Supporting Information for

Evidence for C-H Hydrogen Bonding in t-Butyl Cation Salts

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X-ray structure of [*t*-Bu^+][$CHB_{11}Cl_{11}^-$]

(12 pages total)

X-Ray Structure Determination of [*t*-Bu^+][$CHB_{11}Cl_{11}$]

A colorless fragment of a prism (0.52 x 0.20 x 0.17 mm^3) was used for the single crystal x-ray diffraction study of $(CH_3)_3C^+CHB_{11}Cl_{11}^-$ (sample cr133_0m). The crystal was coated with perfluoropolyethers (PFPE) oil and mounted on to a cryo-loop glass fiber. X-ray intensity data were collected at 100(2) K on a Bruker APEX2 (**ref. 1**) platform-CCD x-ray diffractometer system (Mo-radiation, λ = 0.71073 Å, 50KV/40mA power). The CCD detector was placed at a distance of 5.1000 cm from the crystal.

A total of 4800 frames were collected for a hemisphere of reflections (with scan width of 0.3^o in ω, starting ω at -30^o and -60^o and 2θ at -30^o and -60^o, and ϕ angles of 0^o, 90^o, 180^o, and 270^o for every 600 frames, 10 sec/frame exposure time). The frames were integrated using the Bruker SAINT software package (**ref. 2**) and using a narrow-frame integration algorithm. Based on a monoclinic crystal system, the integrated frames yielded a total of 82310 reflections at a maximum 2θ angle of 80.50^o (0.55 Å resolution), of which 13573 were independent reflections (R_{int} = 0.0375, R_{sig} = 0.0337, redundancy = 6.1, completeness = 99.3%) and 10581 (78.0%) reflections were greater than $2\sigma(I)$. The unit cell parameters were, **a** = 10.8992(2) Å, **b** = 11.9178(3) Å, **c** = 16.9970(4) Å, **β** = 100.315(1)^o**,** V = 2172.13(8) $Å^3$, Z = 4, calculated density D_c = 1.770 g/cm^3. Absorption corrections were applied (absorption coefficient μ = 1.399 mm^{-1}; max/min transmission = 0.8010/0.5272) to the raw intensity data using the SADABS program (**ref. 3**).

The Bruker SHELXTL software package (**ref. 4**) was used for phase determination and structure refinement. The distribution of intensities (E^2-1 = 0.991) and systematic absent reflections indicated one possible space group; P2(1)/c. The space group P2(1)/c (#14) was later determined to be correct. Direct methods of phase determination followed by two Fourier cycles of refinement led to an electron density map from which most of the non-hydrogen atoms were identified in the asymmetry unit of the unit cell. With subsequent isotropic refinement, all of the non-hydrogen atoms were identified. There were one cation of $[CH_3]_3C^+$ and one anion of $CHB_{11}Cl_{11}^-$ present in the asymmetry unit of the unit cell. Because the sample was collected at high resolution (0.55 Å), all tertiary-butyl cation H-atom positions were refined without the H-atom riding model constraints. The possible C-H...Cl hydrogen bond angles and distances were generated using HTAB, which deviated from the normal D-H...A angles and distances using H-atom riding model. The Alerts level B in the checkcif file is flagged because of the unconstrained H-atom positions refinement.

Atomic coordinates, isotropic and anisotropic displacement parameters of all the non-hydrogen atoms were refined by means of a full matrix least-squares procedure on F^2. The H-atom

positions of the cation were refined unconstrained. The refinement converged at R1 = 0.0265, wR2 = 0.0611, with intensity, $I>2\sigma(I)$. The largest peak/hole in the final difference map was 0.635/-0.440 e/Å^3.

The cif file has been deposited with the Cambridge Crystallographic Data Center: # 874494.

REFERENCES

1. *APEX 2,* version 2011.4-1, Bruker (2011), Bruker AXS Inc., Madison, Wisconsin, USA.
2. *SAINT,* version V7.60A, Bruker (2009), Bruker AXS Inc., Madison, Wisconsin, USA.
3. *SADABS,* version 2008/1, Bruker (2008), Bruker AXS Inc., Madison, Wisconsin, USA.
4. *SHELXTL,* version 2008/4, Bruker (2008), Bruker AXS Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for cr133_0m.

Identification code	cr133_0m	
Empirical formula	C5 H10 B11 Cl11	
Formula weight	578.99	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c (#14)	
Unit cell dimensions	a = 10.8992(2) Å	α= 90°.
	b = 11.9178(3) Å	β= 100.315(1)°.
	c = 16.9970(4) Å	γ = 90°.
Volume	2172.13(8) $Å^3$	
Z	4	
Density (calculated)	1.770 Mg/m^3	
Absorption coefficient	1.399 mm^{-1}	
F(000)	1128	
Crystal size	0.52 x 0.20 x 0.17 mm^3	
Theta range for data collection	1.90 to 40.25°.	
Index ranges	-19<=h<=19, -21<=k<=21, -30<=l<=30	
Reflections collected	82310	
Independent reflections	13573 [R(int) = 0.0375]	
Completeness to theta = 40.25°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8010 and 0.5272	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13573 / 0 / 284	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0265, wR2 = 0.0611	
R indices (all data)	R1 = 0.0408, wR2 = 0.0651	
Largest diff. peak and hole	0.635 and -0.440 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for cr133_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1A)	3610(1)	1739(1)	2574(1)	12(1)
B(2)	2354(1)	1207(1)	2937(1)	11(1)
B(3)	2156(1)	1939(1)	2005(1)	12(1)
B(4)	3348(1)	2993(1)	2076(1)	12(1)
B(5)	4275(1)	2916(1)	3056(1)	12(1)
B(6)	3662(1)	1814(1)	3588(1)	12(1)
B(7)	2118(1)	2176(1)	3693(1)	11(1)
B(8)	1178(1)	2265(1)	2712(1)	11(1)
B(9)	1796(1)	3367(1)	2175(1)	12(1)
B(10)	3108(1)	3970(1)	2826(1)	12(1)
B(11)	3312(1)	3238(1)	3769(1)	12(1)
B(12)	1778(1)	3515(1)	3228(1)	11(1)
Cl(1)	2096(1)	-254(1)	2954(1)	15(1)
Cl(2)	1701(1)	1199(1)	1098(1)	16(1)
Cl(3)	4062(1)	3309(1)	1250(1)	17(1)
Cl(4)	5903(1)	3161(1)	3195(1)	18(1)
Cl(5)	4669(1)	945(1)	4259(1)	16(1)
Cl(6)	1479(1)	1715(1)	4529(1)	14(1)
Cl(7)	-444(1)	1957(1)	2547(1)	15(1)
Cl(8)	817(1)	4154(1)	1423(1)	16(1)
Cl(9)	3500(1)	5417(1)	2757(1)	17(1)
Cl(10)	3932(1)	3931(1)	4679(1)	16(1)
Cl(11)	787(1)	4479(1)	3608(1)	15(1)
C(1)	7893(1)	2585(1)	34(1)	19(1)
C(2)	7078(1)	2345(1)	602(1)	31(1)
C(3)	8032(1)	3716(1)	-241(1)	31(1)
C(4)	8571(1)	1674(1)	-259(1)	31(1)

Table 3. Bond lengths [Å] and angles [°] for cr133_0m.

C(1A)-B(6)	1.7160(11)
C(1A)-B(4)	1.7165(11)
C(1A)-B(5)	1.7172(11)
C(1A)-B(3)	1.7186(11)
C(1A)-B(2)	1.7205(11)
C(1A)-H(1)	0.957(12)
B(2)-Cl(1)	1.7649(8)
B(2)-B(7)	1.7802(11)
B(2)-B(3)	1.7873(11)
B(2)-B(8)	1.7897(11)
B(2)-B(6)	1.7929(12)
B(3)-Cl(2)	1.7686(8)
B(3)-B(9)	1.7817(12)
B(3)-B(8)	1.7864(11)
B(3)-B(4)	1.7958(12)
B(4)-Cl(3)	1.7622(8)
B(4)-B(10)	1.7809(12)
B(4)-B(9)	1.7855(12)
B(4)-B(5)	1.7903(12)
B(5)-Cl(4)	1.7719(8)
B(5)-B(11)	1.7806(12)
B(5)-B(10)	1.7810(12)
B(5)-B(6)	1.7897(12)
B(6)-Cl(5)	1.7690(8)
B(6)-B(7)	1.7775(11)
B(6)-B(11)	1.7789(12)
B(7)-Cl(6)	1.7771(8)
B(7)-B(12)	1.7903(11)
B(7)-B(8)	1.7968(11)
B(7)-B(11)	1.8041(12)
B(8)-Cl(7)	1.7777(8)
B(8)-B(12)	1.7922(12)
B(8)-B(9)	1.7987(11)
B(9)-Cl(8)	1.7790(8)
B(9)-B(10)	1.7950(12)
B(9)-B(12)	1.8027(11)
B(10)-Cl(9)	1.7855(8)
B(10)-B(12)	1.7937(11)
B(10)-B(11)	1.8025(12)
B(11)-Cl(10)	1.7775(8)
B(11)-B(12)	1.7886(12)
B(12)-Cl(11)	1.7764(8)
C(1)-C(3)	1.4434(14)
C(1)-C(4)	1.4506(14)
C(1)-C(2)	1.4525(14)
C(2)-H(2A)	0.995(18)
C(2)-H(2B)	0.86(2)
C(2)-H(2C)	0.90(3)
C(3)-H(3A)	0.89(2)
C(3)-H(3B)	0.926(18)
C(3)-H(3C)	1.01(2)
C(4)-H(4A)	0.916(16)
C(4)-H(4B)	0.911(19)
C(4)-H(4C)	0.924(18)

B(6)-C(1A)-B(4)	115.05(6)
B(6)-C(1A)-B(5)	62.84(5)
B(4)-C(1A)-B(5)	62.85(5)
B(6)-C(1A)-B(3)	114.80(6)
B(4)-C(1A)-B(3)	63.04(5)
B(5)-C(1A)-B(3)	115.06(6)
B(6)-C(1A)-B(2)	62.90(5)
B(4)-C(1A)-B(2)	115.18(6)
B(5)-C(1A)-B(2)	115.15(6)
B(3)-C(1A)-B(2)	62.63(5)
B(6)-C(1A)-H(1)	119.3(7)
B(4)-C(1A)-H(1)	116.1(7)
B(5)-C(1A)-H(1)	118.2(7)
B(3)-C(1A)-H(1)	116.1(7)
B(2)-C(1A)-H(1)	117.7(7)
C(1A)-B(2)-Cl(1)	120.60(5)
C(1A)-B(2)-B(7)	104.29(5)
Cl(1)-B(2)-B(7)	125.74(5)
C(1A)-B(2)-B(3)	58.63(4)
Cl(1)-B(2)-B(3)	120.12(5)
B(7)-B(2)-B(3)	108.25(6)
C(1A)-B(2)-B(8)	104.42(5)
Cl(1)-B(2)-B(8)	126.06(5)
B(7)-B(2)-B(8)	60.44(4)
B(3)-B(2)-B(8)	59.92(4)
C(1A)-B(2)-B(6)	58.43(4)
Cl(1)-B(2)-B(6)	119.94(5)
B(7)-B(2)-B(6)	59.66(4)
B(3)-B(2)-B(6)	107.83(6)
B(8)-B(2)-B(6)	107.92(6)
C(1A)-B(3)-Cl(2)	120.55(5)
C(1A)-B(3)-B(9)	104.39(6)
Cl(2)-B(3)-B(9)	125.57(5)
C(1A)-B(3)-B(8)	104.64(5)
Cl(2)-B(3)-B(8)	125.94(5)
B(9)-B(3)-B(8)	60.54(4)
C(1A)-B(3)-B(2)	58.74(4)
Cl(2)-B(3)-B(2)	120.01(5)
B(9)-B(3)-B(2)	108.54(6)
B(8)-B(3)-B(2)	60.10(4)
C(1A)-B(3)-B(4)	58.42(5)
Cl(2)-B(3)-B(4)	119.58(5)
B(9)-B(3)-B(4)	59.88(5)
B(8)-B(3)-B(4)	108.34(6)
B(2)-B(3)-B(4)	108.15(6)
C(1A)-B(4)-Cl(3)	121.38(5)
C(1A)-B(4)-B(10)	104.38(6)
Cl(3)-B(4)-B(10)	124.97(6)
C(1A)-B(4)-B(9)	104.32(5)
Cl(3)-B(4)-B(9)	125.61(6)
B(10)-B(4)-B(9)	60.44(5)
C(1A)-B(4)-B(5)	58.59(5)
Cl(3)-B(4)-B(5)	119.76(5)
B(10)-B(4)-B(5)	59.83(5)
B(9)-B(4)-B(5)	108.14(6)

C(1A)-B(4)-B(3)	58.54(4)
Cl(3)-B(4)-B(3)	120.88(5)
B(10)-B(4)-B(3)	107.96(6)
B(9)-B(4)-B(3)	59.67(5)
B(5)-B(4)-B(3)	107.86(6)
C(1A)-B(5)-Cl(4)	121.68(5)
C(1A)-B(5)-B(11)	104.54(5)
Cl(4)-B(5)-B(11)	124.90(6)
C(1A)-B(5)-B(10)	104.34(6)
Cl(4)-B(5)-B(10)	124.82(5)
B(11)-B(5)-B(10)	60.81(5)
C(1A)-B(5)-B(6)	58.55(4)
Cl(4)-B(5)-B(6)	120.64(5)
B(11)-B(5)-B(6)	59.77(5)
B(10)-B(5)-B(6)	108.20(6)
C(1A)-B(5)-B(4)	58.55(5)
Cl(4)-B(5)-B(4)	119.99(5)
B(11)-B(5)-B(4)	108.60(6)
B(10)-B(5)-B(4)	59.82(5)
B(6)-B(5)-B(4)	107.97(6)
C(1A)-B(6)-Cl(5)	121.47(5)
C(1A)-B(6)-B(7)	104.59(6)
Cl(5)-B(6)-B(7)	124.53(5)
C(1A)-B(6)-B(11)	104.67(6)
Cl(5)-B(6)-B(11)	125.09(5)
B(7)-B(6)-B(11)	60.97(5)
C(1A)-B(6)-B(5)	58.62(4)
Cl(5)-B(6)-B(5)	120.69(5)
B(7)-B(6)-B(5)	108.57(6)
B(11)-B(6)-B(5)	59.86(5)
C(1A)-B(6)-B(2)	58.67(4)
Cl(5)-B(6)-B(2)	119.64(5)
B(7)-B(6)-B(2)	59.81(5)
B(11)-B(6)-B(2)	108.67(6)
B(5)-B(6)-B(2)	108.18(6)
Cl(6)-B(7)-B(6)	121.26(5)
Cl(6)-B(7)-B(2)	120.32(5)
B(6)-B(7)-B(2)	60.52(5)
Cl(6)-B(7)-B(12)	123.28(5)
B(6)-B(7)-B(12)	107.26(5)
B(2)-B(7)-B(12)	107.75(5)
Cl(6)-B(7)-B(8)	121.36(5)
B(6)-B(7)-B(8)	108.28(5)
B(2)-B(7)-B(8)	60.04(4)
B(12)-B(7)-B(8)	59.95(4)
Cl(6)-B(7)-B(11)	122.72(5)
B(6)-B(7)-B(11)	59.55(5)
B(2)-B(7)-B(11)	108.11(5)
B(12)-B(7)-B(11)	59.68(5)
B(8)-B(7)-B(11)	107.99(5)
Cl(7)-B(8)-B(3)	123.08(5)
Cl(7)-B(8)-B(2)	122.83(5)
B(3)-B(8)-B(2)	59.97(5)
Cl(7)-B(8)-B(12)	120.94(5)
B(3)-B(8)-B(12)	107.48(5)
B(2)-B(8)-B(12)	107.25(6)

Cl(7)-B(8)-B(7)	121.29(5)
B(3)-B(8)-B(7)	107.56(5)
B(2)-B(8)-B(7)	59.52(4)
B(12)-B(8)-B(7)	59.84(4)
Cl(7)-B(8)-B(9)	121.55(5)
B(3)-B(8)-B(9)	59.60(4)
B(2)-B(8)-B(9)	107.69(5)
B(12)-B(8)-B(9)	60.27(5)
B(7)-B(8)-B(9)	108.13(5)
Cl(8)-B(9)-B(3)	120.58(5)
Cl(8)-B(9)-B(4)	121.36(5)
B(3)-B(9)-B(4)	60.45(5)
Cl(8)-B(9)-B(10)	122.78(5)
B(3)-B(9)-B(10)	107.96(6)
B(4)-B(9)-B(10)	59.65(5)
Cl(8)-B(9)-B(8)	121.25(5)
B(3)-B(9)-B(8)	59.86(4)
B(4)-B(9)-B(8)	108.25(6)
B(10)-B(9)-B(8)	107.98(6)
Cl(8)-B(9)-B(12)	123.36(5)
B(3)-B(9)-B(12)	107.22(5)
B(4)-B(9)-B(12)	107.29(6)
B(10)-B(9)-B(12)	59.81(4)
B(8)-B(9)-B(12)	59.69(4)
B(4)-B(10)-B(5)	60.35(5)
B(4)-B(10)-Cl(9)	121.13(5)
B(5)-B(10)-Cl(9)	121.76(5)
B(4)-B(10)-B(12)	107.88(6)
B(5)-B(10)-B(12)	107.27(6)
Cl(9)-B(10)-B(12)	122.44(5)
B(4)-B(10)-B(9)	59.91(5)
B(5)-B(10)-B(9)	108.13(6)
Cl(9)-B(10)-B(9)	121.33(5)
B(12)-B(10)-B(9)	60.31(5)
B(4)-B(10)-B(11)	108.04(6)
B(5)-B(10)-B(11)	59.59(5)
Cl(9)-B(10)-B(11)	122.21(5)
B(12)-B(10)-B(11)	59.65(5)
B(9)-B(10)-B(11)	108.19(6)
Cl(10)-B(11)-B(6)	122.26(5)
Cl(10)-B(11)-B(5)	120.92(5)
B(6)-B(11)-B(5)	60.37(5)
Cl(10)-B(11)-B(12)	122.47(5)
B(6)-B(11)-B(12)	107.27(6)
B(5)-B(11)-B(12)	107.51(6)
Cl(10)-B(11)-B(10)	121.08(5)
B(6)-B(11)-B(10)	107.73(6)
B(5)-B(11)-B(10)	59.61(5)
B(12)-B(11)-B(10)	59.93(4)
Cl(10)-B(11)-B(7)	123.04(5)
B(6)-B(11)-B(7)	59.48(4)
B(5)-B(11)-B(7)	107.79(6)
B(12)-B(11)-B(7)	59.77(5)
B(10)-B(11)-B(7)	107.69(6)
Cl(11)-B(12)-B(11)	120.39(5)
Cl(11)-B(12)-B(7)	120.47(5)

B(11)-B(12)-B(7)	60.55(5)
Cl(11)-B(12)-B(8)	121.56(5)
B(11)-B(12)-B(8)	108.89(6)
B(7)-B(12)-B(8)	60.21(4)
Cl(11)-B(12)-B(10)	121.92(5)
B(11)-B(12)-B(10)	60.42(5)
B(7)-B(12)-B(10)	108.69(5)
B(8)-B(12)-B(10)	108.33(6)
Cl(11)-B(12)-B(9)	122.71(5)
B(11)-B(12)-B(9)	108.47(6)
B(7)-B(12)-B(9)	108.24(5)
B(8)-B(12)-B(9)	60.04(4)
B(10)-B(12)-B(9)	59.88(5)
C(3)-C(1)-C(4)	119.90(10)
C(3)-C(1)-C(2)	120.72(10)
C(4)-C(1)-C(2)	119.37(10)
C(1)-C(2)-H(2A)	114.7(10)
C(1)-C(2)-H(2B)	116.5(16)
H(2A)-C(2)-H(2B)	111.8(18)
C(1)-C(2)-H(2C)	101.3(16)
H(2A)-C(2)-H(2C)	104.3(18)
H(2B)-C(2)-H(2C)	106(2)
C(1)-C(3)-H(3A)	106.6(13)
C(1)-C(3)-H(3B)	114.3(11)
H(3A)-C(3)-H(3B)	97.1(16)
C(1)-C(3)-H(3C)	112.2(13)
H(3A)-C(3)-H(3C)	105.8(17)
H(3B)-C(3)-H(3C)	118.5(16)
C(1)-C(4)-H(4A)	112.6(10)
C(1)-C(4)-H(4B)	113.9(11)
H(4A)-C(4)-H(4B)	111.5(14)
C(1)-C(4)-H(4C)	101.1(11)
H(4A)-C(4)-H(4C)	106.4(15)
H(4B)-C(4)-H(4C)	110.7(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cr133_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	11(1)	12(1)	13(1)	0(1)	3(1)	0(1)
B(2)	11(1)	10(1)	12(1)	0(1)	3(1)	0(1)
B(3)	12(1)	13(1)	11(1)	0(1)	2(1)	0(1)
B(4)	12(1)	13(1)	12(1)	1(1)	5(1)	-1(1)
B(5)	10(1)	13(1)	14(1)	0(1)	3(1)	-1(1)
B(6)	11(1)	12(1)	12(1)	1(1)	2(1)	1(1)
B(7)	11(1)	11(1)	11(1)	1(1)	3(1)	0(1)
B(8)	9(1)	12(1)	11(1)	0(1)	2(1)	-1(1)
B(9)	12(1)	12(1)	11(1)	2(1)	2(1)	0(1)
B(10)	12(1)	10(1)	13(1)	0(1)	3(1)	-1(1)
B(11)	12(1)	12(1)	11(1)	0(1)	1(1)	-1(1)
B(12)	10(1)	11(1)	12(1)	0(1)	3(1)	0(1)
Cl(1)	17(1)	10(1)	19(1)	0(1)	5(1)	-1(1)
Cl(2)	18(1)	17(1)	11(1)	-3(1)	3(1)	-3(1)
Cl(3)	19(1)	21(1)	14(1)	2(1)	8(1)	-2(1)
Cl(4)	10(1)	21(1)	23(1)	0(1)	3(1)	-3(1)
Cl(5)	14(1)	17(1)	16(1)	4(1)	0(1)	4(1)
Cl(6)	16(1)	16(1)	11(1)	2(1)	5(1)	0(1)
Cl(7)	9(1)	16(1)	18(1)	-1(1)	2(1)	-2(1)
Cl(8)	17(1)	18(1)	13(1)	5(1)	2(1)	4(1)
Cl(9)	17(1)	11(1)	23(1)	1(1)	6(1)	-3(1)
Cl(10)	17(1)	17(1)	13(1)	-4(1)	0(1)	-3(1)
Cl(11)	15(1)	12(1)	18(1)	0(1)	6(1)	3(1)
C(1)	14(1)	21(1)	20(1)	-1(1)	-2(1)	-2(1)
C(2)	29(1)	41(1)	24(1)	2(1)	7(1)	-6(1)
C(3)	23(1)	22(1)	46(1)	7(1)	3(1)	-3(1)
C(4)	26(1)	27(1)	40(1)	-3(1)	5(1)	6(1)

Table 5. Hydrogen bonds for cr133_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(4)-H(4C)...Cl(6)#1	0.924(18)	3.241(18)	3.7778(13)	119.1(14)
C(4)-H(4C)...Cl(2)#2	0.924(18)	2.910(19)	3.8033(12)	163.0(15)
C(4)-H(4B)...Cl(11)#3	0.911(19)	3.281(18)	3.8082(13)	119.1(13)
C(4)-H(4B)...Cl(2)#4	0.911(19)	3.012(19)	3.6996(12)	133.6(14)
C(4)-H(4A)...Cl(11)#1	0.916(16)	3.070(16)	3.6181(12)	120.2(11)
C(4)-H(4A)...Cl(4)#5	0.916(16)	3.247(15)	3.5582(12)	102.4(11)
C(3)-H(3C)...Cl(6)#6	1.01(2)	2.98(2)	3.7815(12)	136.7(16)
C(3)-H(3C)...Cl(1)#6	1.01(2)	3.23(2)	4.1026(14)	145.6(16)
C(3)-H(3B)...Cl(8)#7	0.926(18)	2.974(18)	3.5989(11)	126.2(13)
C(3)-H(3B)...Cl(6)#1	0.926(18)	3.101(18)	3.8803(12)	142.9(14)
C(3)-H(3A)...Cl(4)#5	0.89(2)	3.32(2)	3.9045(13)	125.4(15)
C(3)-H(3A)...Cl(5)#5	0.89(2)	2.97(2)	3.6339(12)	132.1(16)
C(2)-H(2A)...Cl(1)#6	0.995(18)	2.990(18)	3.7719(13)	136.2(12)
C(2)-H(2A)...Cl(3)	0.995(18)	3.169(17)	3.8265(12)	124.9(12)
C(2)-H(2B)...Cl(7)#2	0.86(2)	3.32(2)	3.9046(12)	127.7(18)
C(2)-H(2B)...Cl(9)#3	0.86(2)	3.03(2)	3.7529(12)	143.3(19)
C(2)-H(2C)...Cl(5)#5	0.90(3)	3.30(3)	3.7566(13)	114(2)
C(2)-H(2C)...Cl(10)#5	0.90(3)	2.95(3)	3.8211(12)	162(2)

Symmetry transformations used to generate equivalent atoms:
#1 x+1,-y+1/2,z-1/2 #2 x+1,y,z #3 -x+1,y-1/2,-z+1/2
#4 -x+1,-y,-z #5 x,-y+1/2,z-1/2 #6 -x+1,y+1/2,-z+1/2
#7 -x+1,-y+1,-z