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Hydrogen-bonded network in the salt 4-methyl-1*H*-imidazol-3-ium picrate

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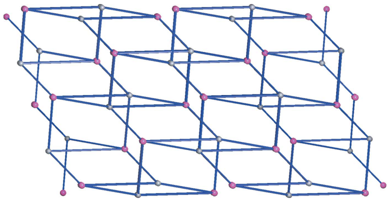
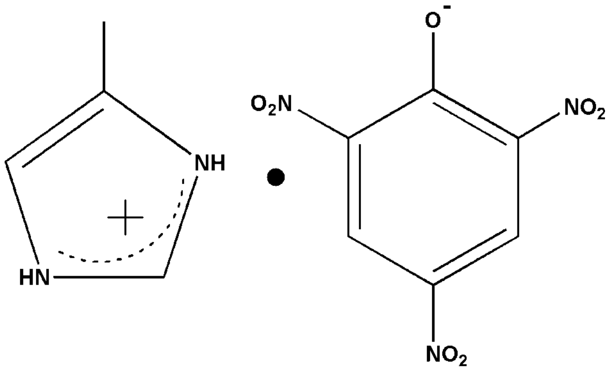
In the title molecular salt, $C_4H_7N_2^+ \cdot C_6H_2N_3O_7^-$, the phenolic proton of the starting picric acid has been transferred to the imidazole N atom. The nitro groups are twisted away from the benzene ring plane, making dihedral angles of 12.8 (2), 9.2 (4) and 29.3 (2)°. In the crystal, the component ions are linked into chains along [010] *via* N—H⋯O and bifurcated N—H⋯(O,O) hydrogen bonds. These chains are further linked by weak C—H⋯O hydrogen bonds into a three-dimensional network. The complex three-dimensional network can be topologically simplified into a 4-connected uninodal net with the point symbol $\{4.8^5\}$.



1. Chemical context

Co-crystallization, the crystallization of more than one solid component into a new compound, forming a new co-crystal or molecular salt, is a well known research field involving, for example, active pharmaceutical ingredients (Aitipamula *et al.*, 2015; Weyna *et al.*, 2012; Robinson, 2010; Arenas-García *et al.*, 2010) and crystal engineering (Manoj *et al.*, 2014). 4-Methylimidazole is an often used pharmaceutical intermediate (Shimpi *et al.*, 2014). The study of its crystallization can facilitate its related organic synthesis and theoretical optimization calculations. Picric acid, as a strong organic proton-donating reagent, is often adopted 2as an organic acid in the synthesis of co-crystallized complexes. Herein, we report the crystal structure of the molecular salt, 4-methylimidazolium picrate, (I). Future work will concentrate on how the crystallization behavior is affected by the solvent and temperature.



2. Structural commentary

The asymmetric unit of (I) consists of one 4-methylimidazolium cation and one picrate anion (Fig. 1). The phenolic proton in the original picric acid starting material was

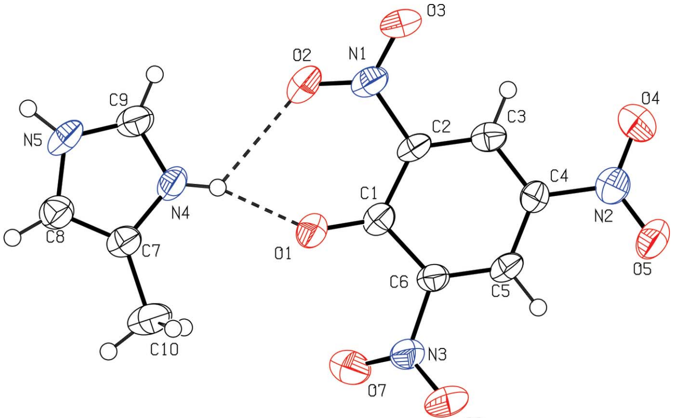


Figure 1
Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

transferred from the picric acid OH group to the imidazole nitrogen atom, forming a molecular salt. In the picrate anion, the C—O$_{\rm phenol}$ bond distance is shorter than in an earlier reported un-deprotonated compound [1.33 (2) Å; Bertolasi *et al.*, 2011] with a value of 1.244 (2) Å in (I). The adjacent C1—C2 [1.453 (2) Å] and C1—C6 [1.457 (3) Å] bonds are also lengthened from the values expected in a completely delocalized benzene ring. The C2—C1—C6 angle [111.0 (2)°] is smaller by *ca* 10° than the average value of the other five phenyl inner angles [121.8 (1)°]. This is mainly due to the electron-withdrawing effect of the three nitro groups attached to the aromatic π system, delocalizing electron density on the phenolate oxygen atom over the π system. The three nitro groups, N1/O2/O3, N2/O4/O5 and N3/O6/O6, are twisted away from the benzene ring plane, making dihedral angles of 12.8 (2), 9.2 (4) and 29.3 (2)°, respectively. In the 4-methylimidazolium cation, the C9—N4 [1.321 (3) Å] and C9—N5 [1.304 (3) Å] bond lengths are similar to each other due to the delocalizing effect; this is in contrast to the un-protonated 4-methylimidazole molecule in the co-crystal of 8-hydroxyquinoline and 5-methyl-1*H*-imidazole [C—N = 1.305 (4) and 1.340 4 Å; Liu & Meng, 2006].

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N4—H4$A\cdots$O2	0.84 (2)	2.46 (2)	3.013 (3)	124 (2)
N4—H4$A\cdots$O1	0.84 (2)	1.88 (2)	2.687 (2)	160 (2)
N5—H5$A\cdots$O3$^{\rm i}$	0.87 (2)	2.07 (3)	2.898 (3)	160 (2)
C8—H8$\cdots$O4$^{\rm ii}$	0.93	2.50	3.302 (3)	145
C9—H9$\cdots$O5$^{\rm iii}$	0.93	2.39	3.242 (3)	152

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

3. Supramolecular features

In the crystal structure of (I), the component ions are linked into chains along [010] by N—H$\cdots$O hydrogen bonds (Table 1, Fig. 2), one of which is bifurcated, N—H$\cdots$(O,O). The chains are linked by C—H$\cdots$O interactions, forming a three-

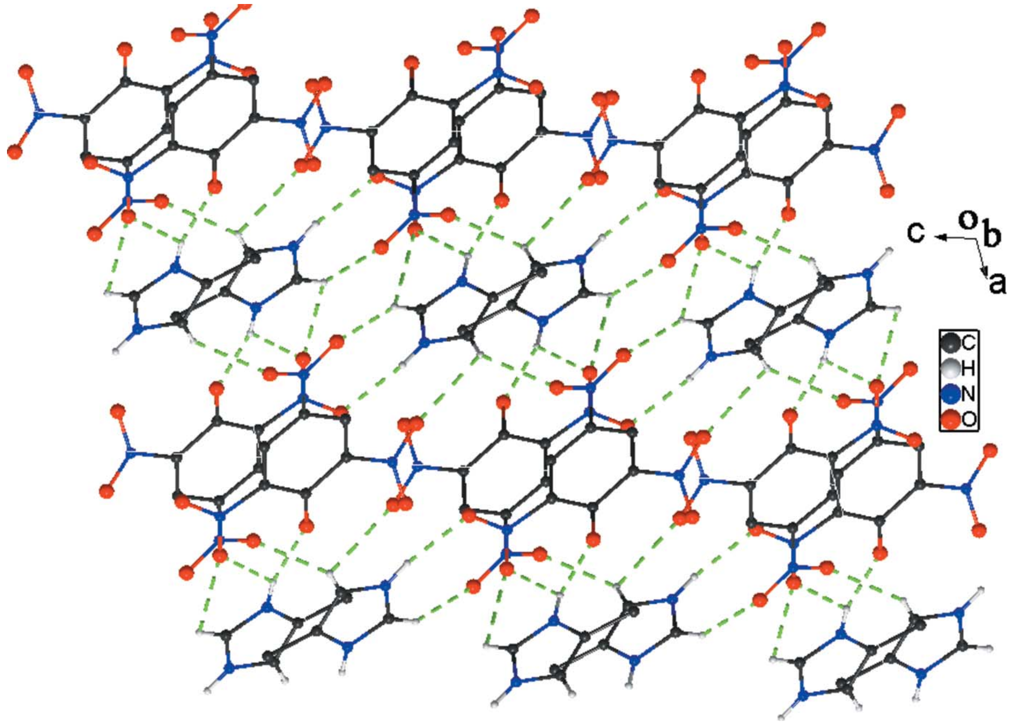


Figure 2
Part of the crystal structure of (I), showing the formation of the three-dimensional network. N—H$\cdots$O Hydrogen bonds and C—H$\cdots$O interactions are shown as green dashed lines. For the sake of clarity, H atoms not involved in the motif have been omitted.

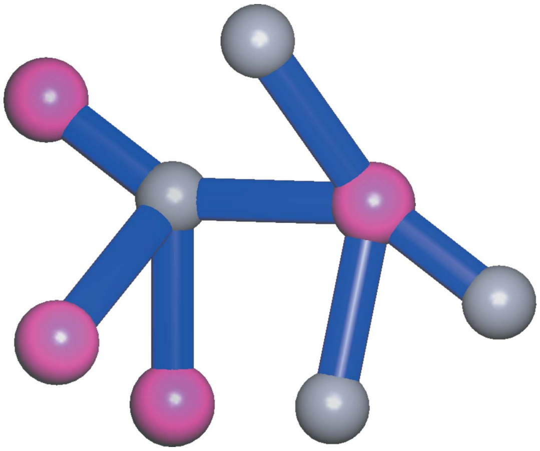


Figure 3
Part of the crystal structure of (I), showing the topologically connected relationship between 4-methylimidazolium and picrate ions (shown as gray and pink balls, respectively).

dimensional framework. In the cation, all H atoms except for the methyl group H atoms act as hydrogen-bond donors. Each cation is bonded to four adjacent picrate anions. In turn, each picrate anion utilizes the one phenolic and four nitro oxygen atoms, acting as hydrogen-bond acceptors, linked to four 4-methylimidazolium cations. No other interactions such as π–π and C—H$\cdots\pi$ are observed (Spek, 2009).

In order to better understand the three-dimensional structure, we can regard both the cation and anion as 4-connected nodes (Fig. 3), *i.e.* each one 4-methylimidazolium ion links with four other picrate ions, and *vice versa*. Thus, the whole network is simplified into a uninodal 4-connected net with the point symbol $\{4.8^5\}$ (Baburin & Blatov, 2007; Blatov *et al.*, 2014) (Fig. 4).

4. Database survey

A CSD search (CSD Version 5.37 plus one update; Groom *et al.*, 2016) found some analogs of the title compound, *viz.* BEZGEU (2-methylimidazolium picrate 2-methylimidazole; Dhanabal *et al.*, 2013) and QAKYOS (2-methyl-1*H*-imidazol-3-ium 2,4,6-trinitrophenolate; Dutkiewicz *et al.*, 2011). A structural comparison indicates that the two nitrogen atoms are preferably hydrogen-bonded to the picrate anions, of which one is bifurcated and the other is linear.

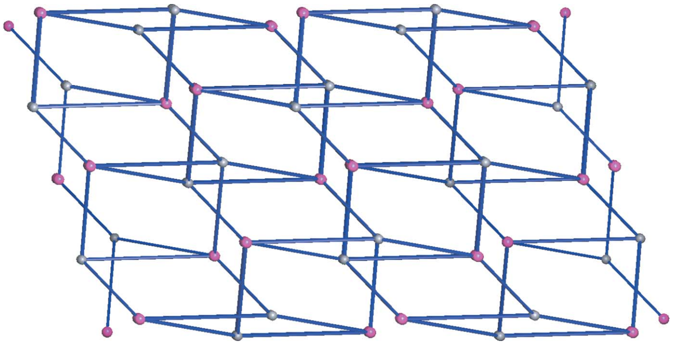


Figure 4
A schematic view of the formation of the 4-connected topological network in (I) when the cations and anions are regarded as four-connected nodes. The gray and pink spheres represent the 4-methylimidazolium cations and picrate anions, respectively.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_4H_7N_2^+ \cdot C_6H_2N_3O_7^-$
M_r	311.22
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, b, c (Å)	9.3079 (17), 9.4339 (17), 15.195 (3)
β (°)	107.835 (2)
V (Å^3)	1270.2 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.14
Crystal size (mm)	0.30 × 0.05 × 0.02
Data collection	
Diffractometer	Bruker *SMART* CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2008)
$T_{\min}$, $T_{\max}$	0.936, 0.992
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12952, 2489, 1539
$R_{\rm int}$	0.142
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.616
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.110, 1.04
No. of reflections	2489
No. of parameters	206
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.25, −0.22

Computer programs: *SMART* and *SAINT-Plus* (Bruker, 2001), *SHELXS* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *DIAMOND* (Brandenburg, 2006).

5. Synthesis and crystallization

Equivalent molar amounts of 4-methyl imidazole (1.0 mmol, 80.0 mg) and picric acid (1 mmol, 230.0mg) were dissolved in 95% methanol (40.0 ml). The mixture was stirred for half an hour at room temperature and then filtered. The resulting yellow solution was kept in air for two weeks. Needle-shaped yellow crystals of (I) suitable for single-crystal X-ray diffraction analysis were grown at the bottom of the vessel by slow evaporation of the solution. The crystals were separated by filtration (yield, 75%, *ca* 0.23 g).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bonded to C atoms were positioned geometrically with C—H = 0.93 Å (aromatic) or 0.96 Å (methyl) and refined using a riding model [$U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(Caromatic) or 1.5$U_{\rm eq}$(Cmethyl)]. H atoms bonded to N atoms were found in Fourier difference maps; N—H distances were refined freely with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(N).

Acknowledgements

We thank Dr Xiang-gao Meng for helpful discussions about this crystal structure.

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Hydrogen-bonded network in the salt 4-methyl-1*H*-imidazol-3-ium picrate

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Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus* (Bruker, 2001); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

4-Methyl-1*H*-imidazol-3-ium 2,4,6-trinitrophenolate

Crystal data

$C_4H_7N_2^+\cdot C_6H_2N_3O_7^-$
$M_r = 311.22$
Monoclinic, $P2_1/c$
$a = 9.3079\ (17)$ Å
$b = 9.4339\ (17)$ Å
$c = 15.195\ (3)$ Å
$\beta = 107.835\ (2)°$
$V = 1270.2\ (4)$ Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.628$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1754 reflections
$\theta = 2.3–22.1°$
$\mu = 0.14$ mm^{-1}
$T = 298$ K
Needle, yellow
0.30 × 0.05 × 0.02 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
$T_{min} = 0.936$, $T_{max} = 0.992$
12952 measured reflections
2489 independent reflections
1539 reflections with $I > 2\sigma(I)$
$R_{int} = 0.142$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.3°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.110$
$S = 1.04$
2489 reflections
206 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0154P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
C1	0.1017 (2)	0.4075 (2)	0.43900 (15)	0.0339 (6)
C2	0.0815 (2)	0.3083 (2)	0.50742 (14)	0.0340 (6)
C3	−0.0320 (2)	0.2096 (2)	0.49046 (15)	0.0350 (6)
H3	−0.0386	0.1486	0.5371	0.042*
C4	−0.1356 (2)	0.2015 (2)	0.40413 (15)	0.0318 (5)
C5	−0.1265 (2)	0.2912 (2)	0.33388 (15)	0.0344 (6)
H5	−0.1983	0.2860	0.2759	0.041*
C6	−0.0126 (2)	0.3863 (2)	0.34989 (14)	0.0326 (6)
C7	0.4896 (2)	0.7421 (2)	0.51495 (15)	0.0367 (6)
C8	0.6087 (3)	0.8040 (3)	0.57572 (16)	0.0420 (6)
H8	0.6633	0.8808	0.5646	0.050*
C9	0.5366 (3)	0.6298 (3)	0.64773 (16)	0.0438 (7)
H9	0.5314	0.5658	0.6932	0.053*
C10	0.4074 (3)	0.7745 (3)	0.41634 (16)	0.0552 (7)
H10A	0.3094	0.8119	0.4116	0.083*
H10B	0.3966	0.6894	0.3803	0.083*
H10C	0.4634	0.8432	0.3936	0.083*
N1	0.1822 (2)	0.3139 (2)	0.60151 (13)	0.0421 (5)
N2	−0.2537 (2)	0.0971 (2)	0.38594 (15)	0.0414 (5)
N3	−0.0051 (3)	0.4734 (2)	0.27120 (13)	0.0438 (5)
N4	0.4464 (2)	0.6333 (2)	0.56162 (13)	0.0390 (5)
H4A	0.369 (3)	0.584 (3)	0.5399 (16)	0.047*
N5	0.6343 (2)	0.7322 (2)	0.65746 (14)	0.0450 (6)
H5A	0.706 (3)	0.757 (3)	0.7063 (18)	0.054*
O1	0.19859 (18)	0.50281 (17)	0.45332 (11)	0.0487 (5)
O2	0.2988 (2)	0.3814 (2)	0.62018 (11)	0.0623 (6)
O3	0.1436 (2)	0.2490 (2)	0.66125 (12)	0.0682 (6)
O4	−0.2498 (2)	0.00651 (19)	0.44540 (13)	0.0600 (5)
O5	−0.35582 (18)	0.10262 (18)	0.31206 (12)	0.0520 (5)
O6	−0.1232 (2)	0.4962 (2)	0.21012 (13)	0.0744 (6)
O7	0.1172 (2)	0.5136 (2)	0.26798 (12)	0.0673 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0342 (14)	0.0300 (14)	0.0336 (13)	0.0044 (11)	0.0044 (11)	−0.0040 (11)
C2	0.0361 (13)	0.0374 (14)	0.0223 (12)	0.0054 (11)	0.0001 (10)	−0.0027 (10)
C3	0.0416 (14)	0.0332 (13)	0.0295 (14)	0.0067 (11)	0.0100 (11)	0.0010 (11)
C4	0.0311 (13)	0.0310 (13)	0.0318 (13)	−0.0012 (11)	0.0074 (11)	−0.0043 (11)

C5	0.0373 (13)	0.0358 (13)	0.0245 (12)	0.0039 (11)	0.0010 (10)	−0.0043 (11)
C6	0.0389 (14)	0.0296 (13)	0.0262 (12)	0.0024 (11)	0.0055 (10)	0.0018 (10)
C7	0.0410 (15)	0.0341 (14)	0.0313 (14)	0.0045 (11)	0.0056 (11)	−0.0018 (11)
C8	0.0456 (15)	0.0401 (15)	0.0371 (15)	−0.0006 (12)	0.0080 (12)	−0.0018 (12)
C9	0.0514 (17)	0.0405 (15)	0.0329 (15)	0.0040 (13)	0.0030 (13)	0.0019 (11)
C10	0.0690 (18)	0.0555 (18)	0.0323 (15)	0.0077 (15)	0.0023 (13)	0.0037 (13)
N1	0.0473 (13)	0.0444 (14)	0.0281 (12)	0.0037 (11)	0.0020 (10)	−0.0017 (10)
N2	0.0427 (13)	0.0394 (13)	0.0421 (13)	0.0010 (10)	0.0131 (11)	−0.0065 (11)
N3	0.0503 (14)	0.0377 (13)	0.0349 (12)	−0.0030 (11)	0.0007 (11)	0.0058 (10)
N4	0.0366 (12)	0.0352 (12)	0.0353 (12)	−0.0032 (10)	−0.0033 (10)	−0.0046 (9)
N5	0.0415 (13)	0.0515 (14)	0.0306 (12)	0.0014 (11)	−0.0058 (10)	−0.0104 (11)
O1	0.0515 (11)	0.0442 (11)	0.0398 (10)	−0.0130 (9)	−0.0017 (8)	−0.0003 (8)
O2	0.0481 (11)	0.0838 (16)	0.0408 (11)	−0.0196 (11)	−0.0074 (9)	0.0005 (10)
O3	0.0797 (14)	0.0853 (15)	0.0274 (10)	−0.0219 (12)	−0.0016 (10)	0.0122 (10)
O4	0.0664 (13)	0.0493 (12)	0.0609 (13)	−0.0107 (10)	0.0144 (10)	0.0134 (10)
O5	0.0459 (11)	0.0590 (13)	0.0428 (11)	−0.0098 (9)	0.0014 (9)	−0.0118 (9)
O6	0.0702 (14)	0.0825 (15)	0.0472 (12)	−0.0069 (11)	−0.0163 (10)	0.0287 (11)
O7	0.0618 (13)	0.0821 (15)	0.0546 (12)	−0.0132 (12)	0.0126 (10)	0.0241 (11)

Geometric parameters (Å, º)

C1—O1	1.244 (2)	C8—H8	0.9300
C1—C2	1.453 (3)	C9—N5	1.304 (3)
C1—C6	1.457 (3)	C9—N4	1.321 (3)
C2—C3	1.372 (3)	C9—H9	0.9300
C2—N1	1.451 (3)	C10—H10A	0.9600
C3—C4	1.372 (3)	C10—H10B	0.9600
C3—H3	0.9300	C10—H10C	0.9600
C4—C5	1.385 (3)	N1—O2	1.214 (2)
C4—N2	1.438 (3)	N1—O3	1.236 (2)
C5—C6	1.353 (3)	N2—O5	1.230 (2)
C5—H5	0.9300	N2—O4	1.236 (2)
C6—N3	1.470 (3)	N3—O7	1.215 (2)
C7—C8	1.340 (3)	N3—O6	1.222 (2)
C7—N4	1.375 (3)	N4—H4A	0.84 (2)
C7—C10	1.491 (3)	N5—H5A	0.87 (2)
C8—N5	1.370 (3)		

O1—C1—C2	125.9 (2)	N5—C9—N4	107.6 (2)
O1—C1—C6	123.1 (2)	N5—C9—H9	126.2
C2—C1—C6	111.0 (2)	N4—C9—H9	126.2
C3—C2—N1	116.0 (2)	C7—C10—H10A	109.5
C3—C2—C1	124.3 (2)	C7—C10—H10B	109.5
N1—C2—C1	119.7 (2)	H10A—C10—H10B	109.5
C4—C3—C2	119.5 (2)	C7—C10—H10C	109.5
C4—C3—H3	120.2	H10A—C10—H10C	109.5
C2—C3—H3	120.2	H10B—C10—H10C	109.5
C3—C4—C5	120.8 (2)	O2—N1—O3	121.9 (2)

C3—C4—N2	119.6 (2)	O2—N1—C2	120.7 (2)
C5—C4—N2	119.6 (2)	O3—N1—C2	117.4 (2)
C6—C5—C4	119.8 (2)	O5—N2—O4	122.5 (2)
C6—C5—H5	120.1	O5—N2—C4	118.5 (2)
C4—C5—H5	120.1	O4—N2—C4	118.9 (2)
C5—C6—C1	124.5 (2)	O7—N3—O6	123.5 (2)
C5—C6—N3	117.02 (19)	O7—N3—C6	119.07 (19)
C1—C6—N3	118.4 (2)	O6—N3—C6	117.4 (2)
C8—C7—N4	106.3 (2)	C9—N4—C7	109.4 (2)
C8—C7—C10	131.6 (2)	C9—N4—H4A	125.9 (17)
N4—C7—C10	122.1 (2)	C7—N4—H4A	124.4 (17)
C7—C8—N5	106.6 (2)	C9—N5—C8	110.0 (2)
C7—C8—H8	126.7	C9—N5—H5A	128.9 (17)
N5—C8—H8	126.7	C8—N5—H5A	121.1 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O2	0.84 (2)	2.46 (2)	3.013 (3)	124 (2)
N4—H4*A*···O1	0.84 (2)	1.88 (2)	2.687 (2)	160 (2)
N5—H5*A*···O3$^{\rm i}$	0.87 (2)	2.07 (3)	2.898 (3)	160 (2)
C8—H8···O4$^{\rm ii}$	0.93	2.50	3.302 (3)	145
C9—H9···O5$^{\rm iii}$	0.93	2.39	3.242 (3)	152

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