Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Acrylamide

Qing-Li Zhou,[a] Zhen-Heng Zhang[b] and Zuo-Liang Jing[c]*

[a]Life College of Sciences and Engineering, Shaanxi University of Science and Technology, Shaanxi 712081, People's Republic of China, and Tianjin Food Engineering Center, Tianjin University of Science and Technology, Tianjin 300457, People's Republic of China, [b]College of Food Engineering and Biotechnology, Tianjin University of Science and Technology, Tianjin 300457, People's Republic of China, and [c]College of Sciences, Tianjin University of Science and Technology, Tianjin 300457, People's Republic of China
Correspondence e-mail: jzl74@tust.edu.cn

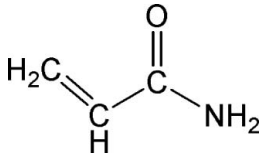
Received 18 May 2007; accepted 21 May 2007

Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.107; data-to-parameter ratio = 17.5.

In the crystal structure of the title compound, C_3H_5NO, the molecules are linked through N—H···O hydrogen bonds, forming a two-dimensional supramolecular network.

Related literature

For related literature, see: Belloni *et al.* (2005); Kahwa *et al.* (1986); Parashar *et al.* (1988); Santos *et al.* (2001); Tynan *et al.* (2005). For a previous (low precision) structure determination, with an R factor of almost 0.20, see: Isakov (1966).



Experimental

Crystal data

C_3H_5NO
M_r = 71.08
Monoclinic, $P2_1/n$
a = 8.2062 (16) Å
b = 5.7480 (11) Å
c = 9.0527 (18) Å
β = 111.37 (3)°
V = 397.65 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 113 (2) K
0.10 × 0.08 × 0.06 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.991, T_{max} = 0.995
2936 measured reflections
943 independent reflections
832 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 1.11
943 reflections
54 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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}	0.886 (8)	1.970 (8)	2.8465 (16)	169.9 (14)
N1—H1B···O1^{ii}	0.894 (8)	2.044 (8)	2.9291 (13)	170.6 (15)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2300).

References

Belloni, M., Kariuki, B. M., Manickam, M., Wilkie, J. & Preece, J. A. (2005). *Cryst. Growth Des.* **5**, 1443–1449.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0). Bruker AXS Inc., Madison, Wisconsin, USA.
Isakov, I. V. (1966). *Zh. Strukt. Khim. (Russian J. Struct. Chem.)*, **7**, 898–900.
Kahwa, I. A., Selbin, J., Hsieh, T. C.-Y. & Laine, R. A. (1986). *Inorg. Chim. Acta*, **118**, 179–185.
Parashar, R. K., Sharma, R. C., Kumar, A. & Mohan, G. (1988). *Inorg. Chim. Acta*, **151**, 201–208.
Santos, M. L. P., Bagatin, I. A., Pereira, E. M. & Ferreira, A. M. D. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 838–844.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tynan, E., Jensen, P., Lees, A. C., Moubaraki, B., Murray, K. S. & Kruger, P. E. (2005). *CrystEngComm*, **7**, 90–95.

 doi:10.1107/S1600536807024816

supplementary materials

Acta Cryst. (2007). E**63**, o3039 [**doi:10.1107/S1600536807024816**]

Acrylamide

Q.-L. Zhou, Z.-H. Zhang and Z.-L. Jing

Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry. Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of the active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of an investigation of the coordination properties of Shiff bases functioning as ligands, we report the synthesis and crystal structure of the title compound, (I).

The expected geometric parameters are observed in (I) (Fig. 1). The molecules are linked through N—H···O hydrogen bonds (Table 2), forming a two-dimensional supramolecular network which leads to stable crystal structure. Fig. 2 shows a portion of this extensively hydrogen-bonded supramolecular assembly.

Experimental

Acrylamide (1 g) was added to a Trichloro-methane (50 ml), with stirring at 350 K. The resulting colourless solution was filtered and the filtrate was allowed to stand in air at room temperature for 10 d, yielding colourless crystals of (I).

Refinement

The H atoms of the NH_2 group were found from a difference Fourier map and refined freely. C-bound H atoms were placed in calculated positions with C—H = 0.93 Å and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

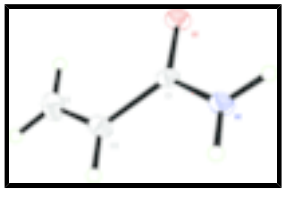


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

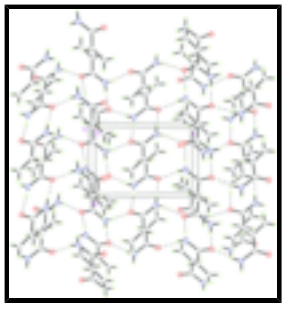


Fig. 2. The crystal packing of (I), viewed down the *a* axis. Hydrogen bonds are indicated by dashed lines.

Acrylamide

Crystal data

C_3H_5NO	$F_{000} = 152$
$M_r = 71.08$	$D_x = 1.187$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1254 reflections
$a = 8.2062$ (16) Å	$\theta = 2.3$–25.0º
$b = 5.7480$ (11) Å	$\mu = 0.09$ mm^{-1}
$c = 9.0527$ (18) Å	$T = 113$ (2) K
$\beta = 111.37$ (3)º	Block, colourless
$V = 397.65$ (16) Å^3	0.10 × 0.08 × 0.06 mm
$Z = 4$	

Data collection

Rigaku Saturn diffractometer	943 independent reflections
Radiation source: rotating anode	832 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{int} = 0.030$
$T = 113$(2) K	$\theta_{max} = 27.9$º
ω scans	$\theta_{min} = 2.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.991$, $T_{max} = 0.995$	$k = -6 \rightarrow 7$
2936 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.107$	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.053P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} < 0.001$
943 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
54 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.01963 (11)	0.26267 (14)	0.86873 (9)	0.0303 (3)
N1	0.21481 (13)	0.36721 (18)	1.10725 (11)	0.0281 (3)
C1	0.15782 (14)	0.2263 (2)	0.98265 (12)	0.0226 (3)
C2	0.26969 (15)	0.0222 (2)	0.98707 (13)	0.0283 (3)
H2	0.3754	0.0058	1.0719	0.034*
C3	0.22422 (19)	−0.1360 (2)	0.87512 (16)	0.0383 (4)
H3A	0.1189	−0.1220	0.7896	0.046*
H3B	0.2972	−0.2623	0.8812	0.046*
H1A	0.3147 (13)	0.344 (2)	1.1876 (13)	0.032 (3)*
H1B	0.1520 (16)	0.492 (2)	1.1129 (17)	0.041 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0228 (4)	0.0377 (6)	0.0219 (4)	0.0031 (3)	−0.0021 (3)	−0.0051 (3)
N1	0.0226 (5)	0.0298 (6)	0.0221 (5)	0.0056 (4)	−0.0034 (4)	−0.0023 (4)
C1	0.0191 (5)	0.0277 (6)	0.0189 (5)	−0.0011 (4)	0.0045 (4)	0.0016 (4)
C2	0.0284 (6)	0.0317 (7)	0.0256 (6)	0.0058 (5)	0.0109 (5)	0.0057 (5)
C3	0.0482 (8)	0.0314 (7)	0.0399 (7)	0.0052 (6)	0.0215 (7)	0.0008 (5)

Geometric parameters (Å, °)

O1—C1	1.2413 (14)	C2—C3	1.3106 (18)
N1—C1	1.3275 (14)	C2—H2	0.9300
N1—H1A	0.886 (8)	C3—H3A	0.9300
N1—H1B	0.894 (8)	C3—H3B	0.9300
C1—C2	1.4815 (16)		
C1—N1—H1A	122.6 (9)	C3—C2—C1	121.98 (12)
C1—N1—H1B	120.3 (9)	C3—C2—H2	119.0
H1A—N1—H1B	117.1 (11)	C1—C2—H2	119.0
O1—C1—N1	122.39 (11)	C2—C3—H3A	120.0
O1—C1—C2	121.69 (10)	C2—C3—H3B	120.0

N1—C1—C2	115.93 (10)	H3A—C3—H3B	120.0
O1—C1—C2—C3	−3.48 (18)	N1—C1—C2—C3	176.71 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.886 (8)	1.970 (8)	2.8465 (16)	169.9 (14)
N1—H1B···O1^{ii}	0.894 (8)	2.044 (8)	2.9291 (13)	170.6 (15)

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

Fig. 1

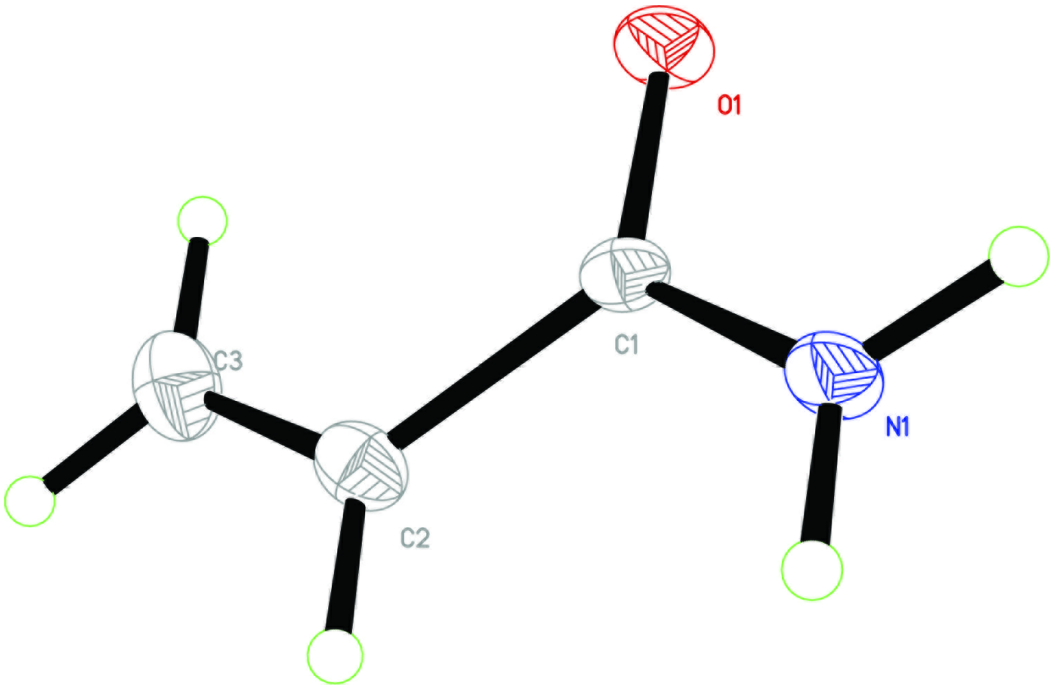


Fig. 2