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Crystal structure of *catena*-poly[*N,N,N',N'*-tetramethylguanidinium [(chloridocadmate)-di- μ -chlorido]]

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Keywords: crystal structure; five-coordinated cadmium; N—H...Cl hydrogen bonds; polyanionic chain

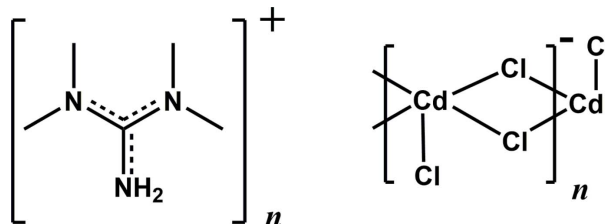
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In the structure of the title salt, $\{(C_5H_{14}N_3)[CdCl_3]\}_n$, the Cd^{II} atom of the complex anion is five-coordinated by one terminal and four bridging Cl atoms. The corresponding coordination polyhedron is a distorted trigonal bipyramid, with Cd—Cl distances in the range 2.4829 (4)–2.6402 (4) Å. The bipyramids are condensed into a polyanionic zigzag chain extending parallel to [101]. The tetramethylguanidinium cations are situated between the polyanionic chains and are linked to them through N—H...Cl hydrogen bonds, forming a layered network parallel to (010).

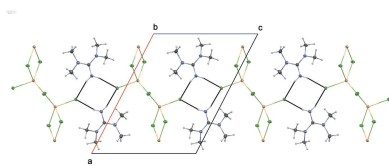
1. Chemical context

Tetramethylguanidine is known to crystallize in its neutral form, as a Lewis base or as a singly protonated cation. Several cationic complexes of Pd, Ga and Pt have been reported with tetramethylguanidine acting as a ligand (Li *et al.*, 2005; Cowley *et al.*, 2005; Eliseev *et al.*, 2013), and halogenidometalates have been reported with tetramethylguanidinium as a counter-cation (Bujak *et al.*, 1999; Bujak & Zaleski, 2007). Since none of these complexes has cadmium as a component, we decided to study the interactions between tetramethylguanidine and $[CdCl_2]\cdot H_2O$, which has yielded the title salt, $(C_5H_{14}N_3)^+[CdCl_3]^-$, (I).



2. Structural commentary

The asymmetric unit of (I) (Fig. 1) consists of a Cd^{II} cation surrounded by four Cl atoms and one *N,N,N',N'*-tetramethylguanidinium cation. The coordination polyhedron around Cd^{II} can be described best as a distorted trigonal bipyramid where atoms Cl1, Cl2 and Cl4 define the equatorial plane while atoms Cl3 and Cl4ⁱ [symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} - y, 1 - z$] are in axial positions with a Cl3—Cd1—Cl4ⁱ angle of 166.347 (10)°. The equatorial Cd—Cl bond lengths range from 2.4829 (4) Å to 2.5829 (4) Å while the axial bond lengths Cd1—Cl3 and Cd1—Cl4ⁱ are 2.5854 (4) Å and 2.6403 (4) Å,



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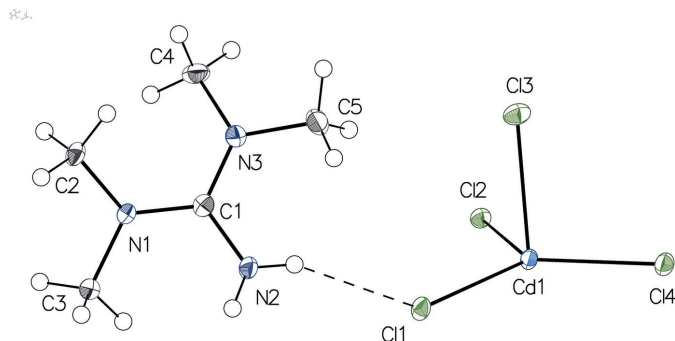


Figure 1
The asymmetric unit of compound (I), with displacement ellipsoids drawn at the 50% probability level. The N—H...Cl hydrogen bond is indicated by a dashed line.

respectively. The CdCl_4 moieties of the asymmetric unit are related by an inversion center, generating an extended zigzag chain of edge-sharing trigonal bipyramids running parallel to [101]. These $[\text{CdCl}_{4/2}\text{Cl}_{1/1}]^-$ chains are formed by the bridging atoms Cl2, Cl3, Cl4 and Cl4ⁱ with a Cd—Cd—Cd angle of 137.893 (6)°. The corrugation of the chains results in rather short Cd...Cd distances of 3.8720 (3) and 3.8026 (3) Å. The same kind of zigzag chain is found, for example, in the $[\text{CdCl}_3]^-$ salt obtained with benzyltriethylammonium as counter-cation (Sun & Jin, 2013) but with a less pronounced corrugation. Accordingly, the angle between two successive rectangular $[\text{Cd}_2\text{Cl}_2]$ units is 57.928 (3)° in the structure of the benzyltriethylammonium compound compared with 129.859 (2)° for the present structure. The tetramethylguanidinium cation has the central atom C1 in an almost trigonal-planar configuration. The three N—C—N angles range from 119.26 (14) to 121.14 (14)° and the r.m.s deviation from the least-squares plane calculated with atoms C1, N1, N2 and N3 is only 0.005 Å. The corresponding C—N bond lengths

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2A...Cl1	0.83 (2)	2.51 (2)	3.2871 (15)	157 (2)
N2—H2B...Cl1 ⁱ	0.83 (2)	2.46 (2)	3.2710 (15)	164 (2)

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

of 1.330 (2), 1.3360 (19), and 1.3441 (19) Å indicate a partial double-bond character. Hence the positive charge may be considered as delocalized in the CN_3 plane (Tiritiris, 2012). The two pairs of dimethylammonium groups are twisted by 24.67 (8) and 27.31 (9)° with respect to this plane.

3. Supramolecular features

The $[\text{CdCl}_{4/2}\text{Cl}_{1/1}]^-$ chains are interconnected through N—H...Cl hydrogen bonds by pairs of tetramethylguanidinium cations linked to symmetry-related Cl1 atoms (Table 1). These interactions define layers extending parallel to (010) (Fig. 2).

4. Database survey

The trichloridocadmate anion, $[\text{CdCl}_3]^-$, may have various discrete or chain structures with tetrahedral, octahedral and trigonal-bipyramidal environments around the central Cd^{II} cation. A search in the Cambridge Structural Database (CSD Version 5.36 with three updates; Groom & Allen, 2014) returned only five entries with the chains having a trigonal-bipyramidal environment for Cd^{II} . The corresponding structures contain different cations such as sulfonium ylide (Sabounchei *et al.*, 2013), tetraethylammonium (Lakshmi *et al.*, 2004), hexadecyl sulfonium (Sokka *et al.*, 2008), benzyltriethylammonium (Sun & Jin, 2013) or trimethylammoniumphenyl-4-thiol (Tang & Lang, 2011).

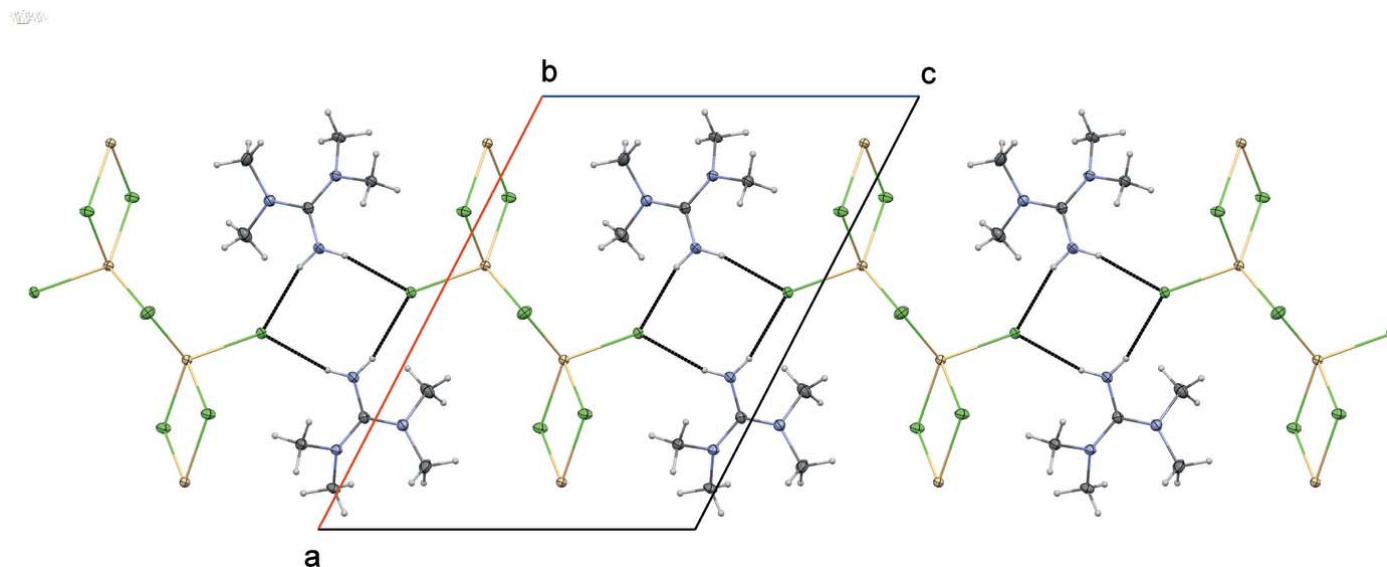


Figure 2
Partial packing diagram of (I), viewed along [010], showing one layer made up of alternating $[\text{CdCl}_{4/2}\text{Cl}_{1/1}]^-$ chains and intermediate tetramethylguanidinium cations. N—H...Cl hydrogen bonds are shown as black dotted lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	(C ₅ H ₁₄ N ₃)[CdCl ₃]
<i>M</i> _r	334.94
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	15.1305 (7), 14.2921 (6), 11.6939 (5)
β (°)	117.370 (2)
<i>V</i> (Å ³)	2245.69 (17)
<i>Z</i>	8
Radiation type	Ga Kα, λ = 1.34139 Å
μ (mm ^{−1})	14.50
Crystal size (mm)	0.19 × 0.10 × 0.10
Data collection	
Diffraction	Bruker Venture Metaljet
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.400, 0.752
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	24837, 2593, 2575
<i>R</i> _{int}	0.043
(sin θ/λ) _{max} (Å ^{−1})	0.650
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.016, 0.040, 1.13
No. of reflections	2593
No. of parameters	122
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.63, −0.40

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2008) and *pubCIF* (Westrip, 2010).

5. Synthesis and crystallization

Crystals suitable for a single-crystal X-ray diffraction study were obtained by mixing stoichiometric amounts of tetramethylguanidine with CdCl₂·H₂O in ethanol and allowing the solvent to evaporate slowly at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H-atom positions of all methyl

groups were placed geometrically and refined with *U*_{iso}(H) = 1.5*U*_{eq}(C). H atoms bonded to the N atoms were located from a Fourier difference map and were refined freely.

Acknowledgements

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

catena-Poly[*N,N,N',N'*-tetramethylguanidinium [(chloridocadmate)-di- μ -chlorido]]

Crystal data

(C₅H₁₄N₃)[CdCl₃]
 $M_r = 334.94$
 Monoclinic, *C2/c*
 $a = 15.1305$ (7) Å
 $b = 14.2921$ (6) Å
 $c = 11.6939$ (5) Å
 $\beta = 117.370$ (2)°
 $V = 2245.69$ (17) Å³
 $Z = 8$

$F(000) = 1312$
 $D_x = 1.981$ Mg m⁻³
 Ga $K\alpha$ radiation, $\lambda = 1.34139$ Å
 Cell parameters from 9941 reflections
 $\theta = 3.9\text{--}60.7^\circ$
 $\mu = 14.50$ mm⁻¹
 $T = 100$ K
 Block, clear light colourless
 $0.19 \times 0.10 \times 0.10$ mm

Data collection

Bruker Venture Metaljet
 diffractometer
 Radiation source: Metal Jet, Gallium Liquid
 Metal Jet Source
 Helios MX Mirror Optics monochromator
 Detector resolution: 10.24 pixels mm⁻¹
 ω and ϕ scans
 Absorption correction: multi-scan
 (*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.400$, $T_{\max} = 0.752$
 24837 measured reflections
 2593 independent reflections
 2575 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$
 $\theta_{\max} = 60.7^\circ$, $\theta_{\min} = 3.9^\circ$
 $h = -19 \rightarrow 19$
 $k = -18 \rightarrow 18$
 $l = -15 \rightarrow 15$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.016$
 $wR(F^2) = 0.040$
 $S = 1.13$
 2593 reflections
 122 parameters
 0 restraints

Primary atom site location: structure-invariant
 direct methods
 Hydrogen site location: mixed
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0144P)^2 + 2.6083P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.63 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.40 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. X-ray crystallographic data for I were collected from a single-crystal sample, which was mounted on a loop fiber. Data were collected using a Bruker Venture diffractometer equipped with a Photon 100 CMOS Detector, a Helios MX optics and a Kappa goniometer. The crystal-to-detector distance was 4.0 cm, and the data collection was carried out in 1024 $\times$ 1024 pixel mode.

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.18403 (9)	0.36639 (9)	0.56127 (12)	0.0134 (2)
N2	0.35116 (10)	0.36153 (11)	0.61584 (14)	0.0191 (3)
N3	0.24068 (10)	0.42244 (9)	0.41914 (13)	0.0150 (3)
C1	0.25851 (11)	0.38434 (10)	0.53204 (15)	0.0132 (3)
C2	0.09488 (11)	0.42502 (11)	0.51613 (15)	0.0153 (3)
H2C	0.1042	0.4816	0.4756	0.023*
H2D	0.0835	0.4425	0.5894	0.023*
H2E	0.0373	0.3901	0.4532	0.023*
C3	0.19647 (12)	0.29906 (11)	0.66197 (15)	0.0152 (3)
H3A	0.2479	0.2535	0.6719	0.023*
H3B	0.1334	0.2664	0.6379	0.023*
H3C	0.2164	0.3322	0.7435	0.023*
C4	0.14557 (12)	0.41074 (12)	0.30272 (15)	0.0200 (3)
H4A	0.1074	0.3604	0.3163	0.030*
H4B	0.1581	0.3948	0.2300	0.030*
H4C	0.1076	0.4692	0.2842	0.030*
C5	0.32011 (13)	0.46786 (12)	0.40087 (17)	0.0212 (3)
H5A	0.3718	0.4902	0.4841	0.032*
H5B	0.2926	0.5210	0.3420	0.032*
H5C	0.3491	0.4228	0.3643	0.032*
Cd1	0.60861 (2)	0.27596 (2)	0.41882 (2)	0.01199 (5)
Cl1	0.54707 (3)	0.30385 (3)	0.57950 (3)	0.01619 (8)
Cl2	0.5000	0.15363 (3)	0.2500	0.01344 (10)
Cl3	0.5000	0.39855 (4)	0.2500	0.01852 (11)
Cl4	0.76617 (3)	0.35865 (2)	0.45006 (4)	0.01607 (8)
H2A	0.3944 (15)	0.3603 (16)	0.591 (2)	0.021 (5)*
H2B	0.3677 (16)	0.3540 (16)	0.694 (2)	0.026 (6)*

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

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0108 (6)	0.0151 (6)	0.0146 (6)	0.0020 (5)	0.0061 (5)	0.0016 (5)
N2	0.0120 (6)	0.0333 (8)	0.0139 (7)	0.0037 (5)	0.0076 (5)	0.0038 (6)
N3	0.0148 (6)	0.0161 (6)	0.0152 (6)	0.0008 (5)	0.0079 (5)	0.0010 (5)

C1	0.0143 (7)	0.0120 (7)	0.0141 (7)	0.0012 (5)	0.0072 (6)	−0.0027 (5)
C2	0.0118 (7)	0.0156 (7)	0.0196 (7)	0.0026 (5)	0.0083 (6)	−0.0001 (6)
C3	0.0140 (7)	0.0174 (7)	0.0151 (7)	0.0016 (6)	0.0073 (6)	0.0020 (6)
C4	0.0200 (8)	0.0249 (8)	0.0124 (7)	0.0067 (6)	0.0052 (6)	0.0027 (6)
C5	0.0232 (8)	0.0210 (8)	0.0254 (8)	0.0017 (6)	0.0163 (7)	0.0050 (7)
Cd1	0.00895 (7)	0.01692 (7)	0.01027 (7)	−0.00065 (3)	0.00457 (5)	−0.00147 (3)
Cl1	0.01164 (16)	0.02608 (19)	0.01180 (16)	0.00064 (14)	0.00620 (13)	−0.00316 (14)
Cl2	0.0121 (2)	0.0156 (2)	0.0115 (2)	0.000	0.00446 (18)	0.000
Cl3	0.0168 (2)	0.0176 (2)	0.0151 (2)	0.000	0.00209 (19)	0.000
Cl4	0.01132 (16)	0.01586 (16)	0.02072 (18)	−0.00045 (12)	0.00710 (14)	0.00232 (13)

Geometric parameters (Å, °)

N1—C1	1.3441 (19)	C4—H4A	0.9800
N1—C2	1.4649 (19)	C4—H4B	0.9800
N1—C3	1.4643 (19)	C4—H4C	0.9800
N2—C1	1.330 (2)	C5—H5A	0.9800
N2—H2A	0.83 (2)	C5—H5B	0.9800
N2—H2B	0.83 (2)	C5—H5C	0.9800
N3—C1	1.3360 (19)	Cd1—Cl1	2.4829 (4)
N3—C4	1.467 (2)	Cd1—Cl2	2.5829 (4)
N3—C5	1.465 (2)	Cd1—Cl3	2.5854 (4)
C2—H2C	0.9800	Cd1—Cl4	2.5323 (4)
C2—H2D	0.9800	Cd1—Cl4 ⁱ	2.6403 (4)
C2—H2E	0.9800	Cl2—Cd1 ⁱⁱ	2.5830 (4)
C3—H3A	0.9800	Cl3—Cd1 ⁱⁱ	2.5854 (4)
C3—H3B	0.9800	Cl4—Cd1 ⁱ	2.6402 (4)
C3—H3C	0.9800		
C1—N1—C2	122.68 (13)	N3—C4—H4B	109.5
C1—N1—C3	121.14 (12)	N3—C4—H4C	109.5
C3—N1—C2	114.98 (12)	H4A—C4—H4B	109.5
C1—N2—H2A	118.6 (14)	H4A—C4—H4C	109.5
C1—N2—H2B	121.6 (15)	H4B—C4—H4C	109.5
H2A—N2—H2B	120 (2)	N3—C5—H5A	109.5
C1—N3—C4	122.47 (13)	N3—C5—H5B	109.5
C1—N3—C5	121.21 (14)	N3—C5—H5C	109.5
C5—N3—C4	115.83 (13)	H5A—C5—H5B	109.5
N2—C1—N1	119.26 (14)	H5A—C5—H5C	109.5
N2—C1—N3	119.57 (14)	H5B—C5—H5C	109.5
N3—C1—N1	121.14 (14)	Cl1—Cd1—Cl2	111.033 (10)
N1—C2—H2C	109.5	Cl1—Cd1—Cl3	98.115 (10)
N1—C2—H2D	109.5	Cl1—Cd1—Cl4 ⁱ	95.516 (13)
N1—C2—H2E	109.5	Cl1—Cd1—Cl4	118.137 (13)
H2C—C2—H2D	109.5	Cl2—Cd1—Cl3	85.262 (13)
H2C—C2—H2E	109.5	Cl2—Cd1—Cl4 ⁱ	89.152 (12)
H2D—C2—H2E	109.5	Cl3—Cd1—Cl4 ⁱ	166.347 (10)
N1—C3—H3A	109.5	Cl4—Cd1—Cl2	130.701 (9)

N1—C3—H3B	109.5	Cl4—Cd1—Cl3	91.126 (11)
N1—C3—H3C	109.5	Cl4—Cd1—Cl4 ⁱ	83.088 (12)
H3A—C3—H3B	109.5	Cd1—Cl2—Cd1 ⁱⁱ	94.798 (17)
H3A—C3—H3C	109.5	Cd1 ⁱⁱ —Cl3—Cd1	94.679 (18)
H3B—C3—H3C	109.5	Cd1—Cl4—Cd1 ⁱ	96.910 (13)
N3—C4—H4A	109.5		
C2—N1—C1—N2	148.47 (15)	C4—N3—C1—N1	−27.1 (2)
C2—N1—C1—N3	−33.2 (2)	C4—N3—C1—N2	151.23 (15)
C3—N1—C1—N2	−18.4 (2)	C5—N3—C1—N1	161.27 (14)
C3—N1—C1—N3	159.92 (14)	C5—N3—C1—N2	−20.4 (2)

Symmetry codes: (i) $-x+3/2, -y+1/2, -z+1$; (ii) $-x+1, y, -z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
C2—H2C $\cdots$ Cl4 ⁱⁱⁱ	0.98	2.87	3.6567 (16)	138
C3—H3B $\cdots$ Cl1 ^{iv}	0.98	2.92	3.7614 (16)	144
C4—H4B $\cdots$ Cl4 ⁱⁱ	0.98	2.87	3.8347 (17)	169
N2—H2A $\cdots$ Cl1	0.83 (2)	2.51 (2)	3.2871 (15)	157 (2)
N2—H2B $\cdots$ Cl1 ^v	0.83 (2)	2.46 (2)	3.2710 (15)	164 (2)

Symmetry codes: (ii) $-x+1, y, -z+1/2$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1/2, -y+1/2, -z+1$; (v) $-x+1, y, -z+3/2$.