Supplementary Information

Loose crystals engineered by mismatched halogen bonds in hexachloroethane

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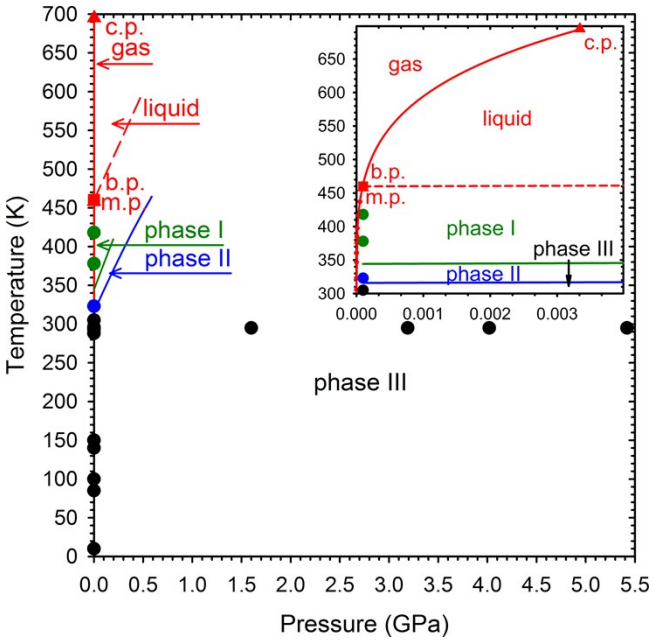


Fig. S1. The phase diagram of HCE. The boiling point at 0.1 MPa, b.p.; the melting point at 0.1 MPa, m.p. and the critical point at 3.34 MPa and 695 K, c.p. after [D. R. Lide, ed., *CRC Handbook of Chemistry and Physics, Internet Version 2007*, Taylor and Francis, Boca Raton, FL, 87th edn, 2007]; unit cell parameters and structure determinations of HCE in: phase I (cubic *Im* $\bar{3}$*m*, green circles [M. Atoji, T. Oda and T. Watanabé, *Acta Crystallogr.*, 1953, **6**, 868]), phase II (monoclinic *C2/m*, blue circles [P. Negrier, J. Ll. Tamarit, M. Barrio and D. Mondieig, *Cryst. Growth Des.*, 2013, **13**, 782−791]) and phase III (orthorhombic *Pnma*, black circles [Y. Sasada and M. Atoji, *J. Chem. Phys.*, 1953, **21**, 145–152; D. Hohlwein, W. Nägele and W. Prandl, *Acta Crystallogr.*, 1979, **B35**, 2975–2978; P. Negrier, J. Ll. Tamarit, M. Barrio and D. Mondieig, *Cryst. Growth Des.*, 2013, **13**, 782−791; this work]); the phase boundary lines (green and blue) after [P. W. Bridgman, *Proc. Amer. Acad. Arts Sci.*, 1915, **51**, 84–90]; the inset magnifies the gas-liquid region after [R. H. Perry and D. W. Green, *Perry's Chemical Engineers' Handbook*, The McGraw Hill Companies, Inc, 7th edn, 1999] and the gas-liquid boundary extrapolation (red line).

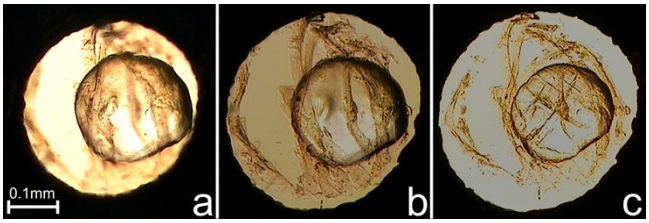


Fig. S2. The crystal sample of HCE in the high-pressure diamond-anvil cell at: 3.19 (a), 4.02 (b) and 5.42 GPa (c). Two small ruby chips, used as pressure markers, are visible in the upper part of the high pressure chamber. The cellulose fibres were used to fix the crystal sample in the cell.

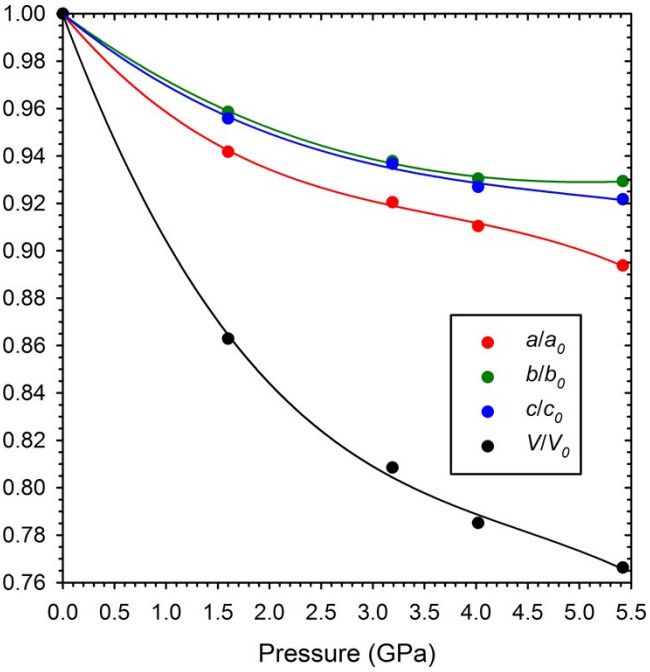
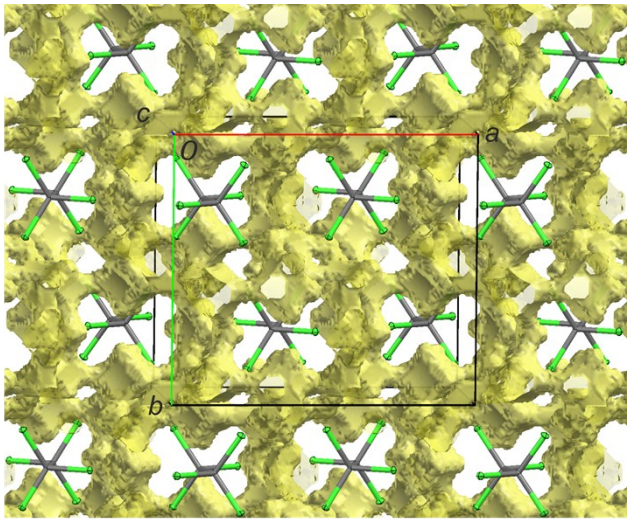
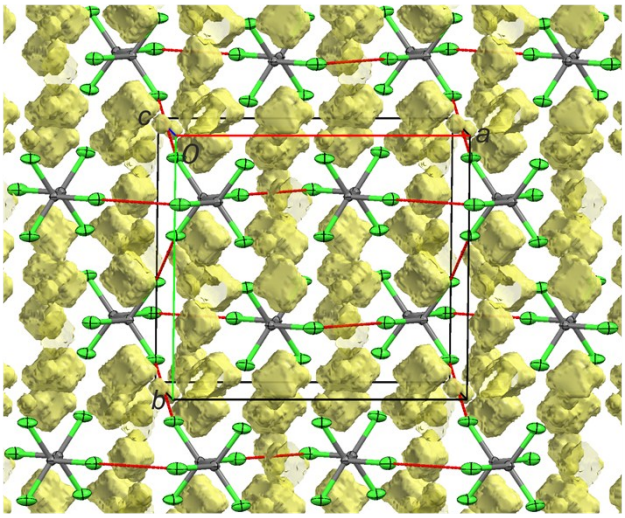


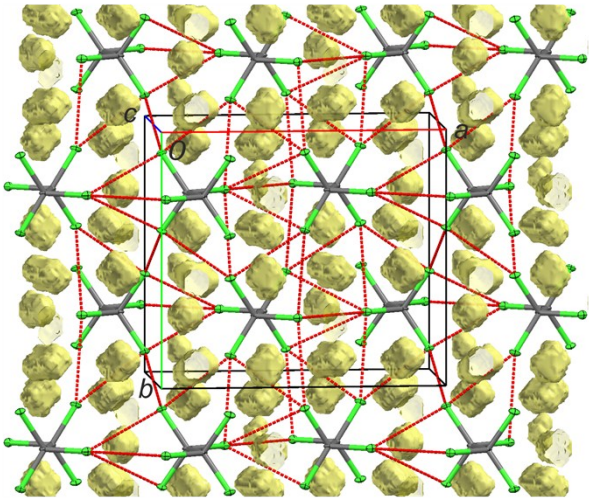
Fig. S3. The pressure dependence of normalized cell volume V_0/V and the three axis length a_0/a, b_0/b and c_0/c of HCE.



(a)



(b)



(c)

Fig. S4. The structures of HCE at: 85 K/0.1MPa (a), 295 K/1.60 GPa (b), and 295 K/4.02 GPa (c). The intermolecular space accessible to a probing sphere of radius 0.35 Å and grid size of 0.1 Å is indicated in yellow [C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek and P. A. Wood, *J. Appl. Crystallogr.*, 2008, **41**, 466−470]. The void volume is: 16.9% (a), 9.0% (b) and 4.7% (c), respectively. The dotted red lines indicate the intermolecular Cl···Cl contacts shorter than the sum van der Waals radii minus 0.05 Å [A. Bondi, *J. Phys. Chem.* 1964, **68**, 441–451; S. C. Nyburg, C. H. Faerman, *Acta Crystallogr.,* 1985, **B41**, 274–279; S. S. Batsanov, *Inorg. Mater.*, 2001, **37**, 871–885; S.-Z. Hu, Z.-H. Zhou, Z.-X. Xie and B. E. Robertson, *Z. Kristallogr.*, 2014, **229**, 517–523]. Displacement ellipsoids are plotted at the 25% probability level.

Table S1. The low-temperature/ambient pressure HCE crystal data and structure determination summary.

temperature, K	305.0(1)	293.0(1)	100.0(1)	85.0(5)
pressure, MPa	0.1	0.1	0.1	0.1
formula	C_2Cl_6	C_2Cl_6	C_2Cl_6	C_2Cl_6
fw, g/mol	236.72	236.72	236.72	236.72
crystal size, mm	0.33 x 0.26 x 0.22	0.33 x 0.26 x 0.22	0.33 x 0.26 x 0.22	0.33 x 0.26 x 0.22
crystal system	orthorhombic	orthorhombic	orthorhombic	orthorhombic
space group, *Z, Z'*	*Pnma,* 4, 0.5	*Pnma,* 4, 0.5	*Pnma,* 4, 0.5	*Pnma,* 4, 0.5
a, Å	11.5785(4)	11.5358(4)	11.2254(2)	11.2102(3)
b, Å	10.1983(4)	10.1791(3)	10.0086(2)	10.0001(3)
c, Å	6.3875(2)	6.4013(2)	6.33713(14)	6.33101(16)
V, Å^3	754.24(5)	751.67(4)	711.98(2)	709.73(3)
ρ, g/cm^3	2.085	2.092	2.208	2.215
μ, mm^{-1}	2.170	2.177	2.298	2.306
θ range, º	3.64 - 28.98	3.64 - 28.97	3.69 - 28.99	3.70 - 28.99
index ranges	$-15 \le h \le 15$	$-15 \le h \le 15$	$-15 \le h \le 14$	$-15 \le h \le 14$
	$-13 \le k \le 13$	$-13 \le k \le 13$	$-13 \le k \le 13$	$-13 \le k \le 13$
	$-7 \le l \le 8$	$-8 \le l \le 7$	$-7 \le l \le 8$	$-8 \le l \le 7$
reflns collected	5691	5656	5308	5304
R_{int}	0.0151	0.0144	0.0110	0.0114
data [$I > 2\sigma(I)$]	746	797	909	900
data/parameters	1034/43	1031/44	981/44	977/44
GOF on F^2	1.098	1.121	1.397	1.148
R_1 [$I > 2\sigma(I)$]	0.0360	0.0286	0.0128	0.0122
R_1 (all data)[a]	0.0487	0.0373	0.0155	0.0144
wR_2 (all data)[a]	0.1114	0.0911	0.0442	0.0318
lrgst diff peak, e/Å^3	0.448	0.380	0.506	0.436
lrgst diff hole, e/Å^3	–0.408	–0.319	–0.425	–0.225

Table S2. The room-temperature/high-pressure HCE crystal data and structure determination summary.

temperature, K	295(2)	295(2)	295(2)	295(2)
pressure, GPa	1.60(2)	3.19(2)	4.02(2)	5.42(2)
formula	C_2Cl_6	C_2Cl_6	C_2Cl_6	C_2Cl_6
fw, g/mol	236.72	236.72	236.72	236.72
crystal size, mm	0.08 x 0.07 x 0.05	0.26 x 0.25 x 0.06	0.26 x 0.25 x 0.06	0.26 x 0.25 x 0.06
crystal system	orthorhombic	orthorhombic	orthorhombic	orthorhombic
space group, *Z, Z'*	*Pnma,* 4, 0.5	*Pnma,* 4, 0.5	*Pnma,* 4, 0.5	*Pnma,* 4, 0.5
a, Å	10.864(16)	10.618(3)	10.502(3)	10.31(18)
b, Å	9.7573(12)	9.5461(3)	9.4708(3)	9.460(8)
c, Å	6.1183(7)	5.9958(2)	5.93353(19)	5.900(5)
V, Å^3	648.6(10)	607.74(17)	590.16(17)	576(10)
ρ, g/cm^3	2.424	2.587	2.664	2.732
μ, mm^{-1}	2.523	2.693	2.773	2.843
θ range, º	3.82 - 28.14	3.90 - 28.32	3.94 - 28.58	–
index ranges	$-3 \le h \le 3$	$-5 \le h \le 5$	$-4 \le h \le 4$	–
	$-12 \le k \le 12$	$-12 \le k \le 12$	$-12 \le k \le 12$	–
	$-8 \le l \le 8$	$-7 \le l \le 7$	$-7 \le l \le 7$	–
reflns collected	4071	3939	3771	–
R_{int}	0.2667	0.0315	0.0308	–
data [$I > 2\sigma(I)$]	136	295	260	–
data/parameters	270/43	337/44	292/44	–
GOF on F^2	1.048	1.137	1.213	–
R_1 [$I > 2\sigma(I)$]	0.0706	0.0201	0.0190	–
R_1 (all data)[a]	0.1526	0.0251	0.0240	–
wR_2 (all data)[a]	0.2183	0.0601	0.0434	–
lrgst diff peak, e/Å^3	0.575	0.223	0.251	–
lrgst diff hole, e/Å^3	–0.496	–0.213	–0.258	–

Table S3. The molecular dimensions (Å, º) of HCE.

temperature, K	305.0(1)	293.0(1)	100.0(1)	85.0(5)	295(2)	295(2)	295(2)
pressure	0.1 MPa	0.1 MPa	0.1 MPa	0.1 MPa	1.60(2) GPa	3.19(2) GPa	4.02(2) GPa
C1–C2	1.554(5)	1.561(4)	1.572(2)	1.5732(18)	1.52(2)	1.559(5)	1.564(5)
C1–Cl1	1.770(3)	1.768(3)	1.7651(17)	1.7650(13)	1.764(13)	1.755(7)	1.759(8)
C1–Cl2	1.7689(19)	1.7665(15)	1.7648(10)	1.7648(8)	1.769(9)	1.758(4)	1.752(5)
C1–Cl2^{i}	1.7689(19)	1.7665(15)	1.7648(10)	1.7648(8)	1.769(9)	1.758(4)	1.752(5)
C2–Cl3	1.765(3)	1.766(3)	1.7711(17)	1.7707(13)	1.777(13)	1.774(7)	1.770(8)
C2–Cl4	1.7677(19)	1.7664(15)	1.7653(10)	1.7657(8)	1.775(10)	1.753(4)	1.752(5)
C2–Cl4^{i}	1.7677(19)	1.7664(15)	1.7653(10)	1.7657(8)	1.775(10)	1.753(4)	1.752(5)
C1–C2–Cl3	108.6(2)	108.86(19)	109.40(11)	109.44(8)	109.4(10)	108.5(5)	108.0(6)
C1–C2–Cl4	108.73(17)	109.05(13)	109.82(7)	109.81(5)	110.9(6)	109.6(2)	109.7(2)
C1–C2–Cl4^{i}	108.73(17)	109.05(13)	109.82(7)	109.81(5)	110.9(6)	109.6(2)	109.7(2)
C2–C1–Cl1	109.3(2)	109.40(18)	109.61(11)	109.61(9)	109.6(10)	109.5(5)	108.8(6)
C2–C1–Cl2	108.95(16)	109.09(12)	109.49(7)	109.46(5)	110.3(6)	109.15(19)	109.1(2)
C2–C1–Cl2^{i}	108.95(16)	109.09(12)	109.49(7)	109.46(5)	110.3(6)	109.15(19)	109.1(2)
Cl1–C1–Cl2	109.74(13)	109.58(10)	109.17(6)	109.20(5)	108.7(6)	109.44(14)	109.51(16)
Cl1–C1–Cl2^{i}	109.74(13)	109.58(10)	109.17(6)	109.20(5)	108.7(6)	109.44(14)	109.51(16)
Cl2–C1–Cl2^{i}	110.10(18)	110.08(14)	109.89(9)	109.91(7)	109.1(9)	110.2(4)	110.9(5)
Cl3–C2–Cl4	110.47(14)	110.10(11)	109.23(6)	109.23(5)	108.8(6)	109.71(14)	109.85(16)
Cl3–C2–Cl4^{i}	110.47(14)	110.10(11)	109.23(6)	109.23(5)	108.8(6)	109.71(14)	109.85(16)
Cl4–C2–Cl4^{i}	109.78(18)	109.66(14)	109.33(9)	109.30(7)	108.0(9)	109.6(4)	109.8(4)
Cl1–C1–C2–Cl3	180.0	180.0	180.0	180.0	180.0	180.0	180.0
Cl1–C1–C2–Cl4	–59.75(15)	–59.86(12)	–60.13(7)	–60.10(5)	–59.9(6)	–60.2(3)	–60.3(4)
Cl1–C1–C2–Cl4^{i}	59.75(15)	59.86(12)	60.13(7)	60.10(5)	59.9(6)	60.2(3)	60.3(4)
Cl2–C1–C2–Cl3	–60.06(14)	–60.14(11)	–60.27(7)	–60.26(5)	–60.3(6)	–60.2(3)	–60.6(4)
Cl2–C1–C2–Cl4	60.2(3)	60.0(2)	59.60(12)	59.64(9)	59.7(11)	59.6(5)	59.1(6)
Cl2–C1–C2–Cl4^{i}	179.68(12)	179.72(10)	179.85(7)	179.85(5)	179.6(6)	179.9(3)	179.7(4)
Cl2^{I}–C1–C2–Cl3	60.06(14)	60.14(11)	60.27(7)	60.26(5)	60.3(6)	60.2(3)	60.6(4)
Cl2^{I}–C1–C2–Cl4	–179.68(12)	–179.72(10)	–179.85(7)	–179.85(5)	–179.6(6)	–179.9(3)	–179.7(4)
Cl2^{I}–C1–C2–Cl4^{i}	–60.2(3)	–60.0(2)	–59.60(12)	–59.64(9)	–59.7(11)	–59.6(5)	–59.1(6)

Symmetry code: (i) $x, -y + 1/2, z$

Table S4. Dimensions (Å, º) of the intra- and intermolecular Cl···Cl contacts in HCE at various temperature/ambient pressure conditions.

temperature, K	305.0(1)	293.0(1)	100.0(1)	85.0(5)
pressure, MPa	0.1	0.1	0.1	0.1
Intramolecular Contacts				
Cl1···Cl4	3.1793(12)	3.1933(9)	3.2259(5)	3.2263(4)
C1–Cl1···Cl4	58.16(10)	58.10(8)	57.90(5)	57.92(4)
Cl1···Cl4–C2	58.57(12)	58.35(9)	57.78(6)	57.79(4)
C1–Cl1···Cl4–C2	–31.36(13)	–31.44(10)	–31.51(6)	–31.51(5)
Cl2···Cl3	3.1702(11)	3.1850(9)	3.2190(5)	3.2195(4)
C1–Cl2···Cl3	58.28(11)	58.22(9)	58.02(5)	58.04(4)
Cl2···Cl3–C2	58.57(10)	58.35(8)	57.89(5)	57.88(4)
C1–Cl2···Cl3–C2	–31.64(13)	–31.68(10)	–31.66(6)	–31.67(5)
Cl2···Cl4	3.1757(11)	3.1873(9)	3.2164(4)	3.2168(3)
C1–Cl2···Cl4	58.26(10)	58.26(8)	58.16(5)	58.17(4)
Cl2···Cl4–C2	58.41(10)	58.29(8)	57.97(5)	57.96(4)
C1–Cl2···Cl4–C2	31.67(19)	31.58(15)	31.28(9)	31.32(7)
Intermolecular Contacts				
Cl1···Cl4^{i}	3.8538(13)	3.8496(10)	3.7479(5)	3.7416(4)
C1–Cl1···Cl4^{i}	115.92(11)	116.09(8)	117.56(5)	117.61(4)
Cl1···Cl4^{i}–C2^{i}	85.39(12)	85.64(9)	85.16(5)	85.09(4)
C1–Cl1···Cl4^{i}–C2^{i}	69.86(11)	70.03(8)	70.93(6)	70.94(4)
Cl1···Cl4^{ii}	3.6969(8)	3.6882(6)	3.5950(3)	3.5901(3)
C1–Cl1···Cl4^{ii}	98.71(2)	98.63(1)	97.48(1)	97.41(1)
Cl1···Cl4^{ii}–C2^{ii}	153.08(10)	152.99(7)	151.85(5)	151.77(4)
C1–Cl1···Cl4^{ii}–C2^{ii}	–164.33(31)	–165.11(24)	–166.06(13)	–166.01(10)
Cl1···Cl2^{iii}	3.7465(12)	3.7324(9)	3.6149(5)	3.6087(4)
C1–Cl1···Cl2^{iii}	129.65(11)	129.44(8)	127.42(5)	127.33(4)
Cl1···Cl2^{iii}–C1^{iii}	96.15(9)	96.00(7)	95.14(5)	95.10(4)
C1–Cl1···Cl2^{iii}–C1^{iii}	130.43(6)	130.48(5)	130.12(3)	130.07(2)
Cl1···Cl3^{iii}	3.6653(15)	3.6648(12)	3.6020(6)	3.5976(4)
C1–Cl1···Cl3^{iii}	179.68(12)	179.49(10)	179.53(6)	179.54(4)
Cl1···Cl3^{iii}–C2^{iii}	116.89(12)	116.28(10)	113.80(6)	113.70(4)
C1–Cl1···Cl3^{iii}–C2^{iii}	180	180	180	180
Cl2···Cl3^{i}	3.8685(12)	3.8633(10)	3.7602(5)	3.7539(4)
C1–Cl2···Cl3^{i}	85.71(12)	85.78(9)	84.93(5)	84.83(4)
Cl2···Cl3^{i}–C2^{i}	115.07(12)	115.42(9)	117.20(5)	117.29(4)
C1–Cl2···Cl3^{i}–C2^{i}	69.80(10)	70.01(8)	70.92(5)	70.95(4)
Cl2···Cl4^{ii}	3.7357(9)	3.7238(7)	3.6102(4)	3.6041(3)
C1–Cl2···Cl4^{ii}	97.38(9)	97.42(7)	96.96(5)	96.92(4)
Cl2···Cl4^{ii}–C2^{ii}	161.08(10)	161.10(8)	160.93(5)	160.94(4)
C1–Cl2···Cl4^{ii}–C2^{ii}	164.89(42)	166.06(32)	167.87(18)	167.82(14)
Cl2···Cl3^{iv}	3.7434(7)	3.7337(6)	3.6317(3)	3.6263(3)
C1–Cl2···Cl3^{iv}	145.47(10)	145.42(8)	145.41(5)	145.44(4)
Cl2···Cl3^{iv}–C2^{iv}	101.59(2)	101.49(2)	100.39(1)	100.33(1)
C1–Cl2···Cl3^{iv}–C2^{iv}	108.71(22)	108.39(17)	108.98(11)	109.10(8)
Cl2···Cl2^{v}	3.6918(12)	3.6893(10)	3.6041(6)	3.5987(4)
C1–Cl2···Cl2^{v}	139.20(12)	139.13(9)	137.51(6)	137.37(4)
Cl2···Cl2^{v}–C1^{v}	139.20(12)	139.13(9)	137.51(6)	137.37(4)
C1–Cl2···Cl2^{v}–C1^{v}	180	180	180	180
Cl2···Cl4^{vi}	3.8579(10)	3.8419(8)	3.7186(4)	3.7127(3)
C1–Cl2···Cl4^{vi}	143.17(11)	143.12(9)	143.30(5)	143.35(4)
Cl2···Cl4^{vi} –C2^{vi}	97.48(10)	97.65(8)	97.44(5)	97.39(4)
C1–Cl2···Cl4^{vi}–C2^{vi}	–113.48(20)	–113.11(16)	–113.02(9)	–113.11(7)
Cl3···Cl4^{vii}	3.9756(12)	3.9546(9)	3.7885(5)	3.7802(4)
C2–Cl3···Cl4^{vii}	158.09(3)	157.90(2)	156.36(2)	156.28(1)
Cl3···Cl4^{vii}–C2^{vii}	103.69(9)	103.69(7)	102.97(5)	102.93(3)
C2–Cl3···Cl4^{vii}–C2^{vii}	163.58(27)	162.77(21)	158.48(12)	158.26(9)

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

Table S5. Dimensions (Å, º) of the intra- and intermolecular Cl···Cl contacts in HCE at room-temperature/high-pressure conditions.

temperature, K	295(2)	295(2)	295(2)
pressure, GPa	1.60(2)	3.19(2)	4.02(2)
Intramolecular Contacts			
Cl1···Cl4	3.2053(45)	3.1970(8)	3.1901(8)
C1–Cl1···Cl4	57.91(43)	57.94(14)	58.22(16)
Cl1···Cl4–C2	56.94(49)	57.90(13)	57.95(14)
C1–Cl1···Cl4–C2	–30.57(61)	–31.55(24)	–31.79(28)
Cl2···Cl3	3.1987(43)	3.1789(7)	3.1684(8)
C1–Cl2···Cl3	57.38(47)	58.40(12)	58.41(14)
Cl2···Cl3–C2	57.64(44)	58.27(14)	58.46(14)
C1–Cl2···Cl3–C2	–30.86(61)	–31.77(25)	–32.18(29)
Cl2···Cl4	3.222(10)	3.1840(15)	3.1760(17)
C1–Cl2···Cl4	57.47(45)	58.29(15)	58.61(18)
Cl2···Cl4–C2	57.03(46)	58.15(15)	58.27(16)
C1–Cl2···Cl4–C2	30.30(72)	31.34(28)	31.19(34)
Intermolecular Contacts			
Cl1···Cl4^{i}	3.5599(44)	3.4535(8)	3.4036(8)
C1–Cl1···Cl4^{i}	118.71(58)	118.70(17)	118.73(19)
Cl1···Cl4^{i}–C2^{i}	84.43(49)	82.45(9)	81.74(9)
C1–Cl1···Cl4^{i}–C2^{i}	71.65(50)	72.15(24)	72.29(26)
Cl1···Cl4^{ii}	3.4618(32)	3.3532(7)	3.3123(6)
C1–Cl1···Cl4^{ii}	95.94(23)	94.94(3)	94.42(4)
Cl1···Cl4^{ii}–C2^{ii}	149.81(55)	149.68(20)	149.29(23)
C1–Cl1···Cl4^{ii}–C2^{ii}	–167.3(11)	–165.87(28)	–165.78(32)
Cl1···Cl2^{iii}	3.474(14)	3.3835(21)	3.3383(24)
C1–Cl1···Cl2^{iii}	124.88(45)	123.83(15)	123.47(17)
Cl1···Cl2^{iii}–C1^{iii}	93.90(40)	93.23(22)	92.62(26)
C1–Cl1···Cl2^{iii}–C1^{iii}	130.30(27)	129.26(7)	129.07(8)
Cl1···Cl3^{iii}	3.449 (16)	3.3416(24)	3.3009(26)
C1–Cl1···Cl3^{iii}	179.91(58)	179.72(19)	179.45(21)
Cl1···Cl3^{iii}–C2^{iii}	112.46(55)	112.58(16)	112.30(17)
C1–Cl1···Cl3^{iii}–C2^{iii}	180	180	180
Cl2···Cl3^{i}	3.5743(46)	3.4826(8)	3.4364(8)
C1–Cl2···Cl3^{i}	84.10(48)	82.26(9)	81.46(10)
Cl2···Cl3^{i}–C2^{i}	118.14(61)	117.41(15)	117.55(17)
C1–Cl2···Cl3^{i}–C2^{i}	71.81(52)	71.56(24)	71.95(28)
Cl2···Cl4^{ii}	3.462(11)	3.3508(15)	3.3027(18)
C1–Cl2···Cl4^{ii}	95.85(47)	94.97(22)	94.89(26)
Cl2···Cl4^{ii}–C2^{ii}	160.76(47)	159.47(21)	159.16(24)
C1–Cl2···Cl4^{ii}–C2^{ii}	170.8(16)	167.89(30)	167.53(32)
Cl2···Cl3^{iv}	3.4918(36)	3.3741(6)	3.3302(6)
C1–Cl2···Cl3^{iv}	144.12(54)	144.84(18)	145.17(22)
Cl2···Cl3^{iv}–C2^{iv}	98.86(27)	97.77(4)	97.24(5)
C1–Cl2···Cl3^{iv}–C2^{iv}	109.9(10)	113.75(33)	114.72(37)
Cl2···Cl2^{v}	3.4004(57)	3.3044(10)	3.2617(10)
C1–Cl2···Cl2^{v}	136.39(54)	133.86(13)	132.97(14)
Cl2···Cl2^{v}–C1^{v}	136.39(54)	133.86(13)	132.97(14)
C1–Cl2···Cl2^{v}–C1^{v}	180	180	180
Cl2···Cl4^{vi}	3.561(10)	3.4438(15)	3.3931(18)
C1–Cl2···Cl4^{vi}	142.84(47)	143.45(16)	143.51(19)
Cl2···Cl4^{vi} –C2^{vi}	96.53(46)	95.78(21)	95.44(24)
C1–Cl2···Cl4^{vi}–C2^{vi}	–112.27(92)	–115.92(31)	–117.24(35)
Cl3···Cl4^{vii}	3.578(14)	3.4529(21)	3.3935(23)
C2–Cl3···Cl4^{vii}	154.55(20)	153.81(6)	153.24(6)
Cl3···Cl4^{vii}–C2^{vii}	102.36(42)	100.68(19)	100.10(21)
C2–Cl3···Cl4^{vii}–C2^{vii}	156.3(11)	156.51(42)	155.99(46)

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