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# *N,N,N',N',N'',N''*-Hexamethylguanidinium 1,1,3,3-tetracyanoprop-2-en-1-ide

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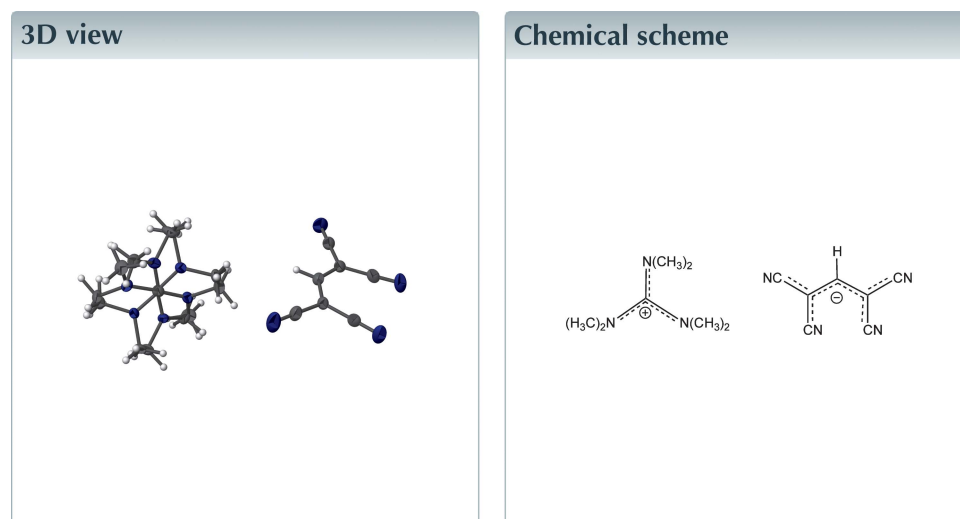
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Keywords: crystal structure; hexamethylguanidinium salt; 1,1,3,3-tetracyano-prop-2-en-1-ide.

CCDC reference: 1469774

Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

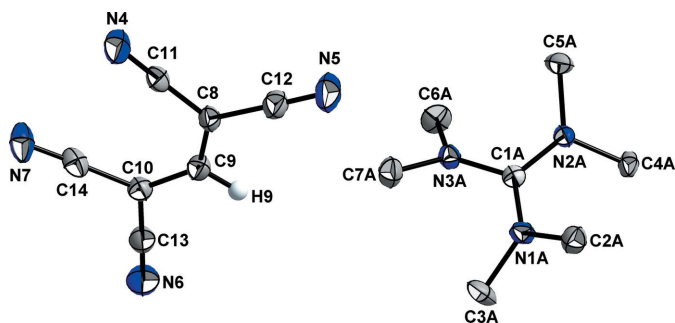
The asymmetric unit of the title salt,  $C_7H_{18}N_3^+ \cdot C_7HN_4^-$ , comprises one cation and one anion. The *N,N,N',N',N'',N''*-hexamethylguanidinium ion shows orientational disorder and two sets of N- and C-atom positions were found, with an occupancy ratio of 0.535 (3):0.465 (3). The C–N bond lengths in the guanidinium ion range from 1.339 (16) to 1.35 (2) Å, indicating partial double-bond character pointing towards charge delocalization within the NCN planes. The negative charge in the 1,1,3,3-tetracyanoprop-2-en-1-ide ion is delocalized within the CCC planes with the C–C bonds ranging in length from 1.379 (3) to 1.427 (3) Å, also indicating partial double-bond character.



## Structure description

The reaction of phosgene with *N,N,N',N'*-tetramethylurea yields *N,N,N',N'*-tetramethylchloroformamidinium chloride (Tiritiris & Kantlehner, 2008), which can be transformed by a mixture of dimethylamine and triethylamine into a mixture of *N,N,N',N',N'',N''*-hexamethylguanidinium chloride and triethylamine hydrochloride. Treating the salt mixture with an aqueous sodium hydroxide solution leads, after work up, to the pure guanidinium chloride. A further anion exchange was possible by reacting *N,N,N',N',N'',N''*-hexamethylguanidinium chloride with sodium 1,1,3,3-tetracyano-prop-2-en-1-ide in acetonitrile. According to the structure analysis, the asymmetric unit contains one *N,N,N',N',N'',N''*-hexamethylguanidinium ion and one 1,1,3,3-tetracyano-prop-2-en-1-ide ion (Fig. 1).

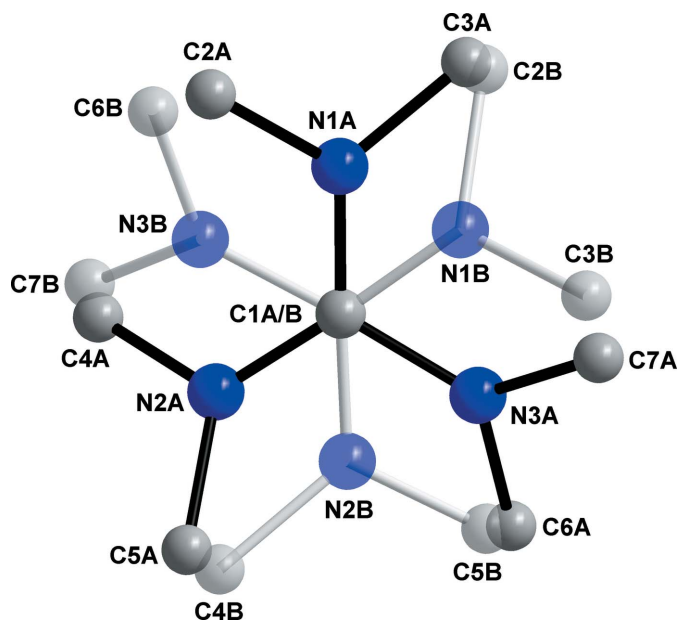
The cation shows orientational disorder and two sets of N and C positions were found, with an occupancy ratio of 0.535 (3):0.465 (3) (Fig. 2). The C–N bond lengths in the guanidinium ion range from 1.339 (16) to 1.35 (2) Å, indicating partial double-bond character. The N–C–N angles range from 119 (2) to 121.0 (15)°, indicating a nearly ideal trigonal–planar surrounding of the carbon atom C1 by the nitrogen atoms. The



**Figure 1**  
The structure of the title compound, with displacement ellipsoids at the 50% probability level. All H atoms have been omitted for clarity (except for H9). Only the major orientation of the disordered cation is shown.

positive charge is completely delocalized in the  $CN_3$  planes. The C–N bond lengths in the cation are in very good agreement with the data from the crystal structure analysis of known  $N,N,N',N',N'',N''$ -hexamethylguanidinium salts [see, for example: tetraphenylborate: Frey *et al.* (1998); chloride: Oelkers & Sundermeyer (2011); cyanate: Tiritiris & Kantlehner (2015)].

The negative charge in the 1,1,3,3-tetracyano-prop-2-en-1-ide ion is delocalized within the CCC planes and the C–C bond distances also indicate partial double-bond character [ $d(C8-C9) = 1.386(3) \text{ \AA}$ ;  $d(C9-C10) = 1.379(3) \text{ \AA}$ ;  $d(C8-C11) = 1.421(3) \text{ \AA}$ ;  $d(C8-C12) = 1.425(3) \text{ \AA}$ ;  $d(C10-C13) = 1.426(3) \text{ \AA}$ ;  $d(C10-C14) = 1.427(3) \text{ \AA}$ ]. The C–N bond lengths are in the range 1.148(3) to 1.153(3)  $\text{ \AA}$  and are characteristic for a triple bond. The dihedral angle between the C11–C8–C12 and the C13–C10–C14 planes is  $2.38(1)^\circ$ , indicating that the anion is nearly flat. A similar anionic



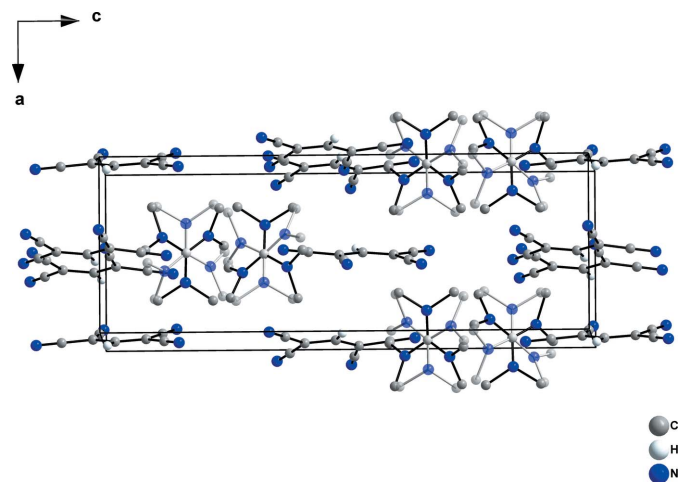
**Figure 2**  
The structure of the orientationally disordered  $N,N,N',N',N'',N''$ -hexamethylguanidinium ion. The C and N atoms are disordered between the dark (major orientation) and the opaque (minor orientation) positions. All H atoms have been omitted for clarity.

**Table 1**  
Experimental details.

Crystal data	
Chemical formula	$C_7H_{18}N_3^+ \cdot C_7HN_4^-$
$M_r$	285.36
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
$a, b, c$ ( $\text{ \AA}$ )	7.7705 (5), 9.8189 (6), 21.5478 (14)
$V$ ( $\text{ \AA}^3$ )	1644.05 (18)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	0.08
Crystal size (mm)	$0.20 \times 0.14 \times 0.10$
Data collection	
Diffractometer	Bruker Kappa APEXII DUO
Absorption correction	Multi-scan (Blessing, 1995)
$T_{\min}, T_{\max}$	0.720, 0.745
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	12519, 3368, 2709
$R_{\text{int}}$	0.039
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{ \AA}^{-1}$ )	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.036, 0.076, 1.02
No. of reflections	3368
No. of parameters	293
No. of restraints	171
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ( $e \text{ \AA}^{-3}$ )	0.11, $-0.13$

Computer programs: APEX2 and SAINT (Bruker, 2008), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015) and DIAMOND (Brandenburg & Putz, 2005).

arrangement was observed in the crystal structure of the compound 2,2'-bipyridin-1-ium 1,1,3,3-tetracyano-2-ethoxy-prop-2-en-1-ide, with the C–C bond lengths ranging from 1.3956(16) to 1.4261(17)  $\text{ \AA}$  and the C–N bond lengths in the range 1.1471(17) to 1.1522(16)  $\text{ \AA}$  (Setifi *et al.*, 2015). Since no significant hydrogen bonding exists in the title compound, the crystal packing results from electrostatic interactions between the cations and anions (Fig. 3).



**Figure 3**  
Molecular packing of the title compound (view along  $ac$ ). Both orientations of the disordered  $N,N,N',N',N'',N''$ -hexamethylguanidinium ion are shown.

## Synthesis and crystallization

The title compound was obtained by mixing an acetonitrile solution of *N,N,N',N',N'',N''*-hexamethylguanidinium chloride with sodium 1,1,3,3-tetracyano-prop-2-en-1-ide dissolved in acetonitrile and stirring it for 18 h at room temperature. The precipitated sodium chloride was removed by filtration. After removal of the acetonitrile, the colorless residue was crystallized from an ethanolic solution. After evaporation of the solvent at ambient temperature, colorless single crystals suitable for X-ray analysis emerged.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The title compound crystallizes in the non-centrosymmetric space group  $P2_12_12_1$ ; however, in the absence of significant anomalous scattering effects, the determined Flack parameter  $x = -0.4(10)$  (Parsons *et al.*, 2013) is essentially meaningless. The atoms C1–C7 and N1–N3 of the cation are disordered over two sets of sites (C1A/C1B–C7A/C7B and N1A/N1B–N3A/N3B) with refined occupancies of 0.535(3):0.465(3). The major and minor disordered components were each restrained to have similar geometries

and the  $U^{ij}$  components of the ADPs of the corresponding atoms were restrained to be similar if closer than 1.7 Å.

## Acknowledgements

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## full crystallographic data

*IUCrData* (2016). **1**, x160478 [doi:10.1107/S2414314616004788]

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*N,N,N',N',N'',N''*-hexamethylguanidinium 1,1,3,3-tetracyanoprop-2-en-1-ide

*Crystal data*

$C_7H_{18}N_3^+ \cdot C_7HN_4^-$

$M_r = 285.36$

Orthorhombic,  $P2_12_12_1$

$a = 7.7705$  (5) Å

$b = 9.8189$  (6) Å

$c = 21.5478$  (14) Å

$V = 1644.05$  (18) Å<sup>3</sup>

$Z = 4$

$F(000) = 608$

$D_x = 1.153$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 12519 reflections

$\theta = 1.9$ – $26.4^\circ$

$\mu = 0.08$  mm<sup>-1</sup>

$T = 100$  K

Block, colorless

$0.20 \times 0.14 \times 0.10$  mm

*Data collection*

Bruker Kappa APEXII DUO  
diffractometer

Radiation source: fine-focus sealed tube

Triumph monochromator

$\varphi$  scans, and  $\omega$  scans

Absorption correction: multi-scan  
(Blessing, 1995)

$T_{\min} = 0.720$ ,  $T_{\max} = 0.745$

12519 measured reflections

3368 independent reflections

2709 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 26.4^\circ$ ,  $\theta_{\min} = 1.9^\circ$

$h = -9 \rightarrow 9$

$k = -12 \rightarrow 11$

$l = -26 \rightarrow 25$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.076$

$S = 1.02$

3368 reflections

293 parameters

171 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 0.107P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.11$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.13$  e Å<sup>-3</sup>

*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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1A	0.473 (2)	0.769 (4)	0.1683 (15)	0.018 (2)	0.535 (3)
C2A	0.727 (2)	0.7960 (18)	0.1024 (8)	0.034 (4)	0.535 (3)
H2A	0.7249	0.8883	0.1197	0.051*	0.535 (3)
H2B	0.7264	0.8011	0.0570	0.051*	0.535 (3)
H2C	0.8315	0.7491	0.1163	0.051*	0.535 (3)
C3A	0.5426 (8)	0.5938 (8)	0.0903 (4)	0.0299 (15)	0.535 (3)
H3A	0.4501	0.5437	0.1111	0.045*	0.535 (3)
H3B	0.6473	0.5381	0.0899	0.045*	0.535 (3)
H3C	0.5082	0.6143	0.0476	0.045*	0.535 (3)
C4A	0.201 (2)	0.727 (2)	0.2239 (7)	0.028 (3)	0.535 (3)
H4A	0.1281	0.6456	0.2203	0.042*	0.535 (3)
H4B	0.1284	0.8074	0.2293	0.042*	0.535 (3)
H4C	0.2774	0.7170	0.2598	0.042*	0.535 (3)
C5A	0.209 (2)	0.7339 (19)	0.1085 (9)	0.027 (3)	0.535 (3)
H5A	0.2879	0.7514	0.0739	0.041*	0.535 (3)
H5B	0.1173	0.8023	0.1084	0.041*	0.535 (3)
H5C	0.1588	0.6429	0.1040	0.041*	0.535 (3)
C6A	0.7115 (10)	0.8155 (9)	0.2409 (4)	0.0289 (15)	0.535 (3)
H6A	0.7554	0.7291	0.2246	0.043*	0.535 (3)
H6B	0.7045	0.8105	0.2863	0.043*	0.535 (3)
H6C	0.7893	0.8895	0.2290	0.043*	0.535 (3)
C7A	0.446 (2)	0.9560 (16)	0.2432 (9)	0.027 (3)	0.535 (3)
H7A	0.3447	0.9769	0.2179	0.040*	0.535 (3)
H7B	0.5214	1.0361	0.2449	0.040*	0.535 (3)
H7C	0.4098	0.9316	0.2853	0.040*	0.535 (3)
N1A	0.5760 (4)	0.7210 (3)	0.12360 (16)	0.0251 (8)	0.535 (3)
N2A	0.3046 (3)	0.7416 (3)	0.16741 (14)	0.0207 (8)	0.535 (3)
N3A	0.5401 (4)	0.8415 (3)	0.21540 (14)	0.0222 (8)	0.535 (3)
C1B	0.465 (2)	0.764 (5)	0.1653 (18)	0.020 (3)	0.465 (3)
C2B	0.7389 (14)	0.7854 (11)	0.2214 (4)	0.031 (2)	0.465 (3)
H2B1	0.6659	0.7618	0.2569	0.047*	0.465 (3)
H2B2	0.7886	0.8760	0.2278	0.047*	0.465 (3)
H2B3	0.8315	0.7183	0.2174	0.047*	0.465 (3)
C3B	0.735 (3)	0.805 (2)	0.1080 (9)	0.035 (4)	0.465 (3)
H3B1	0.6567	0.8222	0.0733	0.052*	0.465 (3)
H3B2	0.8028	0.7227	0.0994	0.052*	0.465 (3)
H3B3	0.8132	0.8827	0.1130	0.052*	0.465 (3)
C4B	0.411 (2)	0.9432 (18)	0.2423 (10)	0.027 (3)	0.465 (3)
H4B1	0.4591	0.9251	0.2835	0.040*	0.465 (3)
H4B2	0.3064	0.9983	0.2465	0.040*	0.465 (3)

H4B3	0.4955	0.9927	0.2172	0.040*	0.465 (3)
C5B	0.218 (3)	0.743 (3)	0.2362 (9)	0.030 (3)	0.465 (3)
H5B1	0.2096	0.6533	0.2168	0.045*	0.465 (3)
H5B2	0.1137	0.7959	0.2267	0.045*	0.465 (3)
H5B3	0.2284	0.7328	0.2813	0.045*	0.465 (3)
C6B	0.213 (2)	0.729 (2)	0.0983 (11)	0.032 (4)	0.465 (3)
H6B1	0.1353	0.6535	0.1091	0.048*	0.465 (3)
H6B2	0.2127	0.7416	0.0532	0.048*	0.465 (3)
H6B3	0.1737	0.8122	0.1186	0.048*	0.465 (3)
C7B	0.4713 (9)	0.5843 (10)	0.0862 (5)	0.0338 (19)	0.465 (3)
H7B1	0.5800	0.5614	0.1067	0.051*	0.465 (3)
H7B2	0.4942	0.6119	0.0432	0.051*	0.465 (3)
H7B3	0.3955	0.5045	0.0863	0.051*	0.465 (3)
N1B	0.6359 (4)	0.7857 (4)	0.16509 (19)	0.0248 (10)	0.465 (3)
N2B	0.3689 (5)	0.8151 (4)	0.21212 (17)	0.0214 (10)	0.465 (3)
N3B	0.3883 (4)	0.6959 (3)	0.11918 (17)	0.0227 (10)	0.465 (3)
N4	0.4223 (3)	-0.0855 (2)	-0.00048 (8)	0.0491 (6)	
N5	0.5394 (3)	0.2260 (2)	0.13383 (9)	0.0584 (6)	
N6	0.5537 (3)	0.46050 (19)	-0.16125 (9)	0.0439 (5)	
N7	0.4329 (3)	0.03094 (18)	-0.15091 (8)	0.0419 (5)	
C8	0.5027 (3)	0.1647 (2)	0.01848 (9)	0.0269 (5)	
C9	0.5256 (3)	0.2613 (2)	-0.02772 (9)	0.0277 (5)	
H9	0.5563	0.3494	-0.0133	0.033*	
C10	0.5110 (2)	0.2500 (2)	-0.09130 (9)	0.0255 (5)	
C11	0.4570 (3)	0.0269 (2)	0.00714 (9)	0.0299 (5)	
C12	0.5233 (3)	0.1998 (2)	0.08220 (11)	0.0366 (6)	
C13	0.5355 (3)	0.3669 (2)	-0.12963 (9)	0.0308 (5)	
C14	0.4672 (3)	0.1278 (2)	-0.12346 (9)	0.0284 (5)	

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1A	0.022 (4)	0.013 (4)	0.019 (4)	0.002 (4)	-0.002 (4)	0.002 (4)
C2A	0.026 (6)	0.029 (5)	0.048 (7)	-0.006 (4)	0.010 (5)	-0.004 (5)
C3A	0.037 (4)	0.023 (3)	0.029 (3)	0.003 (3)	0.004 (4)	-0.007 (2)
C4A	0.028 (4)	0.038 (6)	0.019 (5)	-0.003 (3)	0.003 (3)	0.003 (4)
C5A	0.033 (5)	0.025 (4)	0.022 (5)	-0.007 (4)	-0.004 (3)	-0.001 (3)
C6A	0.023 (3)	0.036 (4)	0.028 (4)	0.003 (3)	-0.014 (3)	-0.002 (3)
C7A	0.027 (5)	0.022 (4)	0.032 (4)	0.001 (3)	-0.003 (4)	-0.008 (3)
N1A	0.0233 (17)	0.0238 (16)	0.0282 (18)	0.0004 (13)	0.0053 (14)	-0.0020 (14)
N2A	0.0192 (15)	0.0254 (16)	0.0176 (17)	-0.0042 (13)	0.0006 (13)	0.0001 (14)
N3A	0.0190 (16)	0.0221 (15)	0.0255 (17)	0.0000 (13)	-0.0064 (14)	-0.0002 (13)
C1B	0.025 (5)	0.017 (5)	0.019 (5)	0.000 (4)	0.001 (5)	0.002 (4)
C2B	0.030 (4)	0.031 (5)	0.034 (5)	0.000 (3)	-0.003 (3)	-0.004 (3)
C3B	0.024 (7)	0.058 (10)	0.021 (5)	0.002 (5)	0.008 (4)	0.003 (5)
C4B	0.042 (7)	0.018 (4)	0.020 (4)	-0.004 (4)	0.003 (5)	-0.001 (3)
C5B	0.027 (5)	0.032 (6)	0.031 (7)	-0.003 (4)	0.012 (6)	0.002 (6)
C6B	0.019 (5)	0.046 (7)	0.032 (7)	0.002 (4)	-0.010 (4)	0.002 (5)

C7B	0.038 (5)	0.030 (3)	0.033 (4)	0.002 (4)	0.000 (5)	-0.009 (2)
N1B	0.0181 (18)	0.032 (2)	0.025 (2)	0.0000 (15)	0.0009 (16)	0.0008 (18)
N2B	0.026 (2)	0.0186 (19)	0.019 (2)	-0.0001 (15)	0.0034 (16)	-0.0007 (15)
N3B	0.0215 (18)	0.0236 (19)	0.023 (2)	0.0026 (15)	0.0003 (16)	-0.0021 (17)
N4	0.0887 (17)	0.0356 (11)	0.0229 (10)	-0.0180 (12)	-0.0009 (11)	0.0039 (9)
N5	0.1007 (17)	0.0476 (12)	0.0270 (12)	-0.0207 (14)	-0.0035 (12)	-0.0047 (9)
N6	0.0597 (13)	0.0333 (10)	0.0389 (11)	-0.0060 (10)	0.0021 (11)	0.0079 (10)
N7	0.0726 (15)	0.0281 (10)	0.0248 (10)	0.0068 (10)	-0.0085 (10)	0.0000 (9)
C8	0.0345 (12)	0.0271 (10)	0.0190 (10)	-0.0037 (9)	0.0001 (9)	-0.0024 (8)
C9	0.0289 (11)	0.0244 (10)	0.0298 (11)	-0.0020 (9)	-0.0001 (9)	-0.0030 (9)
C10	0.0300 (12)	0.0220 (10)	0.0245 (10)	0.0011 (9)	0.0018 (8)	0.0018 (8)
C11	0.0395 (11)	0.0352 (12)	0.0150 (10)	-0.0053 (11)	-0.0001 (10)	0.0032 (9)
C12	0.0519 (15)	0.0290 (11)	0.0290 (12)	-0.0100 (11)	0.0002 (11)	-0.0009 (9)
C13	0.0357 (11)	0.0287 (11)	0.0281 (11)	-0.0008 (10)	0.0005 (10)	-0.0007 (10)
C14	0.0385 (11)	0.0270 (11)	0.0198 (10)	0.0080 (10)	-0.0005 (10)	0.0064 (9)

*Geometric parameters (Å, °)*

C1A—N2A	1.339 (17)	C2B—H2B3	0.9800
C1A—N1A	1.339 (16)	C3B—N1B	1.466 (16)
C1A—N3A	1.34 (3)	C3B—H3B1	0.9800
C2A—N1A	1.459 (14)	C3B—H3B2	0.9800
C2A—H2A	0.9800	C3B—H3B3	0.9800
C2A—H2B	0.9800	C4B—N2B	1.453 (16)
C2A—H2C	0.9800	C4B—H4B1	0.9800
C3A—N1A	1.464 (8)	C4B—H4B2	0.9800
C3A—H3A	0.9800	C4B—H4B3	0.9800
C3A—H3B	0.9800	C5B—N2B	1.466 (17)
C3A—H3C	0.9800	C5B—H5B1	0.9800
C4A—N2A	1.466 (15)	C5B—H5B2	0.9800
C4A—H4A	0.9800	C5B—H5B3	0.9800
C4A—H4B	0.9800	C6B—N3B	1.470 (16)
C4A—H4C	0.9800	C6B—H6B1	0.9800
C5A—N2A	1.472 (15)	C6B—H6B2	0.9800
C5A—H5A	0.9800	C6B—H6B3	0.9800
C5A—H5B	0.9800	C7B—N3B	1.457 (10)
C5A—H5C	0.9800	C7B—H7B1	0.9800
C6A—N3A	1.464 (8)	C7B—H7B2	0.9800
C6A—H6A	0.9800	C7B—H7B3	0.9800
C6A—H6B	0.9800	N4—C11	1.148 (3)
C6A—H6C	0.9800	N5—C12	1.149 (3)
C7A—N3A	1.468 (15)	N6—C13	1.153 (3)
C7A—H7A	0.9800	N7—C14	1.151 (3)
C7A—H7B	0.9800	C8—C9	1.386 (3)
C7A—H7C	0.9800	C8—C11	1.421 (3)
C1B—N1B	1.349 (19)	C8—C12	1.425 (3)
C1B—N2B	1.35 (2)	C9—C10	1.379 (3)
C1B—N3B	1.34 (3)	C9—H9	0.9500

C2B—N1B	1.452 (11)	C10—C13	1.426 (3)
C2B—H2B1	0.9800	C10—C14	1.427 (3)
C2B—H2B2	0.9800		
N2A—C1A—N1A	120 (2)	H2B1—C2B—H2B3	109.5
N2A—C1A—N3A	119.9 (12)	H2B2—C2B—H2B3	109.5
N1A—C1A—N3A	120.1 (13)	N1B—C3B—H3B1	109.5
N1A—C2A—H2A	109.4	N1B—C3B—H3B2	109.4
N1A—C2A—H2B	109.4	H3B1—C3B—H3B2	109.5
H2A—C2A—H2B	109.5	N1B—C3B—H3B3	109.5
N1A—C2A—H2C	109.5	H3B1—C3B—H3B3	109.5
H2A—C2A—H2C	109.5	H3B2—C3B—H3B3	109.5
H2B—C2A—H2C	109.5	N2B—C4B—H4B1	109.4
N1A—C3A—H3A	109.5	N2B—C4B—H4B2	109.5
N1A—C3A—H3B	109.5	H4B1—C4B—H4B2	109.5
H3A—C3A—H3B	109.5	N2B—C4B—H4B3	109.5
N1A—C3A—H3C	109.5	H4B1—C4B—H4B3	109.5
H3A—C3A—H3C	109.5	H4B2—C4B—H4B3	109.5
H3B—C3A—H3C	109.5	N2B—C5B—H5B1	109.5
N2A—C4A—H4A	109.5	N2B—C5B—H5B2	109.5
N2A—C4A—H4B	109.5	H5B1—C5B—H5B2	109.5
H4A—C4A—H4B	109.5	N2B—C5B—H5B3	109.5
N2A—C4A—H4C	109.5	H5B1—C5B—H5B3	109.5
H4A—C4A—H4C	109.5	H5B2—C5B—H5B3	109.5
H4B—C4A—H4C	109.5	N3B—C6B—H6B1	109.5
N2A—C5A—H5A	109.5	N3B—C6B—H6B2	109.5
N2A—C5A—H5B	109.5	H6B1—C6B—H6B2	109.5
H5A—C5A—H5B	109.5	N3B—C6B—H6B3	109.5
N2A—C5A—H5C	109.5	H6B1—C6B—H6B3	109.5
H5A—C5A—H5C	109.5	H6B2—C6B—H6B3	109.5
H5B—C5A—H5C	109.5	N3B—C7B—H7B1	109.5
N3A—C6A—H6A	109.5	N3B—C7B—H7B2	109.5
N3A—C6A—H6B	109.5	H7B1—C7B—H7B2	109.5
H6A—C6A—H6B	109.5	N3B—C7B—H7B3	109.5
N3A—C6A—H6C	109.5	H7B1—C7B—H7B3	109.5
H6A—C6A—H6C	109.5	H7B2—C7B—H7B3	109.5
H6B—C6A—H6C	109.5	C1B—N1B—C2B	122.7 (18)
N3A—C7A—H7A	109.4	C1B—N1B—C3B	123.0 (19)
N3A—C7A—H7B	109.5	C2B—N1B—C3B	114.3 (10)
H7A—C7A—H7B	109.5	C1B—N2B—C4B	122.2 (19)
N3A—C7A—H7C	109.5	C1B—N2B—C5B	121.8 (19)
H7A—C7A—H7C	109.5	C4B—N2B—C5B	116.0 (12)
H7B—C7A—H7C	109.5	C1B—N3B—C7B	122.8 (15)
C1A—N1A—C3A	123.4 (15)	C1B—N3B—C6B	122.0 (17)
C1A—N1A—C2A	121.7 (17)	C7B—N3B—C6B	115.1 (10)
C3A—N1A—C2A	114.8 (8)	C9—C8—C11	124.07 (18)
C1A—N2A—C5A	121.1 (17)	C9—C8—C12	120.82 (18)
C1A—N2A—C4A	123.0 (16)	C11—C8—C12	115.10 (18)



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C5A—N2A—C4A	115.7 (11)	C10—C9—C8	130.39 (19)
C1A—N3A—C6A	123.0 (13)	C10—C9—H9	114.8
C1A—N3A—C7A	121.4 (15)	C8—C9—H9	114.8
C6A—N3A—C7A	115.6 (8)	C9—C10—C13	119.99 (18)
N1B—C1B—N2B	119 (2)	C9—C10—C14	124.71 (18)
N1B—C1B—N3B	121.0 (15)	C13—C10—C14	115.28 (17)
N2B—C1B—N3B	119.8 (14)	N4—C11—C8	178.1 (2)
N1B—C2B—H2B1	109.5	N5—C12—C8	178.9 (2)
N1B—C2B—H2B2	109.5	N6—C13—C10	179.0 (2)
H2B1—C2B—H2B2	109.5	N7—C14—C10	178.1 (2)
N1B—C2B—H2B3	109.5		
N2A—C1A—N1A—C3A	-29 (5)	N2B—C1B—N1B—C3B	-146 (3)
N3A—C1A—N1A—C3A	148 (3)	N3B—C1B—N1B—C3B	32 (6)
N2A—C1A—N1A—C2A	148 (3)	N1B—C1B—N2B—C4B	33 (6)
N3A—C1A—N1A—C2A	-35 (5)	N3B—C1B—N2B—C4B	-145 (3)
N1A—C1A—N2A—C5A	-36 (5)	N1B—C1B—N2B—C5B	-146 (3)
N3A—C1A—N2A—C5A	146 (3)	N3B—C1B—N2B—C5B	36 (6)
N1A—C1A—N2A—C4A	148 (3)	N1B—C1B—N3B—C7B	34 (6)
N3A—C1A—N2A—C4A	-29 (5)	N2B—C1B—N3B—C7B	-148 (3)
N2A—C1A—N3A—C6A	144 (3)	N1B—C1B—N3B—C6B	-146 (3)
N1A—C1A—N3A—C6A	-33 (5)	N2B—C1B—N3B—C6B	31 (6)
N2A—C1A—N3A—C7A	-38 (5)	C11—C8—C9—C10	0.1 (4)
N1A—C1A—N3A—C7A	144 (3)	C12—C8—C9—C10	-179.4 (2)
N2B—C1B—N1B—C2B	38 (6)	C8—C9—C10—C13	177.8 (2)
N3B—C1B—N1B—C2B	-144 (3)	C8—C9—C10—C14	-0.3 (4)

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