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N,*N*-Bis[2-(2-furyl)-2-(hydroxyimino)-ethyl]aniline

Özden Özel Güven,[a] Nagihan Çaylak[b] and Tuncer Hökelek[c]*

[a]Zonguldak Karaelmas University, Department of Chemistry, 67100 Zonguldak, Turkey, [b]Sakarya University, Faculty of Arts and Sciences, Department of Physics, 54187 Esentepe, Adapazarı, Turkey, and [c]Hacettepe University, Department of Physics, 06800 Beytepe, Ankara, Turkey
Correspondence e-mail: merzifon@hacettepe.edu.tr

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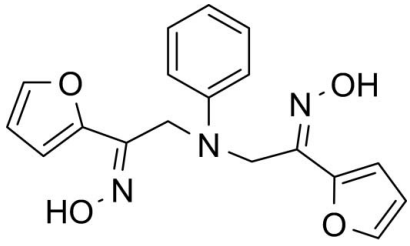
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.110; data-to-parameter ratio = 9.5.

In the crystal structure of the title compound, $C_{18}H_{17}N_3O_4$, intramolecular C—H···O hydrogen bonds cause the formation of two planar five-membered rings, which are also coplanar with the adjacent rings. The oxime units have *E* configurations and their bond lengths and angles compare well with those in related compounds. In this configuration, the oxime groups are involved as donors in O—H···N hydrogen bonds, linking the molecules into chains extending approximately parallel to the *c* axis and stacked along the *b* axis.

Related literature

For general background, see: Sevagapandian *et al.* (2000); Marsman *et al.* (1999); Coşkun *et al.* (1999); Karle *et al.* (1996); Etter *et al.* (1990); Chertanova *et al.* (1994); Balsamo *et al.* (1990); Lipshutz (1986); Holan *et al.* (1984); Forman (1964). For related literature, see: Sarıkavaklı *et al.* (2007); Özel Güven *et al.* (2007); Hökelek, Batı *et al.* (2001); Hökelek, Zülfikaroğlu & Batı (2001); Büyükgüngör *et al.* (2003); Hökelek *et al.* (2004); Hökelek *et al.* (2004*a*,*b*). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{17}N_3O_4$
M_r = 339.35
Monoclinic, $P2_1/n$
a = 11.2363 (2) Å
b = 11.9889 (3) Å
c = 12.8785 (4) Å
β = 109.886 (10)°
V = 1631.43 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.976, T_{max} = 0.985
2933 measured reflections
2801 independent reflections
1518 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.110
S = 0.99
2801 reflections
294 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N3^{i}	0.88 (4)	2.00 (4)	2.795 (3)	150 (3)
O4—H4A···N2^{ii}	0.94 (4)	1.90 (4)	2.771 (3)	154 (3)
C4—H4···O2	0.86 (2)	2.38 (2)	2.797 (4)	110.5 (19)
C16—H16···O4	0.97 (2)	2.38 (2)	2.822 (4)	107.5 (17)

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

Table 2
Comparison of the bond lengths and angles (Å, °) in the oxime group of (I) with the corresponding values in the related compounds (II)–(VII).

Bond/Angle	(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)
N2—O2	1.401 (2)	1.403 (2)	1.423 (3)	1.417 (1)	1.429 (4)	1.424 (2)	1.416 (3)
N3—O4	1.400 (2)	1.396 (2)	1.396 (3)				1.397 (3)
N2—C2	1.285 (3)	1.281 (2)	1.290 (3)	1.290 (1)	1.241 (6)	1.289 (2)	1.282 (3)
N3—C14	1.283 (3)	1.281 (2)	1.282 (3)				1.289 (3)
C1—C2	1.512 (3)	1.477 (3)	1.489 (3)	1.510 (1)	1.551 (7)	1.513 (2)	1.501 (4)
	1.515 (3)	1.473 (3)					1.502 (4)
C1—C2—N2	115.9 (2)	115.2 (2)	116.6 (2)	114.3 (1)	118.3 (5)	113.2 (1)	114.4 (2)
C13—C14—N3	116.4 (2)	115.0 (2)	115.0 (2)				113.4 (2)
C2—N2—O2	113.6 (2)	112.4 (1)	109.4 (2)	110.7 (1)	112.2 (4)	110.6 (1)	110.7 (2)
C14—N3—O4	113.4 (2)	112.2 (1)	111.5 (2)				111.1 (2)

Notes: (II), 2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek, Batı *et al.*, 2001); (III), 1-(2,6-dimethylphenylamino)propane-1,2-dione dioxime (Hökelek, Zülfikaroğlu & Batı, 2001); (IV), *N*-hydroxy-2-oxo-2,*N*′-diphenylacetamidine (Büyükgüngör *et al.*, 2003); (V), *N*-(3,4-dichlorophenyl)-*N*′-hydroxy-2-oxo-2-phenylacetamidine (Hökelek *et al.*, 2004); (VI), *N*-hydroxy-*N*′-(1-naphthyl)-2-phenylacetamidin-2-one (Hökelek *et al.*, 2004*a*); (VII), *N*-(3-chloro-4-methylphenyl)-*N*′-hydroxy-2-oxo-2-phenylacetamidine-2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek *et al.*, 2004*b*).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2310).

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supplementary materials

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N,*N*-Bis[2-(2-furyl)-2-(hydroxyimino)ethyl]aniline

Ö. Özel Güven, N. Çaylak and T. Hökelek

Comment

Furans, oximes and amines are very important compounds in organic chemistry. Furan is a relatively highly reactive heteroaromatic compound and is frequently used as an intermediate in organic synthesis (Lipshutz, 1986). In literature, Beckmann fragmentation reaction of *N*-aryl-*N*,*N*-diphenacylamine dioximes has been reported as a new method for the synthesis of imidazooxadiazolones which are imidazole derivatives (Coşkun *et al.*, 1999).

Oxime and dioxime derivatives are very important compounds in the chemical industry and medicine (Sevagapandian *et al.*, 2000). They have a broad pharmacological activity spectrum, encompassing antibacterial, antidepressant and antifungal activities (Forman, 1964; Holan *et al.*, 1984; Balsamo *et al.*, 1990). The oxime (–C=N—OH) moiety is potentially ambidentate, with possibilities of coordination through nitrogen and/or oxygen atoms. It is a functional group that has not been extensively explored in crystal engineering. In the solid state, oximes are usually associated *via* O—H···N hydrogen bonds of length 2.8 Å.

Oxime groups possess stronger hydrogen-bonding capabilities than alcohols, phenols, and carboxylic acids (Marsman *et al.*, 1999), in which intermolecular hydrogen bonding combines moderate strength and directionality (Karle *et al.*, 1996) in linking molecules to form supramolecular structures; this has received considerable attention with respect to directional noncovalent intermolecular interactions (Etter *et al.*, 1990).

The structures of oxime and dioxime derivatives have been the subject of much interest in our laboratory; examples are 2,3-dimethylquinoxaline-dimethyl- glyoxime (1/1), [(II) Hökelek, Batı *et al.*, 2001], 1-(2,6-dimethylphenylamino)propane-1,2-dione dioxime, [(III) (Hökelek, Zülfikaroğlu & Batı, 2001), *N*-hydroxy-2-oxo-2,*N*'-diphenylacetamidine, [(IV) (Büyükgüngör *et al.*, 2003], *N*-(3,4-dichlorophenyl)-*N*'-hydroxy-2-oxo-2-phenylacetamidine, [(V) Hökelek *et al.*, 2004], *N*-hydroxy-*N*'-(1-naphthyl)-2-phenylacetamidin-2-one [(VI) Hökelek *et al.*, 2004*a*], *N*-(3-chloro-4-methylphenyl)-*N*'-hydroxy-2 -oxo-2-phenylacetamidine [(VII) Hökelek *et al.*, 2004*b*], 2-(1*H*-benzimidazol −1-yl)-1-phenylethanone oxime [(VIII) Özel Güven *et al.*, 2007] and (1*Z*,2E)-1-(3,5-dimethyl-1*H*-pyrazole-1-yl)ethane-1,2-dione dioxime [(IX) Sarıkavaklı *et al.*, 2007]. The structure determination of the title molecule, (I) was carried out in order to investigate the strength of the hydrogen bonding capability of the oxime groups and to compare the geometry of the oxime moieties with the previously reported ones.

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). The intramolecular C—H···O hydrogen bonds (Table 1) cause the formation of two planar five-membered rings A (O2/N2/C2—C4/H4) and B (O4/N3/C14—C16/H16). The rings C (O1/C3—C6), D (C7—C12) and E (O3/C15—C18) are, of course, planar and rings A, C and B, D are also coplanar with dihedral angles of A/C = 1.11 (10)° and B/D = 5.60 (10)°. The coplanar ring systems containing rings A and B are oriented at a dihedral angle of 47.76 (5)°, their orientations with respect to ring C may also be given by the dihedral angles of 89.01 (9)° and 78.73 (9)°, respectively.

Some significant changes in the geometry of the oxime moieties are evident when the bond lengths and angles are compared with the corresponding values in compounds (II)-(VII) (Table 2). The oxime moieties have E configurations

[C1—C2—N2—O2 − 177.9 (2)° and C13—C14—N3—O4 − 179.2 (2)°; Chertanova *et al.*, 1994]. In this configuration, the oxime groups are involved as donors in O—H···N intermolecular hydrogen bondings (Table 1).

In the crystal structure, the intermolecular O—H···N hydrogen bonds (Table 1) link the molecules into chains elongated approximately parallel to the *c* axis and stacked along the *b* axis (Fig. 2). The intra- and intermolecular hydrogen bonds seem to be effective in the stabilization of the crystal structure.

Experimental

For the preparation of the title compound, 2-bromo-1-(2-furanyl)ethanone oxime (81 mg, 0.399 mmol) was added portion-wise to a solution of aniline (56 mg, 0.599 mmol) in ethanol (50%, 0.4 ml) within 5 min, at room temperature. Reaction mixture was stirred at room temperature for 1 night. The formed precipitate was filtered and recrystallized from DMSO to obtain brown crystals (yield; 40 mg, 30%).

Refinement

H atoms were located in difference syntheses and refined isotropically [O—H = 0.89 (3) and 0.94 (3) Å, U_{iso}(H) = 0.106 (13) and 0.101 (12) Å^2 and C—H = 0.86 (2)–1.02 (2) Å, U_{iso}(H) = 0.040 (7)–0.085 (12) Å^2].

Figures

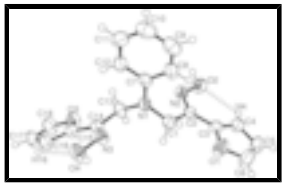

Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

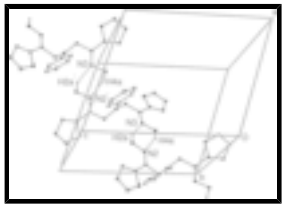

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity [symmetry code: (') *x* + 1/2, −*y* + 1/2, *z* + 1/2].

N,*N*-Bis[2-(2-furyl)-2-(hydroxyimino)ethyl]aniline

Crystal data

$C_{18}H_{17}N_3O_4$	F_{000} = 712
M_r = 339.35	D_x = 1.382 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 486-487 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.2363 (2) Å	Cell parameters from 25 reflections
b = 11.9889 (3) Å	θ = 2.7–21.6º
c = 12.8785 (4) Å	μ = 0.10 mm^{-1}

β = 109.886 (10)º	T = 298 (2) K
V = 1631.43 (13) Å^3	Block, dark-yellow
Z = 4	0.25 × 0.20 × 0.15 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer	R_{int} = 0.026
Radiation source: fine-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 2.4º
T = 298(2) K	h = −12→13
Non–profiled ω scans	k = 0→14
Absorption correction: ψ scan (North *et al.*, 1968)	l = −15→0
T_{min} = 0.976, T_{max} = 0.985	3 standard reflections
2933 measured reflections	every 120 min
2801 independent reflections	intensity decay: 1%
1518 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.042	All H-atom parameters refined
$wR(F^2)$ = 0.110	$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.0438P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max} < 0.001$
2801 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
294 parameters	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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}

O1	−0.22619 (16)	0.61727 (18)	0.45244 (14)	0.0707 (6)
O2	0.15196 (17)	0.66194 (17)	0.58964 (14)	0.0529 (5)
H2A	0.230 (3)	0.687 (3)	0.604 (3)	0.106 (13)*
O3	0.15759 (15)	0.60813 (16)	0.08792 (13)	0.0540 (5)
O4	−0.19768 (17)	0.72757 (18)	−0.06184 (14)	0.0613 (6)
H4A	−0.279 (3)	0.754 (3)	−0.071 (3)	0.101 (12)*
N1	−0.02799 (19)	0.77039 (19)	0.27240 (16)	0.0440 (6)
N2	0.09068 (19)	0.69508 (17)	0.48006 (16)	0.0427 (6)
N3	−0.14059 (18)	0.73967 (18)	0.05252 (15)	0.0451 (6)
C1	−0.0994 (3)	0.7060 (3)	0.3259 (2)	0.0445 (7)
H1A	−0.128 (3)	0.636 (2)	0.286 (2)	0.069 (9)*
H1B	−0.176 (2)	0.7478 (19)	0.3208 (17)	0.043 (7)*
C2	−0.0290 (2)	0.67560 (19)	0.44496 (19)	0.0357 (6)
C3	−0.0995 (2)	0.6263 (2)	0.5084 (2)	0.0392 (6)
C4	−0.0747 (3)	0.5883 (2)	0.6112 (2)	0.0460 (7)
H4	−0.001 (2)	0.588 (2)	0.661 (2)	0.050 (8)*
C5	−0.1896 (3)	0.5536 (3)	0.6213 (2)	0.0562 (8)
H5	−0.197 (2)	0.523 (2)	0.686 (2)	0.051 (7)*
C6	−0.2763 (3)	0.5709 (3)	0.5256 (3)	0.0762 (11)
H6	−0.363 (3)	0.560 (2)	0.492 (2)	0.078 (10)*
C7	−0.0231 (2)	0.8855 (2)	0.27923 (19)	0.0390 (6)
C8	−0.0736 (3)	0.9441 (3)	0.3477 (2)	0.0503 (8)
H8	−0.108 (2)	0.9039 (18)	0.3939 (18)	0.040 (7)*
C9	−0.0730 (3)	1.0586 (3)	0.3505 (3)	0.0620 (9)
H9	−0.106 (3)	1.095 (2)	0.404 (2)	0.079 (10)*
C10	−0.0184 (3)	1.1184 (3)	0.2890 (3)	0.0682 (10)
H10	−0.019 (3)	1.196 (3)	0.288 (2)	0.085 (12)*
C11	0.0357 (3)	1.0632 (3)	0.2229 (3)	0.0616 (9)
H11	0.082 (2)	1.100 (2)	0.184 (2)	0.066 (9)*
C12	0.0337 (2)	0.9481 (3)	0.2178 (2)	0.0499 (8)
H12	0.067 (2)	0.9119 (19)	0.1705 (19)	0.045 (7)*
C13	0.0401 (3)	0.7107 (3)	0.2132 (2)	0.0439 (7)
H13A	0.127 (2)	0.745 (2)	0.2293 (18)	0.053 (7)*
H13B	0.057 (2)	0.634 (2)	0.2408 (18)	0.051 (8)*
C14	−0.0271 (2)	0.7019 (2)	0.08969 (19)	0.0377 (6)
C15	0.0415 (2)	0.6506 (2)	0.02531 (19)	0.0401 (6)
C16	0.0236 (3)	0.6337 (2)	−0.0823 (2)	0.0491 (7)
H16	−0.052 (2)	0.655 (2)	−0.142 (2)	0.067 (8)*
C17	0.1327 (3)	0.5777 (3)	−0.0875 (3)	0.0571 (8)
H17	0.145 (3)	0.554 (2)	−0.151 (2)	0.076 (10)*
C18	0.2093 (3)	0.5647 (3)	0.0156 (3)	0.0604 (9)
H18	0.291 (2)	0.529 (2)	0.048 (2)	0.070 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0385 (11)	0.1210 (19)	0.0489 (12)	−0.0134 (12)	0.0101 (9)	0.0154 (12)
O2	0.0347 (11)	0.0764 (15)	0.0415 (11)	−0.0034 (10)	0.0050 (9)	0.0081 (10)

O3	0.0361 (10)	0.0817 (15)	0.0418 (10)	0.0165 (10)	0.0100 (8)	−0.0058 (11)
O4	0.0412 (11)	0.0971 (17)	0.0376 (10)	0.0189 (11)	0.0028 (9)	−0.0068 (11)
N1	0.0527 (13)	0.0472 (15)	0.0385 (12)	0.0024 (11)	0.0237 (10)	−0.0013 (11)
N2	0.0384 (13)	0.0526 (14)	0.0344 (12)	−0.0021 (10)	0.0089 (10)	−0.0005 (11)
N3	0.0376 (12)	0.0624 (15)	0.0315 (12)	0.0091 (12)	0.0069 (10)	−0.0018 (11)
C1	0.0404 (17)	0.054 (2)	0.0370 (16)	−0.0042 (15)	0.0106 (13)	−0.0001 (14)
C2	0.0315 (14)	0.0380 (15)	0.0374 (14)	0.0001 (12)	0.0113 (11)	−0.0055 (12)
C3	0.0287 (14)	0.0451 (16)	0.0403 (15)	0.0003 (12)	0.0069 (12)	−0.0035 (13)
C4	0.0406 (16)	0.0547 (19)	0.0405 (16)	−0.0023 (15)	0.0109 (14)	0.0040 (15)
C5	0.0562 (19)	0.070 (2)	0.0479 (19)	0.0031 (16)	0.0243 (16)	0.0139 (16)
C6	0.045 (2)	0.125 (3)	0.063 (2)	−0.015 (2)	0.0230 (18)	0.016 (2)
C7	0.0316 (13)	0.0517 (19)	0.0287 (13)	0.0018 (13)	0.0039 (11)	−0.0017 (13)
C8	0.0467 (17)	0.064 (2)	0.0423 (17)	0.0030 (15)	0.0186 (14)	−0.0042 (16)
C9	0.065 (2)	0.060 (2)	0.056 (2)	0.0140 (17)	0.0134 (17)	−0.0082 (18)
C10	0.076 (2)	0.051 (2)	0.065 (2)	0.0048 (19)	0.0077 (19)	−0.003 (2)
C11	0.063 (2)	0.059 (2)	0.055 (2)	−0.0153 (18)	0.0099 (17)	0.0082 (18)
C12	0.0469 (16)	0.064 (2)	0.0399 (16)	−0.0026 (15)	0.0161 (13)	−0.0024 (16)
C13	0.0437 (17)	0.0502 (19)	0.0358 (16)	0.0090 (15)	0.0111 (13)	−0.0004 (14)
C14	0.0334 (14)	0.0430 (16)	0.0357 (14)	0.0017 (12)	0.0103 (11)	0.0001 (12)
C15	0.0302 (14)	0.0492 (17)	0.0390 (15)	0.0048 (12)	0.0091 (11)	−0.0019 (13)
C16	0.0403 (16)	0.069 (2)	0.0370 (16)	0.0037 (15)	0.0117 (13)	−0.0049 (15)
C17	0.0486 (17)	0.082 (2)	0.0460 (18)	0.0007 (16)	0.0225 (15)	−0.0165 (17)
C18	0.0409 (18)	0.087 (3)	0.056 (2)	0.0131 (17)	0.0195 (16)	−0.0115 (17)

Geometric parameters (Å, °)

O1—C3	1.364 (3)	C6—H6	0.94 (3)
O1—C6	1.369 (3)	C7—C8	1.391 (3)
O2—N2	1.401 (2)	C7—C12	1.393 (4)
O2—H2A	0.89 (3)	C8—C9	1.372 (4)
O3—C15	1.376 (3)	C8—H8	0.94 (2)
O3—C18	1.357 (3)	C9—C10	1.361 (4)
O4—H4A	0.94 (3)	C9—H9	0.98 (3)
N1—C1	1.446 (3)	C10—H10	0.93 (3)
N1—C7	1.383 (3)	C11—C10	1.372 (4)
N1—C13	1.441 (3)	C11—H11	0.95 (3)
N2—C2	1.285 (3)	C12—C11	1.381 (4)
N3—O4	1.400 (2)	C12—H12	0.93 (2)
N3—C14	1.283 (3)	C13—H13A	1.02 (2)
C1—H1A	0.98 (3)	C13—H13B	0.98 (3)
C1—H1B	0.98 (2)	C14—C13	1.515 (3)
C2—C1	1.512 (3)	C14—C15	1.447 (3)
C2—C3	1.444 (3)	C15—C16	1.346 (3)
C3—C4	1.337 (3)	C16—C17	1.419 (4)
C4—C5	1.403 (4)	C16—H16	0.97 (2)
C4—H4	0.86 (2)	C17—H17	0.92 (3)
C5—C6	1.301 (4)	C18—C17	1.324 (4)
C5—H5	0.93 (3)	C18—H18	0.97 (3)
C3—O1—C6	105.6 (2)	C7—C8—H8	118.9 (14)

N2—O2—H2A	103 (2)	C10—C9—C8	120.7 (3)
C18—O3—C15	106.3 (2)	C10—C9—H9	121.4 (17)
N3—O4—H4A	99.9 (19)	C8—C9—H9	117.7 (17)
C7—N1—C1	121.3 (2)	C9—C10—C11	119.3 (4)
C7—N1—C13	120.8 (2)	C9—C10—H10	121.8 (19)
C13—N1—C1	117.9 (3)	C11—C10—H10	118.8 (19)
C2—N2—O2	113.6 (2)	C10—C11—C12	120.5 (3)
C14—N3—O4	113.43 (19)	C10—C11—H11	122.9 (17)
N1—C1—C2	115.3 (2)	C12—C11—H11	116.4 (17)
N1—C1—H1B	108.1 (13)	C11—C12—C7	121.0 (3)
C2—C1—H1B	109.6 (13)	C11—C12—H12	119.6 (15)
N1—C1—H1A	110.4 (16)	C7—C12—H12	119.3 (15)
C2—C1—H1A	106.8 (15)	N1—C13—C14	115.2 (2)
H1B—C1—H1A	106 (2)	N1—C13—H13B	110.1 (14)
N2—C2—C3	125.8 (2)	C14—C13—H13B	106.4 (14)
N2—C2—C1	115.9 (2)	N1—C13—H13A	109.9 (13)
C3—C2—C1	118.3 (2)	C14—C13—H13A	110.2 (13)
C4—C3—O1	108.9 (2)	H13B—C13—H13A	104.5 (19)
C4—C3—C2	136.9 (2)	N3—C14—C15	126.3 (2)
O1—C3—C2	114.1 (2)	N3—C14—C13	116.4 (2)
C3—C4—C5	107.8 (3)	C15—C14—C13	117.3 (2)
C3—C4—H4	124.2 (17)	C16—C15—O3	109.1 (2)
C5—C4—H4	128.0 (17)	C16—C15—C14	137.0 (2)
C6—C5—C4	106.3 (3)	O3—C15—C14	113.9 (2)
C6—C5—H5	129.7 (15)	C15—C16—C17	106.9 (2)
C4—C5—H5	124.0 (15)	C15—C16—H16	124.0 (16)
C5—C6—O1	111.5 (3)	C17—C16—H16	129.1 (16)
C5—C6—H6	138.5 (18)	C18—C17—C16	106.6 (3)
O1—C6—H6	110.1 (18)	C18—C17—H17	127.9 (18)
N1—C7—C8	121.9 (2)	C16—C17—H17	125.5 (18)
N1—C7—C12	121.2 (2)	C17—C18—O3	111.0 (3)
C8—C7—C12	116.9 (3)	C17—C18—H18	132.9 (16)
C9—C8—C7	121.5 (3)	O3—C18—H18	116.1 (16)
C9—C8—H8	119.6 (14)		
C6—O1—C3—C4	−0.8 (3)	C3—C2—C1—N1	170.7 (2)
C6—O1—C3—C2	−179.2 (3)	O1—C3—C4—C5	0.1 (3)
C3—O1—C6—C5	1.2 (4)	C2—C3—C4—C5	178.0 (3)
C15—O3—C18—C17	0.0 (3)	C3—C4—C5—C6	0.6 (4)
C18—O3—C15—C16	−0.2 (3)	C4—C5—C6—O1	−1.1 (4)
C18—O3—C15—C14	−179.4 (2)	N1—C7—C8—C9	−177.2 (2)
C7—N1—C1—C2	−86.9 (3)	C12—C7—C8—C9	3.2 (4)
C13—N1—C1—C2	92.0 (3)	N1—C7—C12—C11	178.5 (2)
C13—N1—C7—C8	−171.2 (2)	C8—C7—C12—C11	−2.0 (4)
C1—N1—C7—C8	7.7 (4)	C7—C8—C9—C10	−2.5 (5)
C13—N1—C7—C12	8.4 (3)	C8—C9—C10—C11	0.5 (5)
C1—N1—C7—C12	−172.8 (2)	C12—C11—C10—C9	0.7 (5)
C7—N1—C13—C14	−83.6 (3)	C7—C12—C11—C10	0.1 (4)
C1—N1—C13—C14	97.5 (3)	N3—C14—C13—N1	−5.7 (4)
O2—N2—C2—C3	1.0 (3)	C15—C14—C13—N1	175.1 (2)

O2—N2—C2—C1	−177.9 (2)	N3—C14—C15—C16	6.9 (5)
O4—N3—C14—C15	−0.1 (4)	C13—C14—C15—C16	−174.0 (3)
O4—N3—C14—C13	−179.2 (2)	N3—C14—C15—O3	−174.2 (2)
N2—C2—C3—C4	0.6 (5)	C13—C14—C15—O3	5.0 (3)
C1—C2—C3—C4	179.5 (3)	O3—C15—C16—C17	0.3 (3)
N2—C2—C3—O1	178.4 (2)	C14—C15—C16—C17	179.2 (3)
C1—C2—C3—O1	−2.7 (3)	C15—C16—C17—C18	−0.2 (4)
N2—C2—C1—N1	−10.3 (4)	O3—C18—C17—C16	0.1 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···N3^{i}	0.88 (4)	2.00 (4)	2.795 (3)	150 (3)
O4—H4A···N2^{ii}	0.94 (4)	1.90 (4)	2.771 (3)	154 (3)
C4—H4···O2	0.86 (2)	2.38 (2)	2.797 (4)	110.5 (19)
C16—H16···O4	0.97 (2)	2.38 (2)	2.822 (4)	107.5 (17)

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

Comparison of the bond lengths and angles (Å, °) in the oxime group of (I) with the corresponding values in the related compounds (II)–(VII)

Bond/Angle	(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)
N2-O2	1.401 (2)	1.403 (2)	1.423 (3)	1.417 (1)	1.429 (4)	1.424 (2)	1.416 (3)
N3-O4	1.400 (2)	1.396 (2)	1.396 (3)				1.397 (3)
N2-C2	1.285 (3)	1.281 (2)	1.290 (3)	1.290 (1)	1.241 (6)	1.289 (2)	1.282 (3)
N3-C14	1.283 (3)	1.281 (2)	1.282 (3)				1.289 (3)
C1-C2	1.512 (3)	1.477 (3)	1.489 (3)	1.510 (1)	1.551 (7)	1.513 (2)	1.501 (4)
	1.515 (3)	1.473 (3)					1.502 (4)
C1-C2-N2	115.9 (2)	115.2 (2)	116.6 (2)	114.3 (1)	118.3 (5)	113.2 (1)	114.4 (2)
C13-C14-N3	116.4 (2)	115.0 (2)	115.0 (2)				113.4 (2)
C2-N2-O2	113.6 (2)	112.4 (1)	109.4 (2)	110.7 (1)	112.2 (4)	110.6 (1)	110.7 (2)
C14-N3-O4	113.4 (2)	112.2 (1)	111.5 (2)				111.1 (2)

Notes: (II), 2,3-dimethylquinoxaline-dimethylglyoxime (1/1) (Hökelek, Batı *et al.*, 2001); (III), 1-(2,6-dimethylphenyl-amino)propane-1,2-dione dioxime (Hökelek, Zülfikaroğlu & Batı, 2001); (IV), *N*-hydroxy-2-oxo-2,*N*'-di-phenylacetamidine (Büyükgüngör *et al.*, 2003); (V), *N*-(3,4-di-chloro-phenyl)-*N*'-hydroxy-2-oxo-2-phenylacetamidine (Hökelek *et al.*, 2004); (VI), *N*-hydroxy-*N*'-(1-naphthyl)-2-phenylacetamidin-2-one (Hökelek *et al.*, 2004*a*); (VII), *N*-(3-chloro-4-methylphenyl)-*N*'-hydroxy-2-oxo-2-phenylacetamidine-2,3-dimethylquinoxaline-dimethyl-glyoxime (1/1) (Hökelek *et al.*, 2004*b*).

Fig. 1

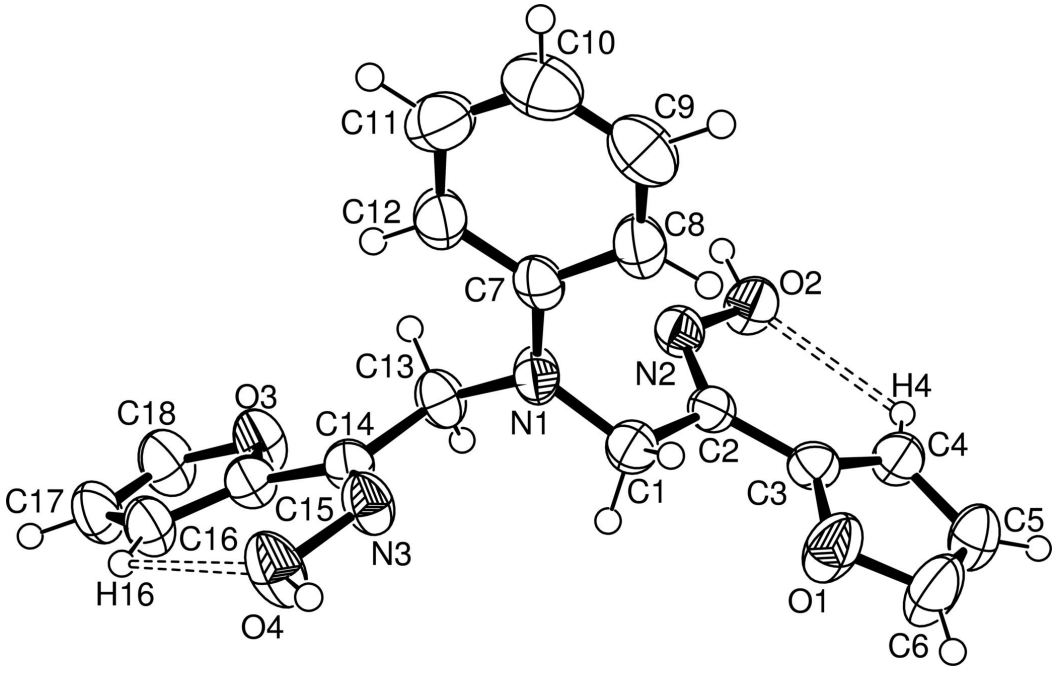
C10
C11
C9
C12
C8
C7
O2
C13
N2
H4
O3
C18
C14
N1
C2
C4
C17
C15
C1
C3
C5
C16
N3
H16
O1
O4
C6

Fig. 2