Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Ureidopyridine *N*-oxide monohydrate

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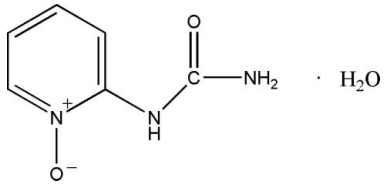
Received 28 October 2007; accepted 5 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.092; data-to-parameter ratio = 11.1.

In the title compound, $C_6H_7N_3O_2\cdot H_2O$, all atoms of 2-ureidopyridine *N*-oxide molecule are approximately coplanar and adjacent molecules are connected by strong hydrogen bonds, resulting in a three-dimensional network.

Related literature

For a related complex, see: Liu *et al.* (2006)).



Experimental

Crystal data

$C_6H_7N_3O_2\cdot H_2O$
M_r = 171.16
Monoclinic, $P2_1/n$
a = 13.1277 (17) Å
b = 4.1085 (5) Å
c = 15.419 (2) Å
β = 114.618 (2)°
V = 756.03 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 (2) K
0.64 × 0.13 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
4130 measured reflections
1316 independent reflections
862 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 0.90
1316 reflections
119 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2^{i}	0.820 (12)	2.347 (12)	3.0763 (18)	149 (2)
N2—H2···O1^{ii}	0.851 (14)	2.223 (9)	3.005 (2)	152.9 (17)
O1—H1B···O2	0.82 (2)	1.911 (19)	2.7310 (19)	179 (2)
N1—H1C···O3^{iii}	0.86	2.06	2.9232 (18)	179
N1—H1D···O1^{ii}	0.86	2.09	2.899 (2)	158

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

The authors are grateful for support from the Key Laboratory of Coordination Chemistry, JingGangShan University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2337).

References

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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

  doi:10.1107/S1600536807055833

supplementary materials

Acta Cryst. (2007). E**63**, o4690 [**doi:10.1107/S1600536807055833**]

2-Ureidopyridine *N*-oxide monohydrate

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Comment

The asymmetric unit of the title compound, (I), there are one 1-(pyridin-2-yl-N-oxide)urea molecule and one discrete water molecule (Fig. 1). All atoms of 1-(pyridin-2-yl-N-oxide)urea molecule are approximately coplanar, the maximum deviation from the least-squares plane through the whole molecule being 0.096Å for O3. In the crystal of (I) adjacent molecules are connected by strong hydrogen bonds, which resulting in a 3-D network (Fig. 2).

Experimental

1-(pyridin-2-yl-N-oxide)urea was obtained commercially. Crystals of the title compound were acquired after 0.153 g (0.001 mol) 1-(pyridin-2-yl-N-oxide)urea were recrystallized in 30 ml e thanol by means of solvent evaporation.

Refinement

The H atoms bonding to C atoms were located at calculated positions and refined as riding on their parent atoms with the bond length fixed to 0.93 Å, with U_{iso}(H) being 1.2 times U_{eq}(C). The H atoms of water molecules were found in electron density maps and refined with bond length fixed to 0.82Å and with i>U_{iso}(H) = 1.2 times U_{eq}(O). The H atoms bonding to N1 were located at calculated positions while the H atoms connect with N2 were found in electron density maps and were refined with the bond lengths fixed to 0.86Å and with i>U_{iso}(H) = 1.5 times U_{eq}(N).

Figures

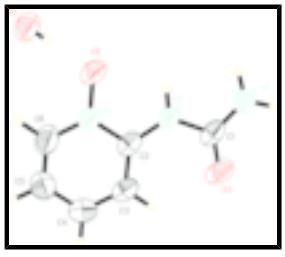

Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids.

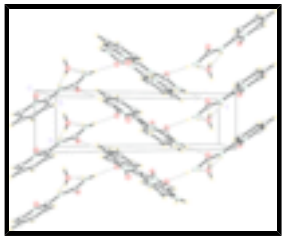

Fig. 2. The packing diagram of (I), viewed along *a* axis. Hydrogen bonds are shown as dash lines.

2-Ureidopyridine N-oxide monohydrate

Crystal data

$C_6H_7N_3O_2 \cdot H_2O$	$F_{000} = 360.0$
$M_r = 171.16$	$D_x = 1.504$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2597 reflections
$a = 13.1277$ (17) Å	$\theta = 1.0$–28.3º
$b = 4.1085$ (5) Å	$\mu = 0.12$ mm^{-1}
$c = 15.419$ (2) Å	$T = 293$ (2) K
$\beta = 114.618$ (2)º	Block, yellow
$V = 756.03$ (17) Å^3	0.64 × 0.13 × 0.09 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	862 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.055$
Monochromator: graphite	$\theta_{max} = 25.0$º
$T = 293(2)$ K	$\theta_{min} = 2.7$º
phi and ω scans	$h = -15 \rightarrow 15$
Absorption correction: none	$k = -4 \rightarrow 4$
4130 measured reflections	$l = -18 \rightarrow 18$
1316 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.90$	$(\Delta/\sigma)_{max} < 0.001$
1316 reflections	$\Delta\rho_{max} = 0.13$ e Å^{-3}
119 parameters	$\Delta\rho_{min} = -0.13$ e Å^{-3}
3 restraints	Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.026 (5)

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}
C1	0.73625 (15)	1.2059 (4)	−0.12921 (12)	0.0502 (5)
C2	0.77990 (14)	0.9178 (4)	0.02165 (11)	0.0455 (4)
C3	0.88443 (14)	0.7903 (4)	0.04058 (12)	0.0544 (5)
H3	0.9173	0.8308	−0.0014	0.065*
C4	0.94047 (15)	0.6049 (5)	0.12032 (13)	0.0607 (5)
H4	1.0110	0.5217	0.1326	0.073*
C5	0.89145 (16)	0.5428 (5)	0.18212 (13)	0.0629 (5)
H5	0.9285	0.4181	0.2366	0.076*
C6	0.78795 (16)	0.6670 (5)	0.16209 (13)	0.0642 (5)
H6	0.7544	0.6248	0.2035	0.077*
H2	0.6539 (8)	1.185 (4)	−0.0503 (12)	0.077*
H1A	0.5125 (18)	0.351 (2)	0.0890 (14)	0.096*
H1B	0.5431 (15)	0.662 (4)	0.0966 (14)	0.096*
N1	0.65659 (13)	1.3944 (4)	−0.19130 (10)	0.0615 (5)
H1C	0.6626	1.4634	−0.2416	0.074*
H1D	0.5991	1.4470	−0.1811	0.074*
N2	0.71368 (11)	1.1122 (4)	−0.05211 (10)	0.0488 (4)
N3	0.73273 (11)	0.8497 (4)	0.08372 (9)	0.0523 (4)
O1	0.50430 (13)	0.5297 (3)	0.10892 (10)	0.0701 (4)
O2	0.63227 (11)	0.9703 (3)	0.06613 (9)	0.0738 (5)
O3	0.82049 (10)	1.1191 (3)	−0.13782 (8)	0.0650 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0547 (11)	0.0590 (12)	0.0452 (9)	−0.0185 (9)	0.0290 (9)	−0.0115 (9)
C2	0.0493 (10)	0.0481 (11)	0.0459 (9)	−0.0121 (8)	0.0267 (8)	−0.0096 (8)
C3	0.0500 (10)	0.0631 (13)	0.0593 (11)	−0.0106 (9)	0.0317 (9)	−0.0091 (9)
C4	0.0488 (10)	0.0634 (13)	0.0691 (13)	−0.0034 (9)	0.0238 (10)	−0.0061 (10)
C5	0.0668 (13)	0.0643 (13)	0.0560 (11)	0.0040 (10)	0.0238 (10)	0.0039 (9)
C6	0.0809 (14)	0.0660 (13)	0.0600 (12)	0.0081 (11)	0.0435 (11)	0.0097 (11)
N1	0.0623 (10)	0.0807 (12)	0.0503 (9)	−0.0052 (9)	0.0323 (8)	0.0089 (8)

N2	0.0503 (8)	0.0583 (10)	0.0474 (8)	−0.0046 (7)	0.0298 (7)	0.0009 (7)
N3	0.0578 (9)	0.0558 (9)	0.0565 (9)	0.0046 (7)	0.0369 (8)	0.0056 (8)
O1	0.0862 (10)	0.0710 (11)	0.0706 (9)	0.0079 (8)	0.0501 (8)	0.0049 (8)
O2	0.0744 (9)	0.0859 (10)	0.0886 (10)	0.0275 (7)	0.0611 (8)	0.0305 (7)
O3	0.0600 (8)	0.0930 (11)	0.0574 (8)	−0.0076 (7)	0.0396 (7)	−0.0073 (7)

Geometric parameters (Å, °)

C1—O3	1.2208 (19)	C5—C6	1.361 (2)
C1—N1	1.332 (2)	C5—H5	0.9300
C1—N2	1.394 (2)	C6—N3	1.349 (2)
C2—N2	1.365 (2)	C6—H6	0.9300
C2—N3	1.3681 (19)	N1—H1C	0.8600
C2—C3	1.382 (2)	N1—H1D	0.8600
C3—C4	1.371 (2)	N2—H2	0.851 (14)
C3—H3	0.9300	N3—O2	1.3268 (16)
C4—C5	1.378 (3)	O1—H1A	0.820 (12)
C4—H4	0.9300	O1—H1B	0.82 (2)
O3—C1—N1	124.55 (16)	C4—C5—H5	120.5
O3—C1—N2	122.41 (17)	N3—C6—C5	121.68 (16)
N1—C1—N2	113.04 (15)	N3—C6—H6	119.2
N2—C2—N3	112.69 (14)	C5—C6—H6	119.2
N2—C2—C3	129.02 (15)	C1—N1—H1C	120.0
N3—C2—C3	118.28 (16)	C1—N1—H1D	120.0
C4—C3—C2	120.98 (16)	H1C—N1—H1D	120.0
C4—C3—H3	119.5	C2—N2—C1	125.76 (15)
C2—C3—H3	119.5	C2—N2—H2	117.0 (13)
C3—C4—C5	119.50 (18)	C1—N2—H2	117.2 (13)
C3—C4—H4	120.2	O2—N3—C6	120.56 (13)
C5—C4—H4	120.2	O2—N3—C2	118.79 (14)
C6—C5—C4	118.91 (18)	C6—N3—C2	120.64 (15)
C6—C5—H5	120.5	H1A—O1—H1B	108 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O2^{i}	0.820 (12)	2.347 (12)	3.0763 (18)	149 (2)
N2—H2···O1^{ii}	0.851 (14)	2.223 (9)	3.005 (2)	152.9 (17)
O1—H1B···O2	0.82 (2)	1.911 (19)	2.7310 (19)	179 (2)
N1—H1C···O3^{iii}	0.86	2.06	2.9232 (18)	179
N1—H1D···O1^{ii}	0.86	2.09	2.899 (2)	158

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+1, −*y*+2, −*z*; (iii) −*x*+3/2, *y*+1/2, −*z*−1/2.

Fig. 1

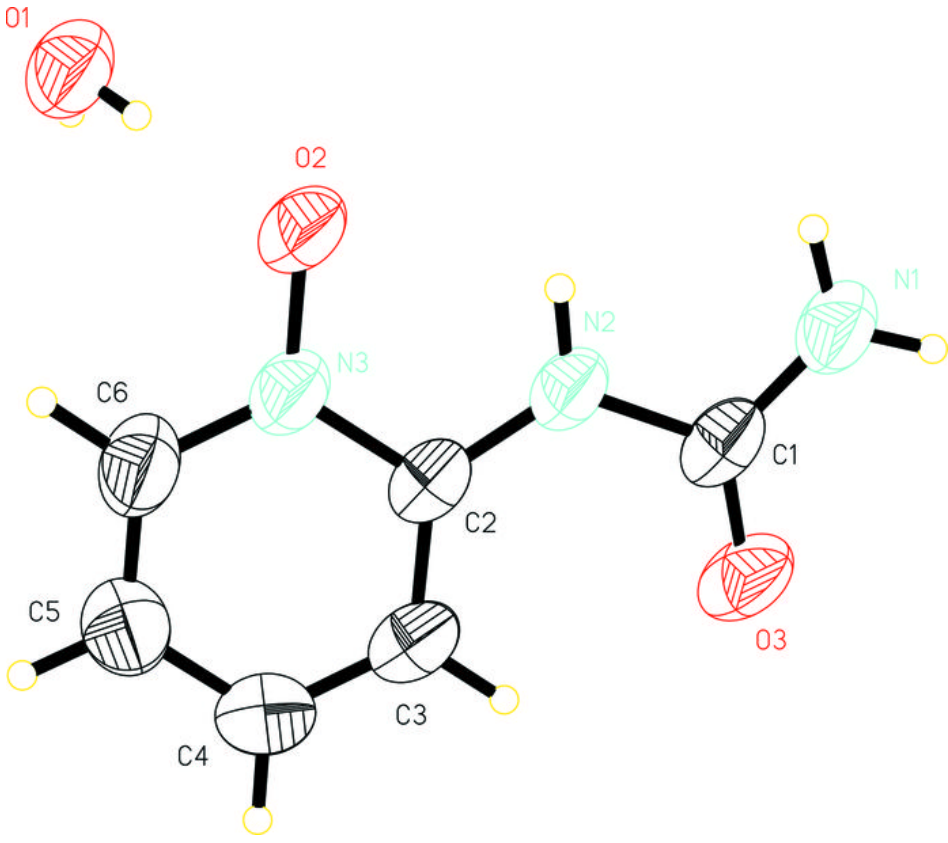

Fig. 2