

***N*-Hydroxy-2-oxo-2,*N'*-diphenylacetamide**

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C})$ = 0.002 Å
R factor = 0.034
wR factor = 0.088
Data-to-parameter ratio = 16.2

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

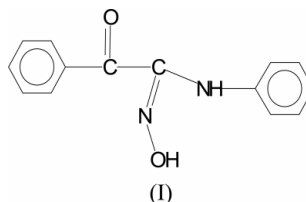
The title compound, C₁₄H₁₂O₂N₂, consists of a phenylamino group and a 2-phenyl-1,2-ethanedione 1-oxime group. Intermolecular O—H···N, N—H···O and intramolecular N—H···O hydrogen bonds [O···N 2.776 (1), 3.086 (1) and 2.574 (1) Å] are highly effective in forming polymeric chains, thereby stabilizing the crystal structure. The oxime group has the *E* configuration.

Comment

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 non-covalent intermolecular interactions (Etter *et al.*, 1990).

The oxime (—C=N—OH) moiety is a functional group that has not been extensively explored in crystal engineering. It is amphiprotic, with a slightly basic N atom and a mildly acidic hydroxyl group. It is also potentially ambident, with possibilities of coordination through nitrogen and/or O atoms. 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). Structurally characterized oxime moieties are much less common than carboxylic acids and amides, but, from a supramolecular perspective, this functionality does have some unique and desirable features (Aakeröy *et al.*, 2001). In general, oxime and dioxime derivatives are very important compounds in chemical industry and medicine (Sevaga-pandian *et al.*, 2000).



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 group and to compare the geometry of the oxime moiety with those found in 2,3-dimethylquinoxaline-dimethylglyoxime (1/1), (II) (Hökelek, Batı *et al.*, 2001), 1-(2,6-dimethylphenylamino)propane-1,2-dione dioxime, (III) (Hökelek, Zülfikaroğlu *et al.*, 2001), and *N*-(3,4-dichlorophenyl)-*N'*-hydroxy-2-oxo-2-phenylacetamide, (IV) (Hökelek *et al.*, 2003).

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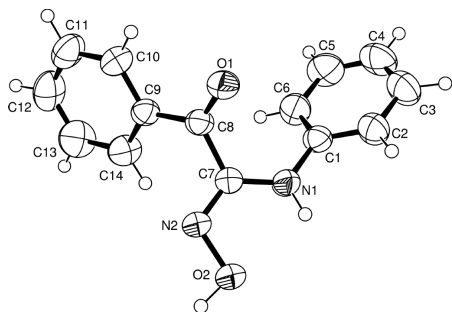


Figure 1

An ORTEP-3 (Farrugia, 1997) drawing of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

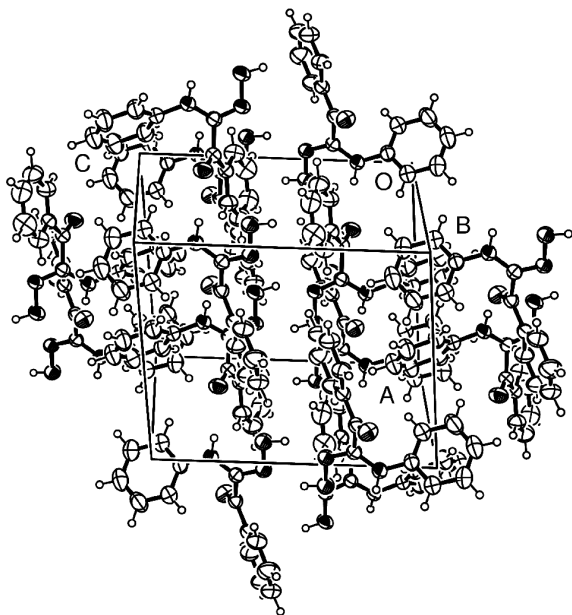


Figure 2

Packing diagram for (I).

The title compound, (I) (Fig. 1), consists of phenylamino and 2-phenyl-1,2-ethanedione 1-oxime moieties. The dihedral angles between the oxime plane *A* (O2/N2/C7) and the non-coplanar phenyl rings *B* (C1–C6) and *C* (C9–C14) are *A/B* = 46.29 (6), *A/C* = 56.43 (7) and *B/C* = 68.02 (4)°.

The steric effects of the substituents bonded to the C atom of the oxime group may influence the bond lengths and angles of the oxime moiety (Table 1). Some significant changes in the geometry of the oxime moiety are evident when the bond lengths and angles are compared with the corresponding values in compounds (II)–(IV) (Table 2).

The oxime moiety has an *E* configuration [C8–C7–N2–O2 = –169.51 (8)°; Chertanova *et al.*, 1994]. In this configuration, the oxime group is involved as a donor in intermolecular hydrogen bonding [O2–H2 0.956 (15) Å, O2···N2ⁱ 2.776 (1) Å, H2···N2ⁱ 1.885 (16) Å and O2–H2···N2ⁱ 153.93(1.37)°; symmetry code: (i) $-x, -y, 1-z$]. There are also N1–H1···O2 intramolecular [N1–H1 0.880 (13) Å, N1···O2 2.574 (1) Å, H1···O2 2.255 (12) Å and N1–H1···O2 101.13 (94)°] and N1–H1···O1ⁱⁱ intermolecular [N1–H1 0.880 (13) Å, N1···O1ⁱⁱ 3.086 (1) Å, H1···O1ⁱⁱ

2.348 (13) Å and N1–H1···O1ⁱⁱ 141.57(1.14)°; symmetry code: (ii) $x + \frac{1}{2}, \frac{1}{2} - y, z$] hydrogen bonds.

The inter- and intramolecular hydrogen bonds are highly effective in forming polymeric chains, thereby stabilizing the crystal structure. As can be seen from the packing diagram (Fig. 2), the chains are approximately parallel to the *a* axis. Dipole–dipole and van der Waals interactions are also effective in the molecular packing in the crystal structure.

Experimental

A solution of aniline (0.03 mol, 2.79 g) in dichloromethane (20 ml) was added dropwise to a solution of ω -chloroisitrosacetophenone (0.015 mol, 2.75 g) in dichloromethane (40 ml). The precipitated product was filtered off, and the resulting solution was allowed to stand for 3 d at room temperature for crystallization to occur.

Crystal data

$C_{14}H_{12}N_2O_2$	$D_x = 1.288 \text{ Mg m}^{-3}$
$M_r = 240.26$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/a$	Cell parameters from 10547 reflections
$a = 10.0106$ (9) Å	$\theta = 1.7\text{--}29.5^\circ$
$b = 10.2280$ (6) Å	$\mu = 0.09 \text{ mm}^{-1}$
$c = 12.1627$ (7) Å	$T = 293$ (2) K
$\beta = 95.763$ (6)°	Block, yellow
$V = 1239.03$ (15) Å ³	$0.35 \times 0.25 \times 0.15 \text{ mm}$
$Z = 4$	

Data collection

Stoe IPDS-II diffractometer	$R_{\text{int}} = 0.036$
φ scans	$\theta_{\text{max}} = 29.5^\circ$
Absorption correction: none	$h = -13 \rightarrow 13$
12031 measured reflections	$k = -14 \rightarrow 14$
3434 independent reflections	$l = -16 \rightarrow 16$
1990 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.088$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 0.81$	$\Delta\rho_{\text{max}} = 0.11 \text{ e \AA}^{-3}$
3434 reflections	$\Delta\rho_{\text{min}} = -0.11 \text{ e \AA}^{-3}$
212 parameters	Extinction correction: <i>SHELXL97</i>
All H-atom parameters refined	Extinction coefficient: 0.062 (5)

Table 1

Selected geometric parameters (Å, °).

O2–N2	1.4167 (10)	N1–C1	1.4145 (13)
O1–C8	1.2147 (12)	C9–C14	1.3841 (16)
N2–C7	1.2897 (12)	C9–C10	1.3866 (15)
C8–C9	1.4768 (14)	C1–C6	1.3765 (16)
C8–C7	1.5098 (13)	C1–C2	1.3795 (17)
C7–N1	1.3475 (13)	C2–C3	1.3786 (17)
C7–N2–O2	110.66 (8)	N1–C7–C8	119.66 (8)
O1–C8–C9	122.67 (9)	C7–N1–C1	125.25 (9)
O1–C8–C7	116.60 (9)	C14–C9–C8	122.40 (9)
C9–C8–C7	120.70 (8)	C10–C9–C8	118.70 (10)
N2–C7–N1	125.09 (9)	C6–C1–N1	121.11 (10)
N2–C7–C8	114.32 (8)	C2–C1–N1	119.13 (10)
O2–N2–C7–C8	–169.51 (8)	N2–C7–N1–C1	169.24 (10)
O1–C8–C7–N2	123.44 (10)	C8–C7–N1–C1	–22.45 (15)
C9–C8–C7–N2	–54.57 (12)	O1–C8–C9–C14	173.21 (10)
O1–C8–C7–N1	–46.09 (13)	O1–C8–C9–C10	–5.16 (15)
C9–C8–C7–N1	135.90 (10)	C7–N1–C1–C2	142.39 (11)

Table 2

Comparison of the bond lengths and angles (Å, °) in the oxime moiety of (I) with those in the related compounds (II), (III) and (IV).

	(I)	(II)	(III)	(IV)
N2—O2	1.4167 (10)	1.4033 (16)/1.3956 (18)	1.423 (3)/1.396 (3)	1.429 (4)
N2—C7	1.2897 (12)	1.2811 (18)/1.2813 (19)	1.290 (3)/1.282 (3)	1.241 (6)
C7—C8	1.5098 (13)	1.477 (3)/1.473 (3)	1.489 (3)	1.551 (7)
C8—C7—N2	114.32 (8)	115.18 (15)/115.03 (17)	116.59 (19)/115.0 (2)	118.3 (5)
C7—N2—O2	110.66 (8)	112.39 (12)/112.15 (13)	109.37 (18)/111.52 (19)	112.2 (4)

The H atoms were located in a difference synthesis and refined isotropically [C—H = 0.929 (15)–0.988 (17) Å].

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); 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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