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Di-μ-chlorido-bis[aqua(2,2′-bipyridine-κ^2N,N')chloridocobalt(II)]

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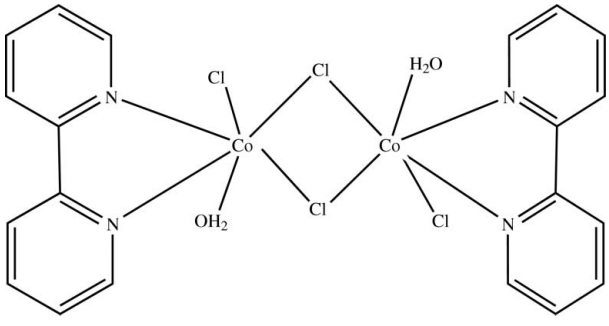
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.085; data-to-parameter ratio = 18.6.

The title complex, $[Co_2Cl_4(C_{10}H_8N_2)_2(H_2O)_2]$, is composed of two Co^{II} atoms, each hexacoordinated by three Cl atoms, one 2,2′-bipyridine (bpy) ligand and one water molecule in a distorted octahedral geometry. Neighboring Co^{II} atoms are linked together by two Cl bridges, forming a dinuclear Co^{II} complex with inversion symmetry. There are intermolecular O—H···Cl hydrogen bonds and intermolecular π–π stacking interactions between adjacent bpy ligands [centroid–centroid distance = 3.617 (2) Å] in the structure.

Related literature

For Cl atoms acting as the bridging anions in transition metal complexes in multi-dimensional molecule-based magnetic materials, see: Jian *et al.* (2005). For related structures, see: Leznoff *et al.* (2003); Liu *et al.*(2004); Puschmann *et al.* (2001).



Experimental

Crystal data

$[Co_2Cl_4(C_{10}H_8N_2)_2(H_2O)_2]$
M_r = 608.06
Monoclinic, $P2_1/n$
a = 11.2939 (10) Å
b = 6.8969 (6) Å
c = 15.1339 (13) Å
β = 91.958 (3)°
V = 1178.14 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 293 K
0.26 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.641, T_{max} = 0.688
11707 measured reflections
2693 independent reflections
2149 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.085
S = 1.03
2693 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···Cl1^{i}	0.82	2.81	3.407 (2)	132
O1—H1C···Cl1^{ii}	0.85	2.39	3.213 (2)	162

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2843).

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supporting information

Acta Cryst. (2009). E**65**, m991 [doi:10.1107/S1600536809027846]

Di-μ-chlorido-bis[aqua(2,2′-bipyridine-κ^2N,N')chloridocobalt(II)]

Li-Li Zhu, Yu Sun, Huai-Hong Zhang, Yun Wang and Bai-Wang Sun

S1. Comment

In the study of multidimensional molecule-based magnetic materials and other areas, the Cl atoms acting as the bridging anions has frequently been used to bridge transition metal complexes (Jian *et al.*, 2005). Many such compounds have been reported (Leznoff *et al.*, 2003; Liu *et al.,* 2004; Puschmann *et al.*, 2001). Herein, we reported the structure of the title Co^{II} compound (I).

The two Co atoms are bridged by two Cl anions into a four-membered Co_2Cl_2 ring. The Co atom is six-coordinated by three Cl atoms, one water molecules and one 2,2′-bipy ligand in an octahedral geometry. The molecule has an inversion symmetry (Fig. 1). In the crystal structure, the intermolecular O—H···Cl hydrogen bonds connect the molecules of (I) into a one-dimensional chain structure. There are π-π stacking interactions between adjacent bpy (2,2′-bipyridine) ligands, where the centroid–centroid separations are 3.617 (2) Å. π-π stacking interaction existing in every two O—H···Cl hydrogen bonds chains, and forming pairs of complex molecules into a two-dimensional structure (Fig. 2). A supramolecular network structure is consolidated by π-π stacking and hydrogen bonds.

S2. Experimental

All chemicals used (reagent grade) were commercially available. To a 10 ml MeCN solution of cobalt dichloride hexahydrate (0.0238 g, 0.1 mmol), a 4 ml CH_2Cl_2 solution of 2,2′-bipyridine (0.0156 g, 0.1 mmol) was added dropwise with stirring. The resulting solution was continuously stirred for about 30 min, and then filtered. The filtrate was slowly evaporated at room temperature over several days, and colourless prism crystals suitable for X-ray analysis were obtained.

S3. Refinement

The positions of the C-bound H atoms were calculated geometrically and refined using a riding model with C-H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C). The positional parameters for the H atoms of the water molecule were placed geometrically and refined with a fixed U_{iso} of 0.05.

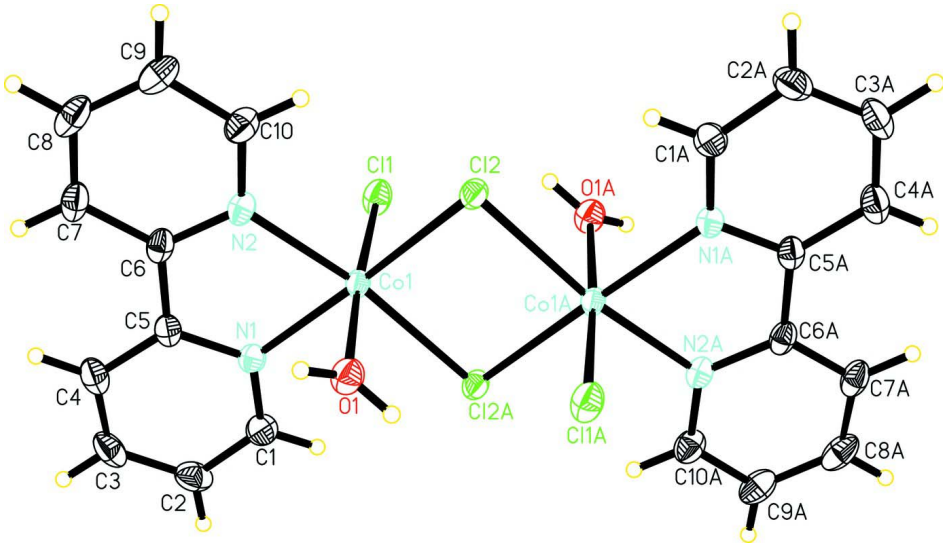

Figure 1

The molecular structure of the title compound with the atom-numbering scheme and all hydrogen atoms. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code A: 2 - *x*, -*y*, 1 - *z*]

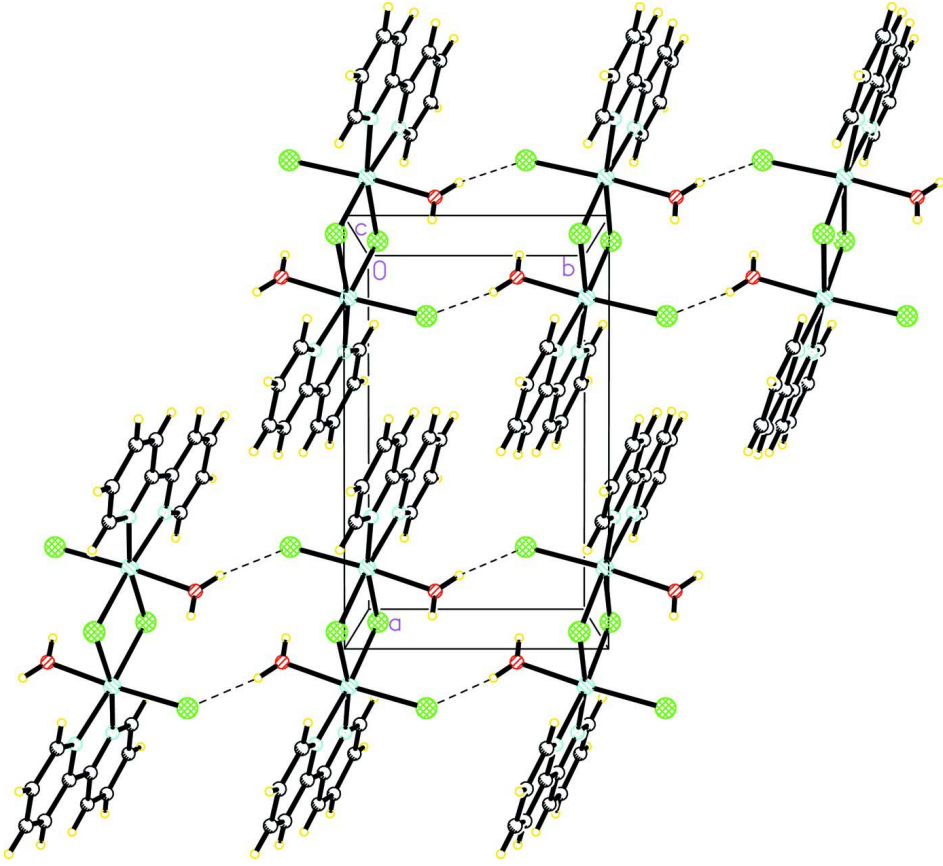

Figure 2

Crystal packing of the compound (I). Hydrogen bonds are shown as dashed lines.

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Crystal data

$[Co_2Cl_4(C_{10}H_8N_2)_2(H_2O)_2]$
M_r = 608.06
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 11.2939 (10) Å
b = 6.8969 (6) Å
c = 15.1339 (13) Å
β = 91.958 (3)°
V = 1178.14 (18) Å^3
Z = 2
$F(000)$ = 612
D_x = 1.714 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 10382 reflections
θ = 3.2–27.7°
μ = 1.89 mm^{-1}
T = 293 K
Prism, colourless
0.26 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.192 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.641, T_{max} = 0.688
11707 measured reflections
2693 independent reflections
2149 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −14→14
k = −8→8
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.085
S = 1.03
2693 reflections
145 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0346P)^2 + 0.3472P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Co1	0.84715 (3)	0.03942 (5)	0.50354 (2)	0.02938 (12)
O1	0.90322 (17)	0.3279 (3)	0.55130 (12)	0.0420 (5)
H1B	0.9629	0.3171	0.5833	0.050*
H1C	0.8639	0.4280	0.5357	0.050*

N1	0.71222 (19)	0.0653 (3)	0.59523 (14)	0.0328 (5)
N2	0.70852 (19)	0.1700 (3)	0.42759 (14)	0.0340 (5)
C1	0.7206 (3)	0.0099 (4)	0.67984 (19)	0.0418 (7)
H1A	0.7894	−0.0524	0.6999	0.050*
C2	0.6322 (3)	0.0407 (5)	0.7389 (2)	0.0504 (8)
H2A	0.6418	0.0035	0.7977	0.060*
C3	0.5291 (3)	0.1284 (4)	0.7079 (2)	0.0500 (8)
H3A	0.4673	0.1493	0.7459	0.060*
C4	0.5178 (3)	0.1848 (4)	0.6209 (2)	0.0441 (7)
H4A	0.4485	0.2437	0.5995	0.053*
C5	0.6114 (2)	0.1524 (4)	0.56541 (18)	0.0325 (6)
C6	0.6095 (2)	0.2104 (4)	0.47093 (19)	0.0345 (6)
C7	0.5126 (3)	0.2985 (4)	0.4275 (2)	0.0430 (7)
H7A	0.4448	0.3272	0.4581	0.052*
C8	0.5184 (3)	0.3423 (4)	0.3396 (2)	0.0513 (9)
H8A	0.4543	0.4011	0.3102	0.062*
C9	0.6192 (3)	0.2994 (4)	0.2947 (2)	0.0493 (8)
H9A	0.6242	0.3275	0.2348	0.059*
C10	0.7123 (3)	0.2134 (4)	0.34111 (19)	0.0430 (7)
H10A	0.7807	0.1842	0.3113	0.052*
Cl1	0.79648 (6)	−0.29082 (10)	0.45617 (5)	0.0445 (2)
Cl2	0.99818 (6)	0.07599 (10)	0.39243 (4)	0.03617 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0223 (2)	0.0359 (2)	0.0300 (2)	0.00151 (15)	0.00089 (14)	0.00302 (16)
O1	0.0374 (11)	0.0386 (11)	0.0496 (12)	−0.0004 (9)	−0.0023 (9)	−0.0006 (10)
N1	0.0269 (12)	0.0365 (12)	0.0349 (12)	−0.0016 (10)	0.0014 (9)	−0.0011 (10)
N2	0.0264 (12)	0.0348 (12)	0.0405 (13)	−0.0018 (9)	−0.0020 (10)	0.0042 (10)
C1	0.0373 (17)	0.0510 (17)	0.0373 (15)	−0.0046 (13)	0.0049 (13)	0.0032 (13)
C2	0.052 (2)	0.063 (2)	0.0364 (16)	−0.0128 (17)	0.0123 (15)	−0.0067 (15)
C3	0.0406 (18)	0.0510 (19)	0.060 (2)	−0.0077 (15)	0.0227 (15)	−0.0188 (16)
C4	0.0323 (16)	0.0383 (16)	0.062 (2)	−0.0014 (13)	0.0101 (14)	−0.0134 (15)
C5	0.0263 (14)	0.0254 (13)	0.0459 (15)	−0.0025 (11)	0.0025 (12)	−0.0061 (12)
C6	0.0268 (14)	0.0259 (13)	0.0503 (16)	−0.0012 (11)	−0.0052 (12)	−0.0037 (12)
C7	0.0308 (15)	0.0313 (15)	0.066 (2)	0.0051 (12)	−0.0099 (14)	−0.0088 (14)
C8	0.051 (2)	0.0340 (16)	0.066 (2)	0.0049 (14)	−0.0279 (17)	0.0019 (15)
C9	0.051 (2)	0.0462 (18)	0.0489 (18)	−0.0039 (15)	−0.0170 (15)	0.0133 (15)
C10	0.0374 (16)	0.0493 (18)	0.0420 (16)	−0.0032 (13)	−0.0043 (13)	0.0103 (14)
Cl1	0.0343 (4)	0.0364 (4)	0.0624 (5)	−0.0001 (3)	−0.0050 (3)	−0.0031 (3)
Cl2	0.0264 (3)	0.0535 (4)	0.0286 (3)	0.0013 (3)	0.0003 (3)	0.0078 (3)

Geometric parameters (Å, º)

Co1—N1	2.103 (2)	C2—H2A	0.9300
Co1—N2	2.112 (2)	C3—C4	1.375 (4)
Co1—O1	2.2021 (18)	C3—H3A	0.9300

Co1—Cl2^{i}	2.4445 (7)	C4—C5	1.391 (4)
Co1—Cl2	2.4488 (7)	C4—H4A	0.9300
Co1—Cl1	2.4497 (8)	C5—C6	1.484 (4)
O1—H1B	0.8200	C6—C7	1.396 (4)
O1—H1C	0.8500	C7—C8	1.368 (4)
N1—C1	1.336 (3)	C7—H7A	0.9300
N1—C5	1.351 (3)	C8—C9	1.377 (5)
N2—C10	1.345 (3)	C8—H8A	0.9300
N2—C6	1.345 (3)	C9—C10	1.379 (4)
C1—C2	1.378 (4)	C9—H9A	0.9300
C1—H1A	0.9300	C10—H10A	0.9300
C2—C3	1.380 (5)	Cl2—Co1^{i}	2.4445 (7)

N1—Co1—N2	77.44 (8)	C1—C2—H2A	121.0
N1—Co1—O1	85.04 (8)	C3—C2—H2A	121.0
N2—Co1—O1	89.59 (8)	C4—C3—C2	119.9 (3)
N1—Co1—Cl2^{i}	96.93 (6)	C4—C3—H3A	120.1
N2—Co1—Cl2^{i}	171.68 (7)	C2—C3—H3A	120.1
O1—Co1—Cl2^{i}	83.78 (5)	C3—C4—C5	119.0 (3)
N1—Co1—Cl2	169.00 (6)	C3—C4—H4A	120.5
N2—Co1—Cl2	95.92 (6)	C5—C4—H4A	120.5
O1—Co1—Cl2	86.16 (5)	N1—C5—C4	121.3 (3)
Cl2^{i}—Co1—Cl2	88.66 (2)	N1—C5—C6	115.2 (2)
N1—Co1—Cl1	96.01 (6)	C4—C5—C6	123.5 (3)
N2—Co1—Cl1	94.35 (6)	N2—C6—C7	120.8 (3)
O1—Co1—Cl1	176.05 (5)	N2—C6—C5	115.4 (2)
Cl2^{i}—Co1—Cl1	92.31 (3)	C7—C6—C5	123.8 (3)
Cl2—Co1—Cl1	93.21 (3)	C8—C7—C6	119.4 (3)
Co1—O1—H1B	109.5	C8—C7—H7A	120.3
Co1—O1—H1C	120.1	C6—C7—H7A	120.3
H1B—O1—H1C	130.4	C7—C8—C9	120.0 (3)
C1—N1—C5	118.6 (2)	C7—C8—H8A	120.0
C1—N1—Co1	125.36 (19)	C9—C8—H8A	120.0
C5—N1—Co1	116.00 (17)	C8—C9—C10	118.0 (3)
C10—N2—C6	118.9 (2)	C8—C9—H9A	121.0
C10—N2—Co1	125.24 (19)	C10—C9—H9A	121.0
C6—N2—Co1	115.86 (18)	N2—C10—C9	122.9 (3)
N1—C1—C2	123.2 (3)	N2—C10—H10A	118.6
N1—C1—H1A	118.4	C9—C10—H10A	118.6
C2—C1—H1A	118.4	Co1^{i}—Cl2—Co1	91.34 (2)
C1—C2—C3	118.0 (3)		

N2—Co1—N1—C1	−179.5 (2)	C1—N1—C5—C6	179.7 (2)
O1—Co1—N1—C1	−88.8 (2)	Co1—N1—C5—C6	2.2 (3)
Cl2^{i}—Co1—N1—C1	−5.7 (2)	C3—C4—C5—N1	0.6 (4)
Cl2—Co1—N1—C1	−125.8 (3)	C3—C4—C5—C6	−178.9 (3)
Cl1—Co1—N1—C1	87.3 (2)	C10—N2—C6—C7	−0.9 (4)
N2—Co1—N1—C5	−2.25 (17)	Co1—N2—C6—C7	179.38 (19)

O1—Co1—N1—C5	88.43 (18)	C10—N2—C6—C5	178.2 (2)
Cl2^{i}—Co1—N1—C5	171.53 (17)	Co1—N2—C6—C5	−1.5 (3)
Cl2—Co1—N1—C5	51.4 (4)	N1—C5—C6—N2	−0.5 (3)
Cl1—Co1—N1—C5	−95.39 (17)	C4—C5—C6—N2	179.1 (2)
N1—Co1—N2—C10	−177.7 (2)	N1—C5—C6—C7	178.7 (2)
O1—Co1—N2—C10	97.3 (2)	C4—C5—C6—C7	−1.8 (4)
Cl2—Co1—N2—C10	11.2 (2)	N2—C6—C7—C8	0.7 (4)
Cl1—Co1—N2—C10	−82.5 (2)	C5—C6—C7—C8	−178.4 (3)
N1—Co1—N2—C6	1.99 (18)	C6—C7—C8—C9	0.0 (4)
O1—Co1—N2—C6	−83.02 (18)	C7—C8—C9—C10	−0.4 (4)
Cl2—Co1—N2—C6	−169.12 (17)	C6—N2—C10—C9	0.5 (4)
Cl1—Co1—N2—C6	97.19 (18)	Co1—N2—C10—C9	−179.8 (2)
C5—N1—C1—C2	−1.3 (4)	C8—C9—C10—N2	0.1 (4)
Co1—N1—C1—C2	175.9 (2)	N1—Co1—Cl2—Co1^{i}	120.8 (3)
N1—C1—C2—C3	1.8 (5)	N2—Co1—Cl2—Co1^{i}	173.04 (6)
C1—C2—C3—C4	−1.0 (5)	O1—Co1—Cl2—Co1^{i}	83.85 (5)
C2—C3—C4—C5	−0.1 (4)	Cl2^{i}—Co1—Cl2—Co1^{i}	0.0
C1—N1—C5—C4	0.1 (4)	Cl1—Co1—Cl2—Co1^{i}	−92.24 (3)
Co1—N1—C5—C4	−177.4 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···Cl1^{i}	0.82	2.81	3.407 (2)	132
O1—H1*C*···Cl1^{ii}	0.85	2.39	3.213 (2)	162

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