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2-[Benzoyl(hydroxyimino)methylamino]benzoic acid

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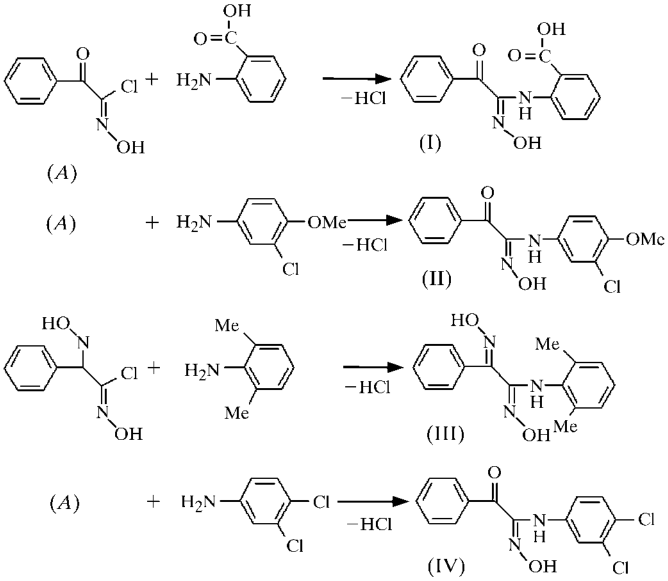
The structure of the title compound, $C_{15}H_{12}N_2O_4$, consists of a polymeric arrangement, around inversion centres, of molecules linked through O—H···N and O—H···O hydrogen bonds; there are also intramolecular hydrogen bonds. All these hydrogen-bond interactions result in the formation of infinite chains parallel to the [010] direction. The oxime group has an *E* conformation.

Comment

In general, oximes and their derivatives are very important compounds for the chemical industry and in medicine, due to their biological activity. Experimental studies on derivatives of oxime groups are numerous (Bertolasi *et al.*, 1982; Gilli *et al.*, 1983; Hökelek, Zülfikaroglu & Batı, 2001). Oximes have various insecticidal, miticidal and nematodicidal activities and are employed as antidotes against organophosphorus poisons. Carbonyl oximes are employed in the separation and spectrophotometric determination of Ni, Pd, Co, Fe and Cu. Besides these properties, the oxime (C═N—OH) group possesses stronger hydrogen-bonding capabilities than the alcohol, phenol and carboxylic acid groups (Marsman *et al.*, 1999). Hydrogen bonding plays a key role in molecular recognition in chemical engineering (Bertolasi *et al.*, 1982; Gilli *et al.*, 1983; Hökelek, Batı *et al.*, 2001). Intermolecular hydrogen bonding has received considerable attention among directional non-covalent intermolecular interactions (Etter *et al.*, 1990), which combine moderate strength and directionality in designing compounds to form supramolecular structures (Karle *et al.*, 1996).

The crystal structure determination of the title compound, (I), was carried out to determine the strength of the hydrogen-bonding capabilities of the oxime group, as well as to establish the molecular arrangement, and also to compare the geometry of the oxime moiety with those found in *N*-(3-chloro-4-methoxyphenyl)-*N*′-hydroxy-2-oxo-2-phenylacetamidine, (II) (Soylu *et al.*, 2003), 1-(2,6-dimethylphenylamino)propane-1,2-dione dioxime, (III) (Hökelek, Zülfikaroglu & Batı, 2001), and *N*-(3,4-dichlorophenyl)-*N*′-hydroxy-2-oxo-2-phenylacetamidine, (IV) (Hökelek *et al.*, 2004).



Compound (I) (Fig. 1) consists of two aromatic groups linked through a monoxime group. The dihedral angles between the oxime plane *A* (O1/N1/C7) and rings *B* (C1–C6) and *C* (C9–C14) are *A*/*B* = 58.61 (10)°, *A*/*C* = 30.13 (11)° and *B*/*C* = 75.30 (9)° (with approximate s.u. values). Rings *B* and *C* are nearly perpendicular to one another. Ring *B* is linked to the C═N—OH group by atom C2(O2). The other ring, *C*, is linked to the same functional group by atom N2(H2). 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.

A comparison of the bond lengths and angles in compounds (I)–(IV) (Table 1) shows significant changes in the geometry of the oxime moiety. The C═N and C—C bond lengths and C═N—O bond angles in (I) and (II) are larger than the corresponding values reported in (III), and smaller than those in (IV). The O—N and C—C═N values in (I) and (II) are smaller than those found in (III) and (IV). The bond lengths and angles of the oxime moiety in (I) are in accord with the reported values for (II). The differences reported here may be partly due to the steric effect of the 2-carboxyl group.

The oxime moiety in (I) has an *E* configuration, with a C2—C1—N1—O1 torsion angle of 169.11 (14)°, which is slightly different from the torsion angles found in related studies (Soylu *et al.*, 2003; Hökelek, Zülfikaroglu & Batı, 2001). In this configuration, atom O1 of the oxime group and atom O3 of the carboxyl group behave as donors in intermolecular hydrogen bonds around the inversion centre [$O1\cdots N1^{i}$ = 2.780 (2) Å and $O3\cdots O4^{ii}$ = 2.644 (3) Å; symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $1 - x, -y, 1 - z$; Fig. 2]. There are also intramolecular N···O hydrogen bonds in the molecule [N2···O1 = 2.548 (2) Å and N2···O4 = 2.667 (2) Å; Table 2].

All the above-mentioned inter- and intramolecular hydrogen bonds in (I) are highly effective in forming polymeric chains, thereby stabilizing the crystal structure. As can

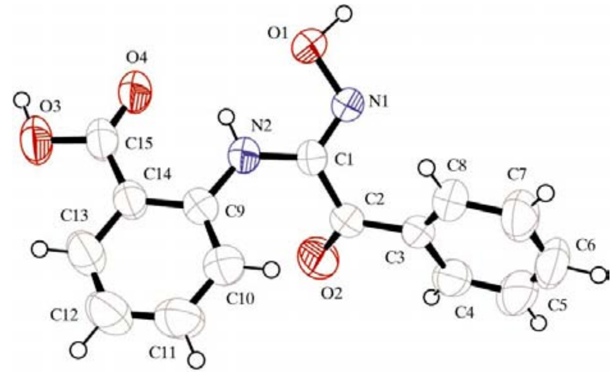


Figure 1
A view of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

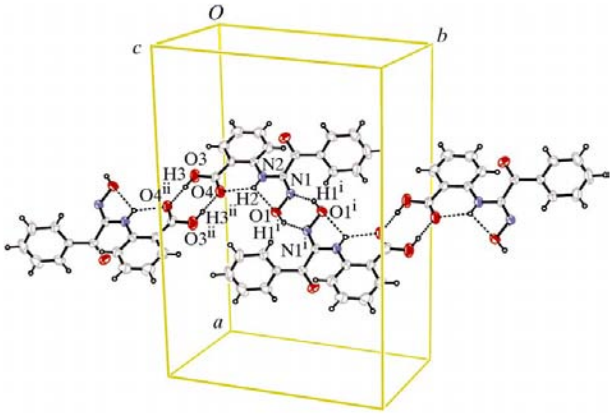


Figure 2
A diagram showing the hydrogen-bonding interactions in (I) [symmetry codes: (i) 1 − *x*, 1 − *y*, 1 − *z*; (ii) 1 − *x*, −*y*, 1 − *z*].

be seen from the packing diagram (Fig. 2), the chains are approximately parallel to the *b* axis. Dipole–dipole and van der Waals interactions are also effective in the molecular packing in the crystal structure.

Experimental

A solution of anthranilic acid (2.06 g, 0.015 mol) in dichloromethane (20 ml) was added dropwise to a solution of ω-chloroisonitrosoacetophenone (2.75 g, 0.015 mol) in ethanol (15 ml). The precipated product was filtered off and the resulting solution was allowed to stand for 1 h at room temperature for crystallization to occur.

Crystal data

$C_{15}H_{12}N_2O_4$
$M_r = 284.27$
Monoclinic, $C2/c$
$a = 20.6850\ (19)$ Å
$b = 13.1680\ (13)$ Å
$c = 10.488\ (11)$ Å
$\beta = 101.921\ (5)$°
$V = 2795\ (3)$ Å^3
$Z = 8$

$D_x = 1.351$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 4812 reflections
$\theta = 1.8$–27.7°
$\mu = 0.10$ mm^{-1}
$T = 293\ (2)$ K
Prism, colourless
0.40 × 0.27 × 0.16 mm

Data collection

Stoe IPDS-2 diffractometer
φ scans
12 250 measured reflections
2477 independent reflections
1472 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.088$
$\theta_{\rm max} = 25.0$°
$h = -24 \rightarrow 24$
$k = -15 \rightarrow 15$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.097$
$S = 0.86$
2477 reflections
202 parameters
H atoms: see below

$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.22$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.22$ e Å^{-3}

Table 1
Comparison of selected geometric parameters (Å, °) in the oxime moiety of (I) with those in the related compounds (II), (III) and (IV).

Bond or angle	(I)	(II)	(III)	(IV)
N1—O1	1.4093 (18)	1.4063 (17)	1.423 (3)	1.429 (4)
N1—C1	1.288 (2)	1.282 (2)	1.290 (3)	1.241 (6)
C1—C2	1.501 (2)	1.502 (2)	1.489 (3)	1.551 (7)
C2—C1—N1	113.21 (15)	113.75 (15)	116.59 (19)	118.3 (5)
C1—N1—O1	111.51 (13)	111.00 (14)	109.37 (18)	112.2 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1$^{\rm i}$	1.02 (3)	1.83 (3)	2.780 (2)	154 (2)
O3—H3···O4$^{\rm ii}$	0.96 (3)	1.68 (3)	2.644 (3)	177 (3)
N2—H2···O1	0.86 (2)	2.18 (2)	2.548 (2)	105.5 (16)
N2—H2···O4	0.86 (2)	2.01 (2)	2.667 (2)	132.0 (18)

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

H atoms on N and O atoms were located from a difference Fourier map and freely refined, giving an N—H distance of 0.86 (2) Å, and O—H distances of 0.96 (3) and 1.02 (3) Å. H atoms bonded to C atoms were treated as riding, with C—H distances of 0.93 Å.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD1303). Services for accessing these data are described at the back of the journal.

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