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Acetamidoxime

Marilyn M. Olmstead[a]* and Javad J. Sahbari[b]

[a]Department of Chemistry, University of California, Davis, CA 95616, USA, and [b]10 Vista Real, Mill Valley, CA 94941, USA
Correspondence e-mail: olmstead@indigo.ucdavis.edu

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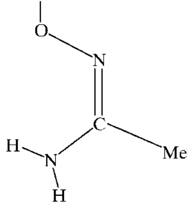
The oxime of acetamide, *viz.* *N*-hydroxyethanimidamide, $C_2H_6N_2O$, has a complex hydrogen-bonding arrangement in its crystal structure, featuring one strong O—H···N hydrogen bond together with weaker hydrogen bonding involving the amide groups. Conjugation effects lead to atypical distances and angles.

Comment

The molecular structure of acetamidoxime, (I), is shown in Fig. 1. The molecular geometry has somewhat atypical distances and angles, which can be explained by a contribution from a resonance form that places partial double-bond character in the C1—N2 bond. The C1—N1 and N1—O1 distances are longer than average, having values of 1.295 (2) and 1.442 (2) Å, respectively, whereas the C1—N2 distance is 1.346 (2) Å. In addition, the C═N—O angle [109.37 (13)°] is more acute than comparable angles in other oxime structures (Chertanova *et al.*, 1994). For a more exact comparison, the structure of *N*,*N*-dimethylacetamidoxime (Bright *et al.*, 1973) differs only in the replacement of NH_2 by $N(CH_3)_2$, yet the C═N and N—O distances are shorter [1.284 (2) and 1.430 (2) Å, respectively], while the C—$N(CH_3)_2$ distance is longer [1.367 (3) Å] and the C═N—O angle is 111.8 (2)°. Excluding the methyl H atoms, the entire molecule of (I) is planar; based on unit weights, the r.m.s. deviation from this plane is 0.069 Å.



(I)

The major form of hydrogen bonding in the structure of (I) (Fig. 2 and Table 1) is between the O—H donor and the oxime N-atom acceptor, as is commonly found. This hydrogen bond consists of a monodirectional interaction along a screw axis of the structure in the *c* direction. The N···O distance is longer than average [2.804 (2) Å; Chertanova *et al.*, 1994]. Weaker hydrogen bonds are apparent for each of the amide H atoms; atom H2*A* participates in an intramolecular hydrogen bond, while atom H2*B* participates in a hydrogen bond to the oxime O-atom acceptor.

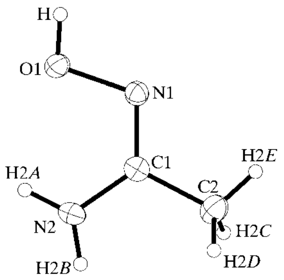


Figure 1
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

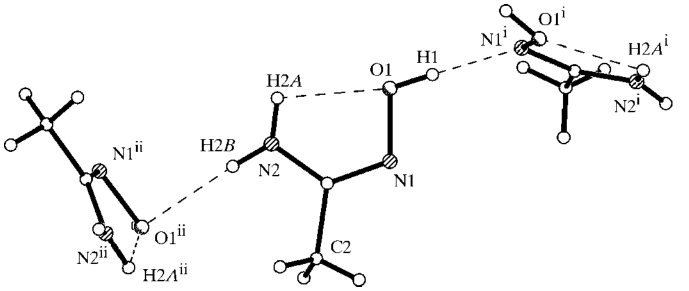


Figure 2
A view of the hydrogen-bonding scheme in the structure of (I). [Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, 1 - z$; (ii) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$.]

Experimental

The title compound was synthesized from acetamide and hydroxylamine according to the method described by Sahbari & Russell (2000, 2001). Hygroscopic crystals were obtained by recrystallization from perfluorocyclohexane.

Crystal data

$C_2H_6N_2O$
M_r = 74.09
Orthorhombic, $P2_12_12_1$
a = 5.0422 (14) Å
b = 8.016 (3) Å
c = 9.284 (3) Å
V = 375.2 (2) Å^3
Z = 4
D_x = 1.311 Mg m^{-3}

Cu *Kα* radiation
Cell parameters from 50 reflections
θ = 7.3–29.9°
μ = 0.89 mm^{-1}
T = 130 (2) K
Parallelepiped, colorless
0.50 × 0.26 × 0.25 mm

Data collection

Syntex $P2_1$ diffractometer
$2\theta-\omega$ scans
886 measured reflections
415 independent reflections
413 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.013
$\theta_{\rm max}$ = 66.7°

$h = -2 \rightarrow 6$
$k = 0 \rightarrow 9$
$l = 0 \rightarrow 11$
2 standard reflections
every 198 reflections
intensity decay: <0.1%

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.072$
$S = 1.26$
415 reflections
60 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.0757P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.008$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.056 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H···N1$^{\text{i}}$	0.91 (3)	1.89 (3)	2.804 (2)	178 (3)
N2—H2A···O1	0.90 (3)	2.21 (3)	2.554 (2)	102 (2)
N2—H2B···O1$^{\text{ii}}$	0.88 (3)	2.20 (3)	3.078 (2)	173 (2)

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

The title molecule crystallized in the chiral space group $P2_12_12_1$, but the absolute structure was indeterminate since only light atoms were present. The merging of Friedel pairs reduced the reflections-to-parameter ratio from 9.15 to 6.92, but the reliability of the structure determination did not change, being based more on the quality of the data than their number. H atoms on atoms N2 and O1 were refined freely, while H atoms on atom C2 were refined using a riding model, with C—H distances of 0.98 Å and U_{iso}(H) values of $1.5U_{\text{eq}}$(C2).

Data collection: *P*3-*PC* (Siemens, 1994); cell refinement: *P*3-*PC*; data reduction: *XDISK* (Siemens, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1994); software used to prepare material for publication: *SHELXL*97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1623). Services for accessing these data are described at the back of the journal.

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