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(*E*)-2-(Hydroxyimino)-*N*-phenylacetamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.139
Data-to-parameter ratio = 12.0

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

The title compound, $C_8H_8N_2O_2$, is a key intermediate in the synthesis of oxindole. The crystal packing is stabilized by O—H···O, N—H···O and N—H···N hydrogen-bond interactions.

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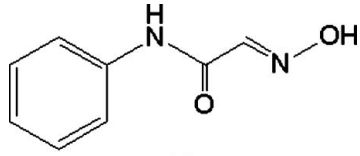
Comment

The title compound, (I), is a key intermediate in the synthesis of oxindole (Marvel & Hiers, 1941). The molecular structure of (I) is illustrated in Fig. 1. The molecule is roughly planar, the largest deviation from the mean plane being 0.224 (2) Å for atom C3. Bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The values of the N1—C7 [1.338 (2) Å] and O1—C7 [1.226(2 Å] bond lengths suggest partial sp^2 character of the N atom. In the crystal structure (Fig. 2), the molecules are linked by intermolecular O—H···O, N—H···O and N—H···N hydrogen-bonding interactions (Table 1).



(I)

Experimental

A mixture of chloral hydrate (90 g, 0.54 mol) in water (1200 ml), sodium sulfate (1300 g), aniline (46.5 g, 0.5 mol) in water (300 ml), hydrochloric acid (43 ml, 0.52 mol) and hydroxylamine hydrochloride (110 g, 1.58 mol) was heated to boiling. After two minutes of vigorous boiling, the reaction was complete. The mixture was cooled to room temperature and the solid collected by vacuum filtration to give the title compound (yield 82%). Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

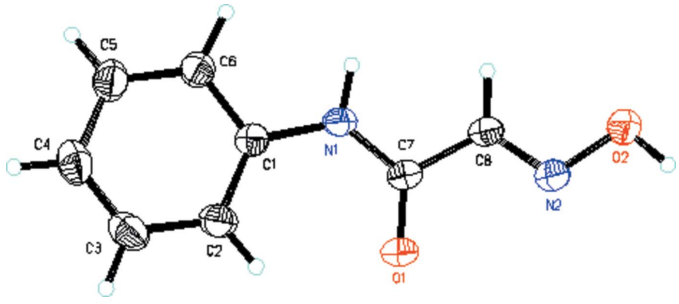


Figure 1
The molecular structure of (I), drawn with 30% probability ellipsoids.

Crystal data

$C_8H_8N_2O_2$
M_r = 164.16
Orthorhombic, *Pbca*
a = 9.6551 (11) Å
b = 9.1665 (10) Å
c = 17.673 (2) Å
V = 1564.1 (3) Å^3
Z = 8
D_x = 1.394 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2586 reflections
θ = 4.6–49.5°
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.51 × 0.47 × 0.33 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.764, T_{max} = 0.970
8540 measured reflections
1710 independent reflections
1316 reflections with $I > 2\sigma(I)$
R_{int} = 0.115
θ_{max} = 27.0°
$h = -9 \rightarrow 12$
$k = -11 \rightarrow 11$
$l = -22 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.139
S = 0.99
1710 reflections
142 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.087P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.014 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1^{i}	0.91 (2)	1.86 (3)	2.7448 (17)	163 (2)
N1—H1···O1^{ii}	0.89 (2)	2.43 (2)	3.1191 (17)	134 (2)
N1—H1···N2^{ii}	0.89 (2)	2.35 (2)	3.1898 (17)	156 (2)

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{5}{2}, -z+1$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, z$.

All H atoms were found in a difference Fourier map and refined isotropically [C—H = 0.93 (2)–1.02 (2) Å].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

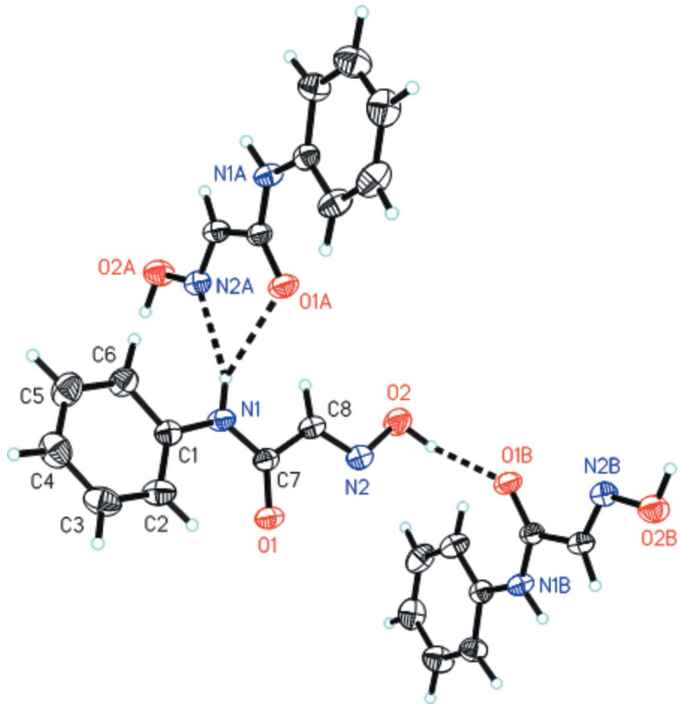


Figure 2
Partial view of the crystal packing in (I), showing the hydrogen-bonding interactions as dashed lines. [Symmetry codes: (A) $\frac{3}{2}-x, y-\frac{1}{2}, z$; (B) $\frac{1}{2}+x, \frac{5}{2}-y, 1-z$.]

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