4—H4'	102 (4)
C8—C9—C10	120.6 (3)		
C2—C1—O1—C4	−0.3 (3)	C6—C7—C8—C9	47.0 (3)
C5—C1—O1—C4	176.3 (2)	C13—C8—C9—C10	0.5 (4)
C1—O1—C4—C3	0.5 (3)	C7—C8—C9—C10	175.1 (2)
O1—C4—C3—C2	−0.5 (3)	C8—C9—C10—C11	−0.6 (4)
O1—C1—C2—C3	0.0 (3)	C9—C10—C11—C12	0.5 (4)
C5—C1—C2—C3	−176.0 (2)	C10—C11—C12—C13	−0.1 (4)
C4—C3—C2—C1	0.4 (3)	C9—C8—C13—C12	−0.1 (4)
C2—C1—C5—N1	176.7 (3)	C7—C8—C13—C12	−174.6 (2)
O1—C1—C5—N1	1.0 (3)	C11—C12—C13—C8	−0.1 (4)
C1—C5—N1—N2	−174.7 (2)	O3—C7—C14—C15	−10.3 (3)
C5—N1—N2—C6	169.5 (2)	C8—C7—C14—C15	112.2 (2)
N1—N2—C6—O2	5.7 (3)	C6—C7—C14—C15	−125.9 (2)
N1—N2—C6—C7	−174.00 (18)	O3—C7—C14—C19	170.6 (2)
O2—C6—C7—O3	176.32 (19)	C8—C7—C14—C19	−66.9 (3)
N2—C6—C7—O3	−4.0 (3)	C6—C7—C14—C19	55.0 (3)
O2—C6—C7—C8	57.9 (3)	C15—C14—C19—C18	0.4 (4)
N2—C6—C7—C8	−122.5 (2)	C7—C14—C19—C18	179.5 (2)
O2—C6—C7—C14	−66.2 (3)	C14—C19—C18—C17	−1.0 (4)
N2—C6—C7—C14	113.5 (2)	C19—C18—C17—C16	0.7 (4)
O3—C7—C8—C13	104.8 (2)	C18—C17—C16—C15	0.1 (4)
C14—C7—C8—C13	−17.6 (3)	C19—C14—C15—C16	0.4 (4)
C6—C7—C8—C13	−138.6 (2)	C7—C14—C15—C16	−178.8 (2)
O3—C7—C8—C9	−69.7 (3)	C17—C16—C15—C14	−0.6 (4)
C14—C7—C8—C9	167.9 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N2—H2A···O4^{i}	0.89 (2)	2.40 (2)	3.248 (3)	159 (2)
O3—H3A···O4^{ii}	0.92 (3)	1.94 (3)	2.776 (2)	151 (3)
O4—H4"···O2	0.86 (5)	2.11 (5)	2.937 (3)	161 (4)
O4—H4"···N1	0.86 (5)	2.38 (5)	2.929 (3)	122 (4)
O4—H4'···O1	0.97 (5)	2.07 (5)	3.003 (3)	163 (4)
O4—H4'···N1	0.97 (5)	2.56 (5)	2.929 (3)	103 (4)
N2—H2A···O3	0.89 (2)	2.09 (2)	2.521 (3)	109 (2)

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

Fig. 1

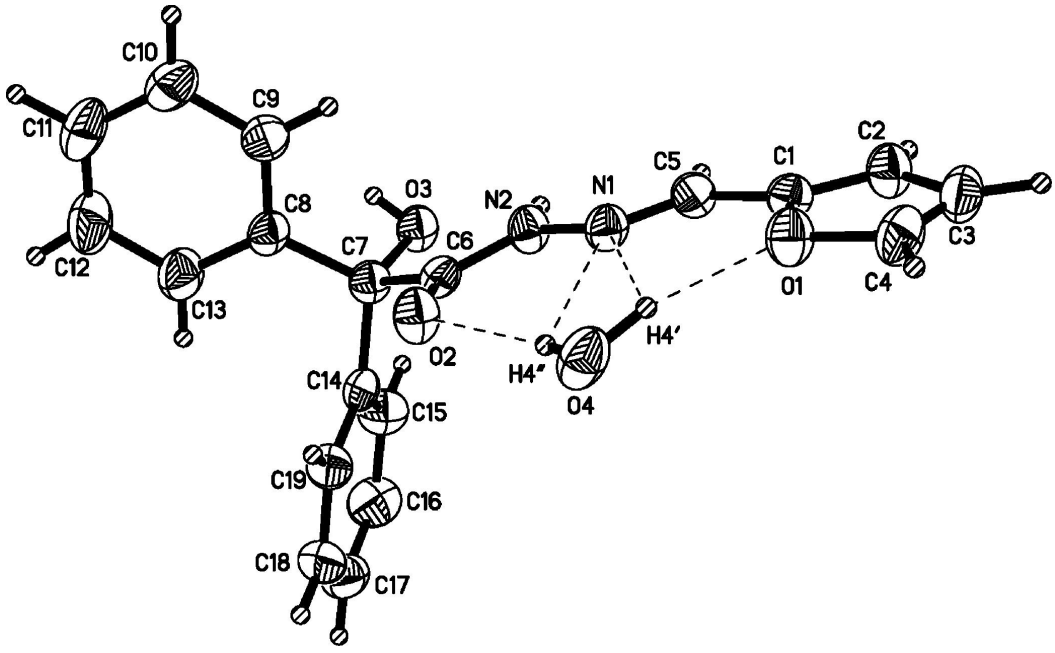
C10
C9
C11
C8
C12
C13
C7
C6
O3
N2
N1
C5
C1
C2
C3
C4
O1
O2
H4'
H4''
O4
C14
C15
C19
C16
C18
C17

Fig. 2