Table 27A-1-001. HCl, DCl. Unit cell parameters [67San1].

Compound	Phase	T [K]	a [Å]	b [Å]	c [Å]
HCl	I	118.5	5.482(1)		
	II	92.4	5.082(1)	5.410(1)	5.826(1)
DCl	I	118.5	5.475(1)		
	II	92.4	5.069(1)	5.399(1)	5.829(1)

Table 27A-1-002. DCl. Positional and temperature parameters. B, β_{ij} are defined by Eqs. (e), (c) in Introduction, respectively.

77.4 K [67San1]. R = 2.9 %

	x	y	z	B [Å^2]
D	0.081(2)	0.170(4)	0	2.7(5)
Cl	0.25	0	0	1.71(1)

111.5 K [67San2]. R = 1.9 %

	x (= y)	z	β_{11} (=β_{22}) [Å^2]	β_{33} [Å^2]	β_{12} [Å^2]	β_{13} (=β_{23}) [Å^2]
D (1/12 atom in 48-fold position)	0.151(5)	0	7.5(15)	15.7(48)	–3.65(180)	0
Cl (in 4-fold position)	0	0	3.55(30)	3.55(30)	0	0

Table 27A-1-003. DCl. Bond lengths and bond angles.

T = 77.4 K [67San1]	
D–Cl	1.25(2) Å
Cl–Cl	3.688(1) Å
Cl–Cl–Cl	93°31(2)'
T = 111.5 K [67San2]	
D–Cl	1.17(4) Å

Table 27A-1-004. HCl, DCl. Transition heat and transition entropy of the II–I transition.

Compound	ΔQ_m [J mol^{-1}]	ΔS_m [J K^{-1} mol^{-1}]	Ref.
HCl	1187	12.1	28Gia
DCl	1338	12.75	47Clu

Table 27A-1-005. HCl. Lattice mode frequencies [cm^{-1}].

Raman [69Ito] T = 77 K	Raman [70Wan] T = 77 K	Raman [72Sun] T = 79 K	Raman [77Ves] T = 74 K	IR [64And]
–	50?	–	49	–
55 (A_2)	59 (A_2)	58 (A_2)	58	–
84 (A_1)	87 (A_1)	84 (A_1)	85	86
–	113 ($2A_2$)	110 (B_1)	110	109
133 ($A_2 + A_1$)	138?	135 (A_2)	134 (A_1)	–
218 (B_2)	221 (B_2)	217 (A_1)	219 (A_2)	217
290 (A_1)	–	–	–	296
–	–	333 (B_2)	–	–
–	408?	399 (B_1)	403 (B_1)	–
–	–	–	–	496