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2-Aminopyrimidinium picrate

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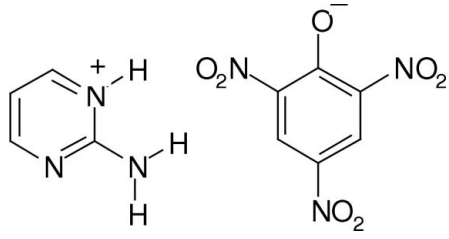
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.099; data-to-parameter ratio = 10.9.

The geometric parameters of the title compound, $C_4H_6N_3^+\cdot C_6H_2N_3O_7^-$, are in the usual ranges. While two nitro groups are almost coplanar with the aromatic picrate ring [dihedral angles 3.0 (2) and 4.4 (3)°], the third is significantly twisted out of this plane [dihedral angle 46.47 (8)°]. Anions and cations are connected *via* N—H···O hydrogen bonds. The molecules crystallize in planes parallel to $(1\bar{2}1)$.

Related literature

For related literature, see: Barraclough & Smith (1995); Etter *et al.* (1990); Fischer *et al.* (2007); Goswami *et al.* (2000); Gueiffier *et al.* (1996); Katritzky *et al.* (2003); Rival *et al.* (1991); Sanfilippo *et al.* (1988); Scheinbeim & Schempp (1976); Schlueter *et al.* (2006); Tully *et al.* (1991); Yathirajan, Bindya *et al.* (2007*a*,*b*); Yathirajan, Mayekar *et al.* (2007); Yathirajan, Narayana *et al.* (2007).



Experimental

Crystal data

$C_4H_6N_3^+\cdot C_6H_2N_3O_7^-$
M_r = 324.22
Triclinic, $P\bar{1}$
a = 5.8803 (7) Å
b = 8.0025 (10) Å
c = 13.8108 (17) Å
α = 88.021 (10)°
β = 82.322 (9)°
γ = 88.739 (10)°
V = 643.59 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 173 (2) K
0.26 × 0.22 × 0.09 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
8757 measured reflections
2402 independent reflections
1927 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.01
2402 reflections
220 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N6^{i}	0.87 (2)	2.09 (2)	2.958 (2)	177.0 (18)
N1—H1B···O11	0.91 (2)	1.97 (2)	2.7577 (19)	143.7 (18)
N1—H1B···O17	0.91 (2)	2.50 (2)	3.2488 (18)	140.0 (17)
N2—H2···O11	0.90 (2)	1.84 (2)	2.6501 (16)	148.6 (19)
N2—H2···O12	0.90 (2)	2.31 (2)	2.9792 (18)	131.6 (17)

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2509).

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supplementary materials

Acta Cryst. (2008). E**64**, o117-o118 [**doi:10.1107/S1600536807062599**]

2-Aminopyrimidinium picrate

B. Narayana, B. K. Sarojini, K. Prakash Kamath, H. S. Yathirajan and M. Bolte

Comment

Pyrimidine is a heterocyclic aromatic organic compound similar to benzene and pyridine, containing two nitrogen atoms at positions 1 and 3 of the six-member ring. A pyrimidine has many properties in common with pyridine, as the number of nitrogen atoms in the ring increases the ring π-electrons become less energetic and electrophilic aromatic substitution gets more difficult while nucleophilic aromatic substitution gets easier. Pyrimidines are important compounds in pharmaceutical chemistry as antiviral agents (Gueiffier *et al.*, 1996), inotropic and β-blocking agents (Barraclough & Smith, 1995), antifungal agents (Rival *et al.* 1991), benzodiazepine receptor agonists (Tully *et al.*1991), and calcium channel blockers (Sanfilippo *et al.*, 1988). The synthesis of imidazo[1,2-*a*]pyrimidines has been widely investigated and one of the most common strategies uses 2-aminopyrimidine as the starting material (Katritzky *et al.*, 2003). The crystal structures of the following compounds have been previously reported, *viz*; 2-aminopyrimidine (Scheinbeim & Schempp, 1976), 1:1 hetero-assembly of 2-aminopyrimidine and (+)-camphoric acid (Goswami, *et al.*, 2000), 2-aminopyrimidine-succinic acid (1:1) cocrystal (Etter *et al.*, 1990), 5-aminopyrimidine (Schlueter *et al.*, 2006), 5-bromopyrimidin-2(1*H*)-one (Yathirajan, Narayana, Ashalatha *et al.*, 2007), ethyl 7-methyl-2-[4-(methylsulfanyl)benzylidene]-5-[4-(methylsulfanyl)phenyl]-3-oxo-2, 3-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidine-6-carboxylate (Fischer *et al.*, 2007), 2-(4-methylbenzoyloxymethyl)-5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1 -yl)tetrahydrofuran-3-yl 4-methylbenzoate (Yathirajan, Mayekar, Sarojini *et al.*, 2007), methyl (4-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazolo[3,4-*d*]pyrimidin-5-yl)acetate (Yathirajan, Bindya, Sarojini *et al.*, 2007*a*), ethyl (4-oxo-1-phenyl-1,4-dihydro-5*H*-pyrazolo[3,4-*d*]pyrimidin-5-yl)acetate (Yathirajan, Bindya, Sarojini *et al.*, 2007*b*). In continuation to our work on picrates of biologically important molecules, we have prepared a new picrate of 2-aminopyrimidine, and its crystal structure is reported.

Geometric parameters of the title compound are in the usual ranges. Whereas two nitrogroups are almost coplanar with the aromatic picrate ring [dihedral angles 3.0 (2)° and 4.4 (3)°] the third one is significantly twisted [dihedral angle 46.47 (8)°] out of this plane Anions and cations are connected *via* N—H···O hydrogen bonds. The molecules crystallize in planes parallel to (1 − 2 1).

Experimental

2-Aminopyrimidine (0.95 g, 0.01 mol) was dissolved in 20 ml of ethanol. Picric acid (2.29 g, 0.01 mol) was dissolved in 10 ml of water. Both the solutions were mixed and to this, 5 ml of 5 *M* HCl was added and stirred for few minutes. The formed complex was filtered, dried and recrystallized from ethanol (m.p.: 413–415 K). Composition: Found (calculated): C 37.01(37.05), H 2.46(2.49), N 25.87% (25.92%).

Refinement

H atoms were found in a difference map, but those bonded to C were geometrically positioned and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2 U_{eq}(C)] using a riding model with C—H = 0.95 Å. The amino H atoms were freely refined.

Figures

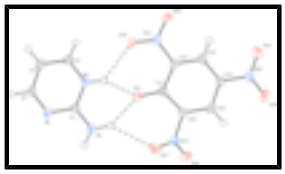


Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. The hydrogen bonds are shown as dashed lines.

2-Aminopyrimidinium picrate

Crystal data

$C_4H_6N_3^+ \cdot C_6H_2N_3O_7^-$	$Z = 2$
$M_r = 324.22$	$F_{000} = 332$
Triclinic, $P\overline{1}$	$D_x = 1.673$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.8803$ (7) Å	Cell parameters from 8213 reflections
$b = 8.0025$ (10) Å	$\theta = 3.5$–25.8º
$c = 13.8108$ (17) Å	$\mu = 0.15$ mm^{-1}
$\alpha = 88.021$ (10)º	$T = 173$ (2) K
$\beta = 82.322$ (9)º	Plate, yellow
$\gamma = 88.739$ (10)º	0.26 × 0.22 × 0.09 mm
$V = 643.59$ (14) Å^3	

Data collection

Stoe IPDSII two-circle diffractometer	1927 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.042$
Monochromator: graphite	$\theta_{max} = 25.6$º
$T = 173$(2) K	$\theta_{min} = 3.5$º
ω scans	$h = -7 \rightarrow 7$
Absorption correction: none	$k = -9 \rightarrow 9$
8757 measured reflections	$l = -16 \rightarrow 16$
2402 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
$R[F^2 > 2\sigma(F^2)] = 0.036$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.099$	$w = 1/[\sigma^2(F_o^2) + (0.0661P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$

2402 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
220 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. ;

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}
N1	0.7277 (3)	0.40774 (18)	0.07873 (11)	0.0279 (3)
H1A	0.799 (3)	0.422 (2)	0.0195 (16)	0.033 (5)*
H1B	0.600 (4)	0.346 (3)	0.0984 (15)	0.039 (5)*
C1	0.8282 (3)	0.47463 (18)	0.14768 (11)	0.0199 (3)
N2	0.7333 (2)	0.45943 (15)	0.24319 (9)	0.0206 (3)
H2	0.604 (4)	0.400 (3)	0.2556 (15)	0.039 (5)*
C3	0.8321 (3)	0.52828 (18)	0.31540 (11)	0.0229 (3)
H3	0.7618	0.5183	0.3814	0.027*
C4	1.0334 (3)	0.61214 (19)	0.29261 (11)	0.0241 (3)
H4	1.1076	0.6609	0.3415	0.029*
C5	1.1247 (3)	0.62249 (18)	0.19338 (12)	0.0229 (3)
H5	1.2654	0.6791	0.1762	0.027*
N6	1.0274 (2)	0.55855 (15)	0.12224 (9)	0.0228 (3)
C11	0.2209 (2)	0.17922 (17)	0.24085 (11)	0.0194 (3)
C12	0.0995 (2)	0.17467 (18)	0.33896 (11)	0.0196 (3)
C13	−0.1064 (2)	0.09207 (18)	0.36532 (11)	0.0201 (3)
H13	−0.1809	0.0931	0.4307	0.024*
C14	−0.2010 (2)	0.00844 (17)	0.29461 (11)	0.0197 (3)
C15	−0.0957 (3)	0.00409 (18)	0.19783 (11)	0.0209 (3)
H15	−0.1612	−0.0560	0.1506	0.025*
C16	0.1043 (2)	0.08881 (18)	0.17311 (11)	0.0197 (3)
N11	0.1908 (2)	0.26127 (16)	0.41664 (10)	0.0238 (3)
N12	−0.4142 (2)	−0.08122 (16)	0.32163 (10)	0.0250 (3)
N13	0.2118 (2)	0.08312 (16)	0.07100 (9)	0.0226 (3)
O11	0.41007 (18)	0.24842 (14)	0.21384 (8)	0.0276 (3)
O12	0.3751 (2)	0.33240 (17)	0.39985 (9)	0.0371 (3)
O13	0.0778 (2)	0.2607 (2)	0.49744 (9)	0.0534 (4)

O14	−0.5137 (2)	−0.07121 (17)	0.40512 (9)	0.0396 (3)
O15	−0.4859 (2)	−0.16322 (15)	0.25825 (10)	0.0366 (3)
O16	0.2234 (2)	−0.05385 (14)	0.03198 (9)	0.0323 (3)
O17	0.2799 (2)	0.21390 (15)	0.02874 (9)	0.0334 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0296 (8)	0.0360 (8)	0.0185 (7)	−0.0172 (6)	−0.0015 (6)	−0.0027 (6)
C1	0.0220 (7)	0.0191 (7)	0.0183 (7)	−0.0042 (5)	−0.0013 (6)	−0.0009 (6)
N2	0.0207 (6)	0.0211 (6)	0.0201 (7)	−0.0059 (5)	−0.0014 (5)	−0.0018 (5)
C3	0.0273 (8)	0.0228 (7)	0.0186 (8)	−0.0021 (6)	−0.0026 (6)	−0.0037 (6)
C4	0.0275 (8)	0.0234 (7)	0.0227 (8)	−0.0042 (6)	−0.0063 (6)	−0.0054 (6)
C5	0.0226 (7)	0.0211 (7)	0.0254 (8)	−0.0073 (6)	−0.0034 (6)	−0.0035 (6)
N6	0.0244 (7)	0.0235 (6)	0.0206 (7)	−0.0087 (5)	−0.0015 (5)	−0.0031 (5)
C11	0.0190 (7)	0.0181 (7)	0.0215 (8)	−0.0028 (5)	−0.0030 (6)	−0.0020 (6)
C12	0.0205 (7)	0.0205 (7)	0.0187 (8)	−0.0034 (6)	−0.0049 (6)	−0.0030 (6)
C13	0.0200 (7)	0.0199 (7)	0.0199 (8)	−0.0011 (5)	−0.0007 (6)	0.0001 (6)
C14	0.0158 (7)	0.0179 (7)	0.0255 (8)	−0.0042 (5)	−0.0022 (6)	−0.0012 (6)
C15	0.0221 (7)	0.0193 (7)	0.0226 (8)	−0.0019 (5)	−0.0063 (6)	−0.0048 (6)
C16	0.0208 (7)	0.0208 (7)	0.0176 (8)	−0.0014 (6)	−0.0025 (6)	−0.0018 (6)
N11	0.0244 (7)	0.0276 (7)	0.0196 (7)	−0.0063 (5)	−0.0023 (5)	−0.0039 (5)
N12	0.0193 (6)	0.0241 (6)	0.0316 (8)	−0.0048 (5)	−0.0031 (5)	−0.0008 (6)
N13	0.0212 (6)	0.0270 (7)	0.0201 (7)	−0.0026 (5)	−0.0035 (5)	−0.0052 (5)
O11	0.0226 (6)	0.0368 (6)	0.0233 (6)	−0.0141 (5)	0.0006 (4)	−0.0050 (5)
O12	0.0342 (7)	0.0518 (8)	0.0267 (6)	−0.0260 (6)	−0.0030 (5)	−0.0070 (5)
O13	0.0449 (8)	0.0925 (12)	0.0221 (7)	−0.0335 (7)	0.0095 (6)	−0.0245 (7)
O14	0.0298 (7)	0.0545 (8)	0.0322 (7)	−0.0175 (6)	0.0075 (5)	−0.0038 (6)
O15	0.0306 (6)	0.0386 (7)	0.0425 (8)	−0.0170 (5)	−0.0067 (5)	−0.0107 (6)
O16	0.0375 (7)	0.0321 (6)	0.0272 (6)	−0.0035 (5)	−0.0006 (5)	−0.0137 (5)
O17	0.0422 (7)	0.0339 (6)	0.0227 (6)	−0.0089 (5)	0.0017 (5)	0.0014 (5)

Geometric parameters (Å, °)

N1—C1	1.320 (2)	C12—C13	1.392 (2)
N1—H1A	0.87 (2)	C12—N11	1.4631 (19)
N1—H1B	0.91 (2)	C13—C14	1.385 (2)
C1—N6	1.3622 (19)	C13—H13	0.9500
C1—N2	1.3643 (19)	C14—C15	1.397 (2)
N2—C3	1.3572 (19)	C14—N12	1.4568 (18)
N2—H2	0.90 (2)	C15—C16	1.368 (2)
C3—C4	1.368 (2)	C15—H15	0.9500
C3—H3	0.9500	C16—N13	1.4682 (19)
C4—C5	1.404 (2)	N11—O13	1.2202 (18)
C4—H4	0.9500	N11—O12	1.2262 (17)
C5—N6	1.324 (2)	N12—O14	1.2258 (18)
C5—H5	0.9500	N12—O15	1.2349 (17)
C11—O11	1.2588 (18)	N13—O17	1.2289 (17)
C11—C12	1.444 (2)	N13—O16	1.2345 (17)

C11—C16	1.452 (2)		
C1—N1—H1A	115.1 (13)	C13—C12—N11	116.45 (13)
C1—N1—H1B	117.1 (13)	C11—C12—N11	120.10 (12)
H1A—N1—H1B	127.5 (19)	C14—C13—C12	118.89 (14)
N1—C1—N6	119.19 (14)	C14—C13—H13	120.6
N1—C1—N2	120.24 (13)	C12—C13—H13	120.6
N6—C1—N2	120.57 (13)	C13—C14—C15	122.04 (13)
C3—N2—C1	121.42 (13)	C13—C14—N12	119.44 (14)
C3—N2—H2	122.1 (13)	C15—C14—N12	118.50 (13)
C1—N2—H2	116.5 (13)	C16—C15—C14	118.09 (13)
N2—C3—C4	119.58 (14)	C16—C15—H15	121.0
N2—C3—H3	120.2	C14—C15—H15	121.0
C4—C3—H3	120.2	C15—C16—C11	124.88 (14)
C3—C4—C5	116.62 (14)	C15—C16—N13	117.24 (13)
C3—C4—H4	121.7	C11—C16—N13	117.85 (12)
C5—C4—H4	121.7	O13—N11—O12	121.68 (13)
N6—C5—C4	124.25 (14)	O13—N11—C12	118.02 (12)
N6—C5—H5	117.9	O12—N11—C12	120.30 (13)
C4—C5—H5	117.9	O14—N12—O15	123.36 (13)
C5—N6—C1	117.53 (13)	O14—N12—C14	118.93 (13)
O11—C11—C12	125.89 (13)	O15—N12—C14	117.70 (13)
O11—C11—C16	121.46 (13)	O17—N13—O16	123.85 (13)
C12—C11—C16	112.63 (13)	O17—N13—C16	118.75 (12)
C13—C12—C11	123.45 (13)	O16—N13—C16	117.38 (12)
N1—C1—N2—C3	−179.40 (14)	C14—C15—C16—C11	2.1 (2)
N6—C1—N2—C3	0.7 (2)	C14—C15—C16—N13	−179.82 (13)
C1—N2—C3—C4	−1.3 (2)	O11—C11—C16—C15	176.85 (14)
N2—C3—C4—C5	0.6 (2)	C12—C11—C16—C15	−1.5 (2)
C3—C4—C5—N6	0.7 (2)	O11—C11—C16—N13	−1.2 (2)
C4—C5—N6—C1	−1.3 (2)	C12—C11—C16—N13	−179.53 (12)
N1—C1—N6—C5	−179.32 (15)	C13—C12—N11—O13	−2.7 (2)
N2—C1—N6—C5	0.6 (2)	C11—C12—N11—O13	176.73 (15)
O11—C11—C12—C13	−178.11 (14)	C13—C12—N11—O12	177.68 (14)
C16—C11—C12—C13	0.2 (2)	C11—C12—N11—O12	−2.9 (2)
O11—C11—C12—N11	2.5 (2)	C13—C14—N12—O14	4.9 (2)
C16—C11—C12—N11	−179.19 (12)	C15—C14—N12—O14	−176.38 (14)
C11—C12—C13—C14	0.4 (2)	C13—C14—N12—O15	−175.46 (14)
N11—C12—C13—C14	179.81 (13)	C15—C14—N12—O15	3.2 (2)
C12—C13—C14—C15	0.2 (2)	C15—C16—N13—O17	133.79 (15)
C12—C13—C14—N12	178.82 (13)	C11—C16—N13—O17	−48.03 (19)
C13—C14—C15—C16	−1.4 (2)	C15—C16—N13—O16	−44.61 (19)
N12—C14—C15—C16	179.93 (13)	C11—C16—N13—O16	133.57 (14)

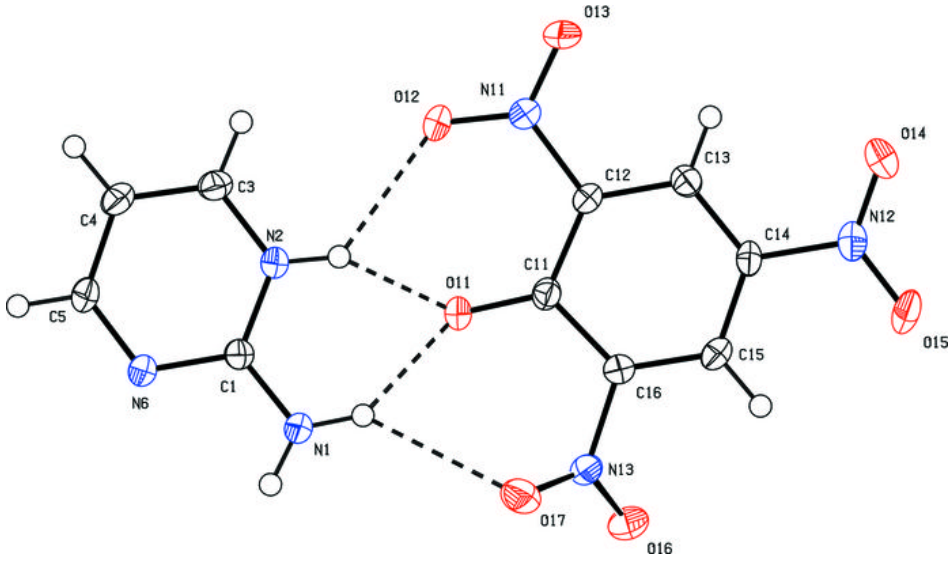
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···N6^{i}	0.87 (2)	2.09 (2)	2.958 (2)	177.0 (18)
N1—H1B···O11	0.91 (2)	1.97 (2)	2.7577 (19)	143.7 (18)

N1—H1B···O17	0.91 (2)	2.50 (2)	3.2488 (18)	140.0 (17)
N2—H2···O11	0.90 (2)	1.84 (2)	2.6501 (16)	148.6 (19)
N2—H2···O12	0.90 (2)	2.31 (2)	2.9792 (18)	131.6 (17)

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

Fig. 1


O13
O12
N11
O14
C13
C12
C3
C4
N2
C14
N12
C11
O11
C5
O15
C15
C16
N6
C1
N1
N13
O17
O16