Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Information

Negative linear compression and expanding NH···N bond in an imidazoline compound

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Table S1 Crystal data and structure-refinements details of ambient- and high-pressure measurements of $C_9H_9N_2Cl$ (compound **I**) at 296 K.

Pressure	0.1 MPa	0.08 GPa	1.20 GPa
Formula weight	180.63	180.63	180.63
Wavelength (Å)	1.54178	0.71073	0.71073
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*Fdd*2	*Fdd*2	*Fdd*2
Unit cell dimensions (Å,) *a*	19.8523(3)	19.875(6)	19.659(9)
b	39.3437(7)	39.36(3)	38.94(4)
c	4.46970(10)	4.398(4)	4.070(5)
Volume ($Å^3$)	3491.12(11)	3441(5)	3115(5)
Z	16	16	16
Calculated density (g/cm^3)	1.375	1.395	1.540
Absorption coefficient (mm^{-1})	3.392	0.384	0.424
F(000) (e)	1504	1504	1504
Crystal size (mm)	0.62/0.21/0.09	0.42/0.37/0.23	0.42/0.37/0.23
θ-range for data collection (°)	4.50 to 73.79	4.10 to 17.90	4.65 to 24.68
Min/max indices: h, k, l	-24/24,-48/42,-5/5	-17/17,-20/20,-3/3	-22/22,-11/11,-4/4
Reflect. Collected/unique	35785 / 1764	2242 / 340	2892 / 373
R_{int}	0.1654	0.2946	0.3073
Refinement method	Full-matrix least squares		
Completeness (%)	99.9	54.0	27.0
Data/restrains/parameters	1764 / 1 / 114	340 / 1 / 45	373 / 16 / 33
Goodness-of-fit on F^2	1.110	1.291	1.224
Final R_1/wR_2 ($I>2\sigma_1$)	0.0579/ 0.1695	0.0994/0.2218	0.1266/0.2628
R_1/wR_2 (all data)	0.0591/ 0.1714	0.1145/0.2367	0.1802/0.2861
Largest diff. peak/hole ($e.Å^{-3}$)	0.233/-0.227	0.186/-0.200	0.427/-0.381

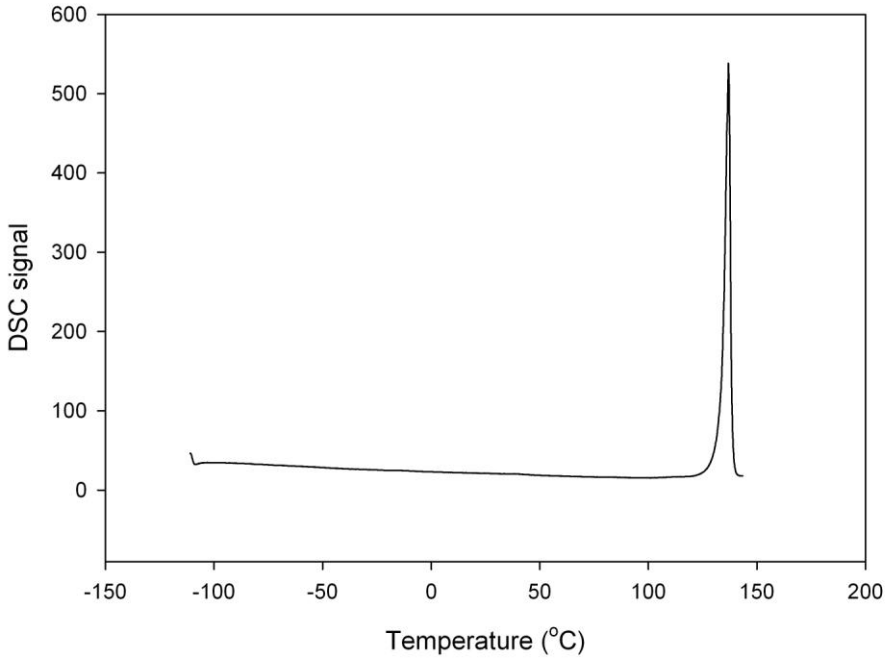

Fig. S1 DSC signal of 2-(3'-chlorophenyl)-imidazoline (compound **I**).

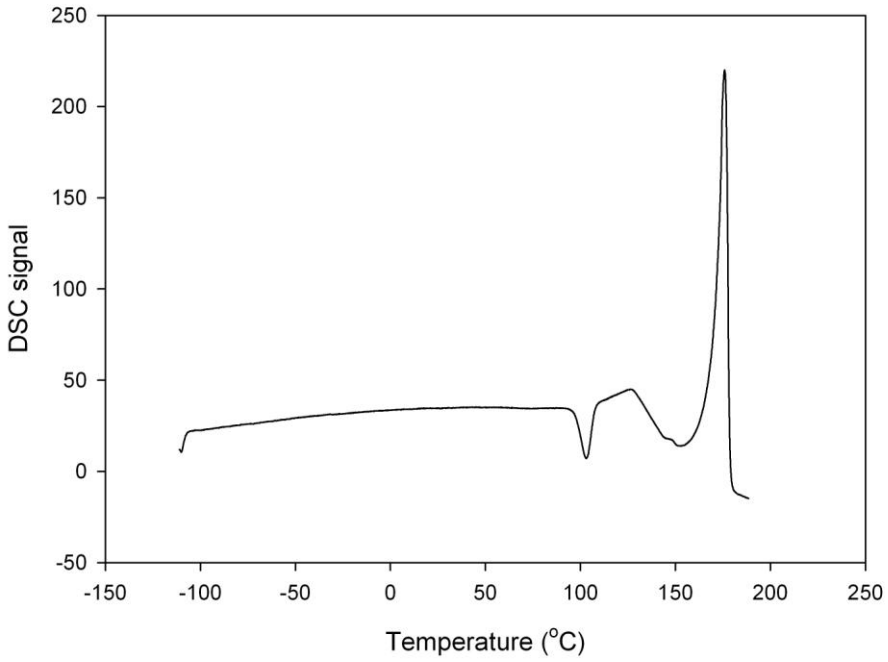

Fig. S2 DSC signal of 2-(4,5-dihydro-1H-imidazol-2-yl)-pyridine (compound **II**).

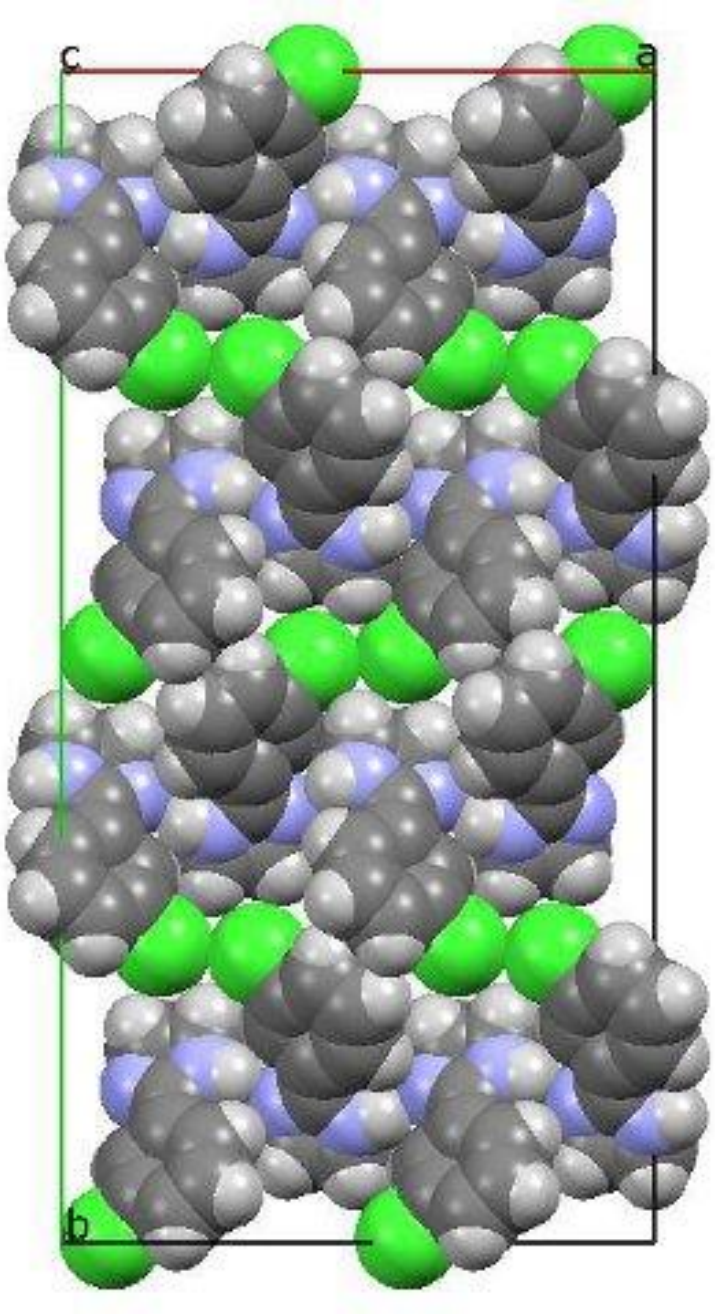

Fig. S3 The space-filling representation of the unit-cell contents of 2-(3'-chlorophenyl)-imidazoline (compound **I**) viewed down [z].

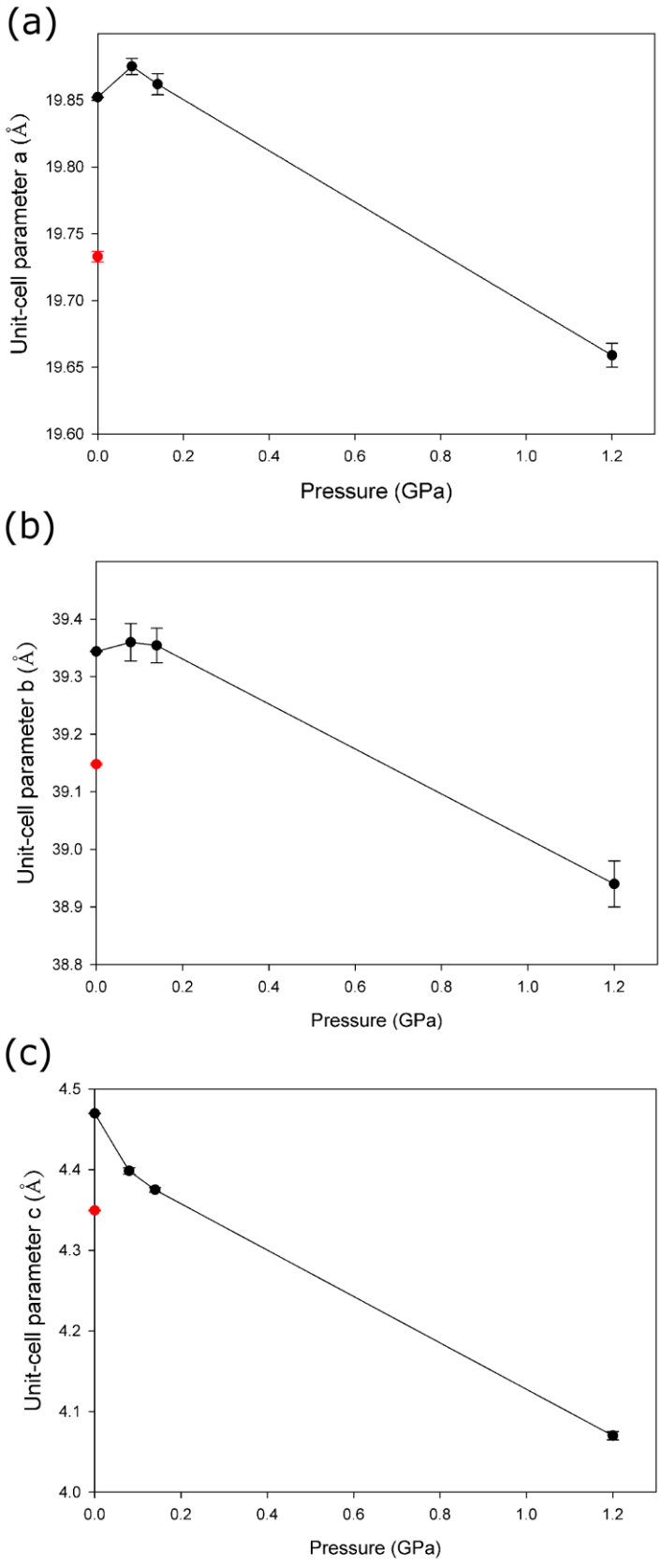

Fig. S4 Unit-cell parameters in the function of pressure at 296 K (black dots), and at lower temperature at 100 K (red dots): (a) parameter *a*; (b) parameter *b* and (c) parameter *c*.

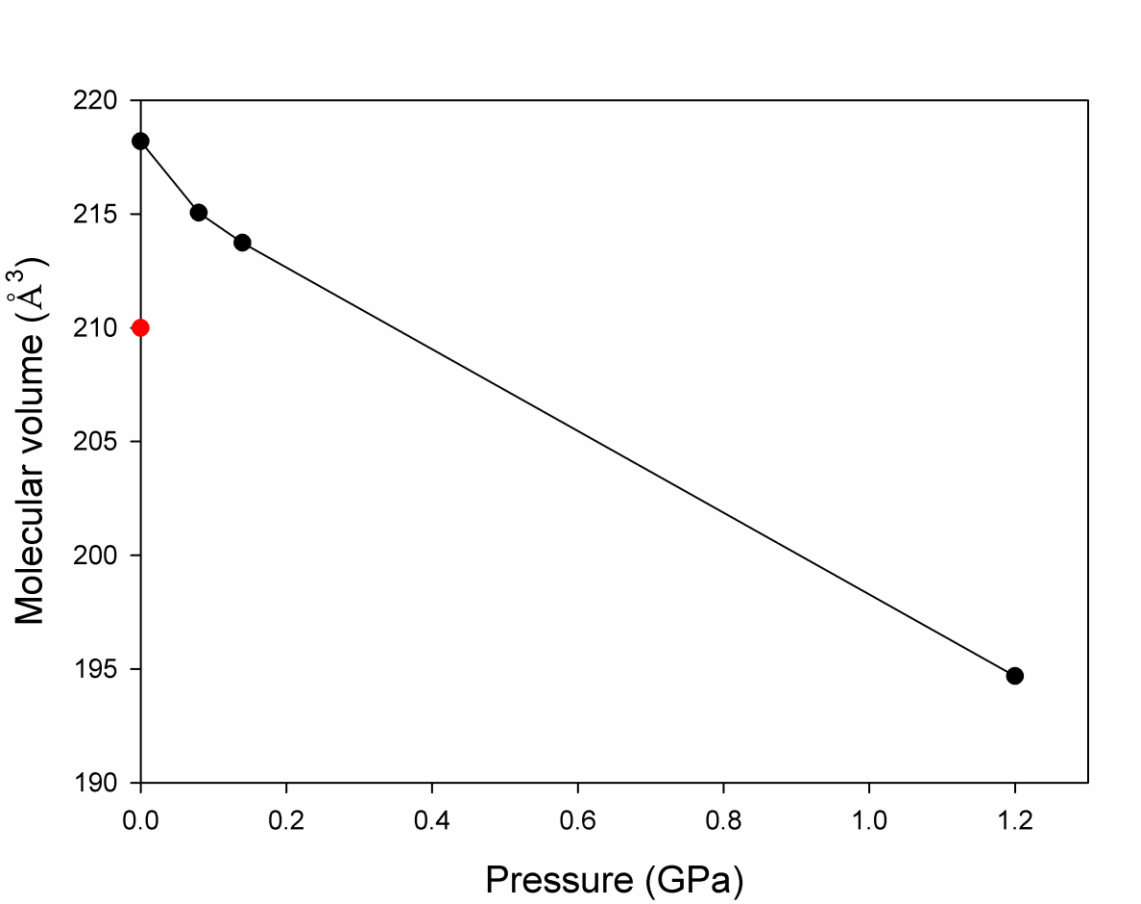

Fig. S5 The pressure dependence of molecular volume (unit-cell volume/Z) of $C_9H_9N_2Cl$ (compound **I**) at 296 K, measured by single-crystal x-ray diffraction (black dots). The V_m value previously measured at 100 K (red dots) has also been shown.