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N-(2-Formamidoethyl)formamide

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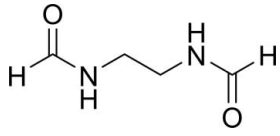
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.027; wR factor = 0.073; data-to-parameter ratio = 11.7.

The complete molecule of the title compound, $C_4H_8N_2O_2$, is generated by a crystallographic inversion center. The occurence of N—H···O hydrogen bonds results in the formation of a two-dimensional infinite network parallel to the (010) plane. In this plane, the hydrogen bonds define graph-set motif $R_4^4(22)$ in a centrosymmetric array by the association of four molecules.

Related literature

For general background, see: Yang *et al.* (2007). For related structures, see: Goss *et al.* (1996). For graph-set notation, see: Bernstein *et al.* (1995); Etter *et al.* (1990).



Experimental

Crystal data

$C_4H_8N_2O_2$
M_r = 116.12
Orthorhombic, *Pbca*
a = 8.7138 (17) Å
b = 6.6714 (13) Å
c = 9.3162 (19) Å
V = 541.58 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 113 (2) K
0.32 × 0.26 × 0.16 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.964, T_{max} = 0.982
2736 measured reflections
467 independent reflections
431 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.073
S = 1.11
467 reflections
40 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.844 (15)	2.062 (16)	2.8570 (13)	156.9 (12)

Symmetry code: (i) $-x+\frac{1}{2}, -y+1, z-\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2396).

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supplementary materials

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N-(2-Formamidoethyl)formamide

J. Yang, Y. Chen, S. Wang and J. Wang

Comment

N-(2-Formylaminoethyl)formamide is a plasticizer to prepare thermoplastic starch. The mechanical properties of N-(2-Formylaminoethyl)formamide plasticized starch were enhanced compared with the conventional glycerol plasticized one (Yang,*et al.*, 2007).

The molecule of (I) has a center of symmetry at the mid-point of the central C2—C2^{i} bond (Fig. 1).

Intermolecular N—H···O hydrogen bonds link the molecule to form a two dimensionnal network parallel to the (0 1 0) plane. In this plane, the hydrogen bonds define rings by associating 4 molécules displaying graph set motif $R_4^4(21)$ (Etter *et al.*, 1990; Bernstein *et al.*, 1995).

Therefore, the OH group of the starch can also form intermolecular O—H···O hydrogen bonds with the *N*-(2-Formylaminoethyl)formamide, the mechanical properties of the plasticized starch is then enhanced.

Experimental

Methyl formate (500 ml) was placed in a 1000 ml flask cooled by ice-bath and ethylenediamine (250 ml) was slowly added. Subsequently, ice-bath was removed and the mixture was refluxed for 10 h. After standing overnight, the product was isolated by filtration. The solids obtained by filtration were recrystallized from anhydrous ethyl alcohol in 95% yield. Colorless crystals of *N*-(2-Formylaminoethyl)formamide were obtained by slow evaporation of a solution of anhydrous methyl alcohol at 278 k(m.p. 381 k).

Refinement

The N-bound H atoms were located in a difference map and freely refined with U_{iso}(H) = 1.2 U_{eq}(N)], H atoms attached to carbon were positioned geometrically and treated as riding on their parent atoms [C—H distances are 0.93 Å for CH and 0.97 Å for CH_2 groups, both with U_{iso}(H) = 1.2 U_{eq}(C)].

Figures

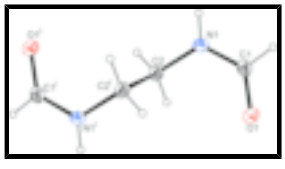

Fig. 1. A view of the molecular structure of (I) with the atom-labeling scheme. Displacement ellopsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry code:(i) 1-*x,* 1-*y*, 1-*z*]

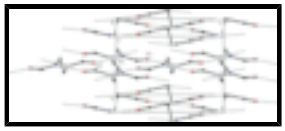

Fig. 2. Partial packing view showing the formation of the two dimensional network through N-H···O hydrogen bonds which are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (i) -x+1/2, -y+1, z-1/2]

N-(2-Formamidoethyl)formamide

Crystal data

$C_4H_8N_2O_2$	F_{000} = 248
M_r = 116.12	D_x = 1.424 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 1513 reflections
a = 8.7138 (17) Å	θ = 3.1–27.8º
b = 6.6714 (13) Å	μ = 0.12 mm^{-1}
c = 9.3162 (19) Å	*T* = 113 (2) K
V = 541.58 (19) Å^3	Block, colorless
Z = 4	0.32 × 0.26 × 0.16 mm

Data collection

Rigaku Saturn diffractometer	467 independent reflections
Radiation source: rotating anode	431 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.035
T = 113(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 4.4º
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	*h* = −10→7
T_{min} = 0.964, T_{max} = 0.982	*k* = −7→7
2736 measured reflections	*l* = −9→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.027	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.073	$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 0.1199P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.11	$(\Delta/\sigma)_{max} < 0.001$
467 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
40 parameters	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > \sigma(F^2)$ 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}
C1	0.26367 (12)	0.50564 (15)	0.69236 (11)	0.0165 (3)
H1	0.1616	0.4744	0.7110	0.020*
C2	0.45751 (11)	0.59669 (16)	0.51762 (12)	0.0158 (3)
H2A	0.5102	0.6659	0.5948	0.019*
H2B	0.4575	0.6835	0.4341	0.019*
N1	0.30073 (10)	0.55554 (13)	0.56027 (10)	0.0160 (3)
H1A	0.2325 (15)	0.5444 (19)	0.4965 (17)	0.019*
O1	0.35499 (8)	0.49743 (11)	0.79307 (8)	0.0209 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0155 (5)	0.0165 (6)	0.0175 (6)	0.0003 (4)	0.0024 (5)	−0.0025 (4)
C2	0.0170 (6)	0.0170 (6)	0.0133 (6)	−0.0011 (4)	0.0004 (4)	0.0009 (4)
N1	0.0140 (5)	0.0196 (5)	0.0143 (5)	0.0010 (4)	−0.0027 (3)	−0.0015 (4)
O1	0.0200 (4)	0.0288 (5)	0.0139 (5)	−0.0006 (3)	−0.0002 (3)	0.0012 (3)

Geometric parameters (Å, °)

C1—O1	1.2314 (13)	C2—C2^{i}	1.523 (2)
C1—N1	1.3151 (14)	C2—H2A	0.9700
C1—H1	0.9300	C2—H2B	0.9700
C2—N1	1.4490 (15)	N1—H1A	0.844 (15)
O1—C1—N1	124.44 (10)	N1—C2—H2B	109.5
O1—C1—H1	117.8	C2^{i}—C2—H2B	109.5
N1—C1—H1	117.8	H2A—C2—H2B	108.0
N1—C2—C2^{i}	110.91 (11)	C1—N1—C2	122.41 (9)
N1—C2—H2A	109.5	C1—N1—H1A	117.6 (9)
C2^{i}—C2—H2A	109.5	C2—N1—H1A	119.2 (9)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{ii}	0.844 (15)	2.062 (16)	2.8570 (13)	156.9 (12)

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

Fig. 1

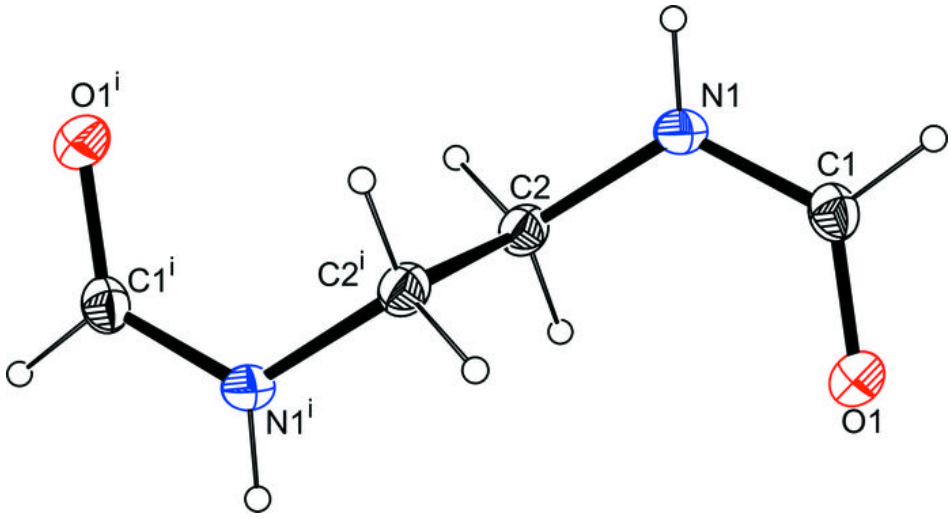

Fig. 2