Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information

High temperature phase transitions in N, N-diisopropylpropan-1-ammonium perchlorate

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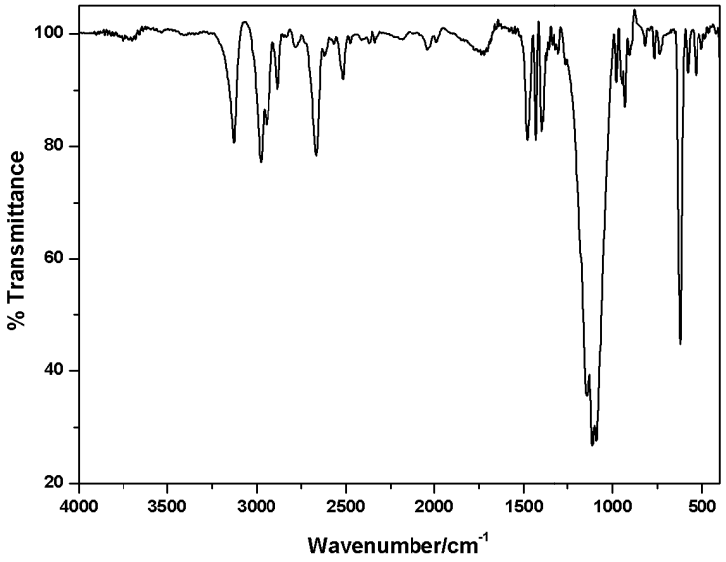

Fig S1 IR for N, N-diisopropylpropan-1-ammonium perchlorate (DAP)

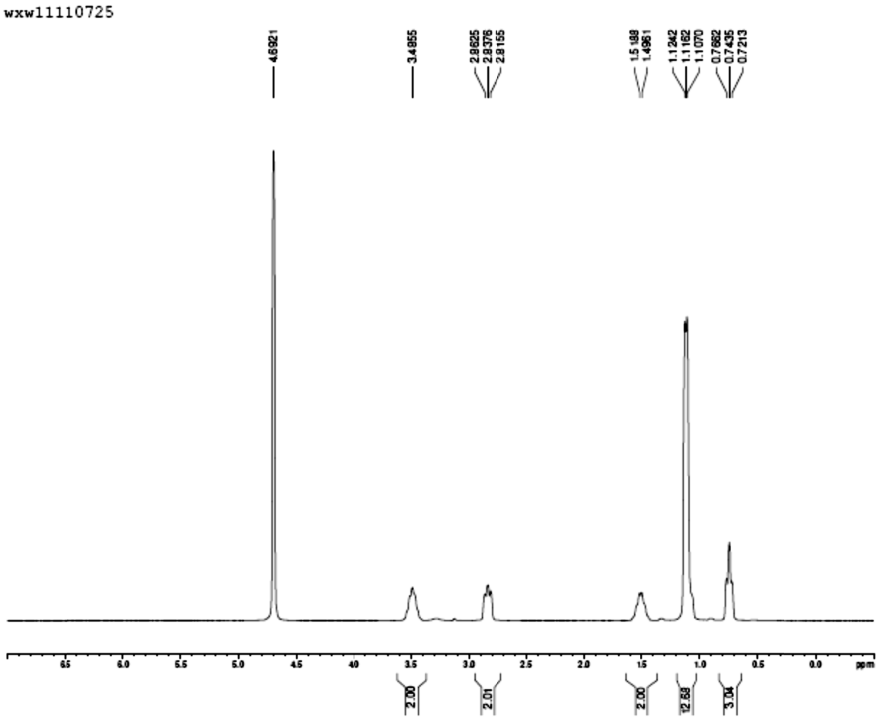

Fig S2 ^{1}H NMR for DAP

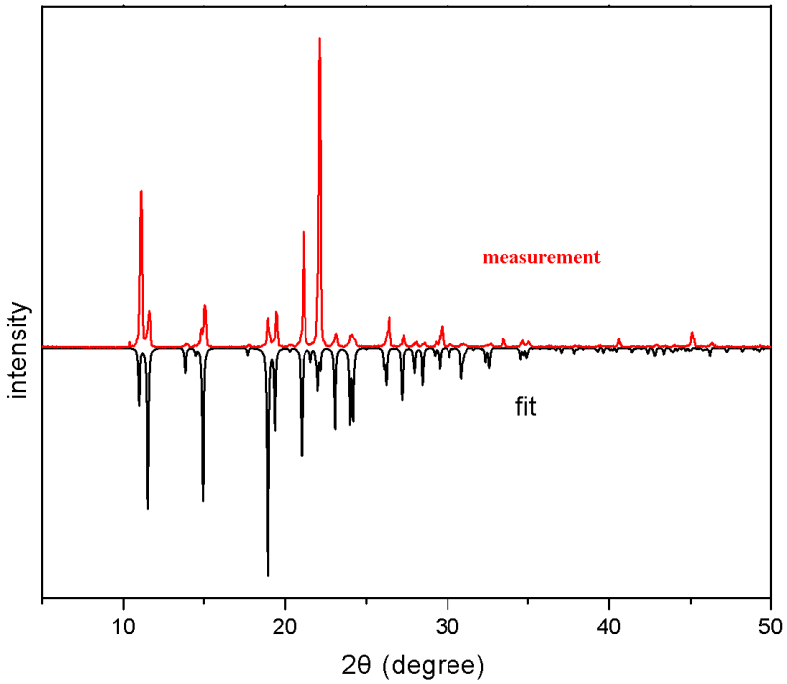

Fig S3 X-ray powder diffraction (XRPD) of DAP

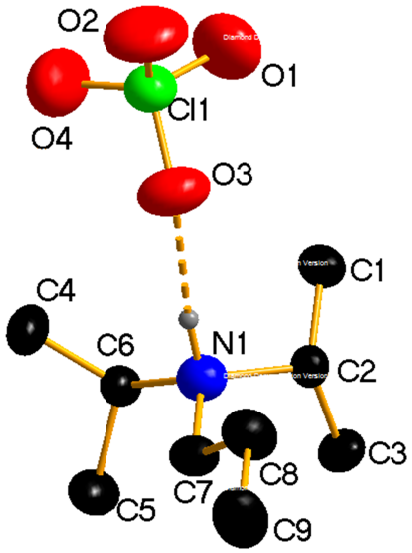

Fig S4 Asymmetric unit of DAP at 293K

The crystal structure was solved by direct methods and refined by the full-matrix method based on F^2 using the SHELXL2014 software package (Sheldrick, 1997). Displacement ellipsoids are drawn at the 50% probability level.

All H atoms attached to C atoms were omitted. The N-H···O hydrogen bond are indicated by a dotted line.

Table S1 Summary of crystallographic data for DAP

	I
Molecular formula	$C_9H_{22}NClO_4$
Formular weigh	243.73
Crystal system, space group	Orthorhombic *P*na2$_1$
Temperature (K)	293(2)
a(Å)	16.126(3),
b(Å)	8.7468(17),
c (Å)	9.3691(19)
α (º)	90,
β (º)	90,
γ (º)	90
V (Å^3)	1321.5(5)
Z	4
Calculated density(Mg/m^3)	1.225
Flack parameter	0.13(8)
F(000)	528
h, *k*, *l* (min, max)	(-20, 20); (-11, 11); (-12, 12)
Reflections collected / unique	13071 / 3018 [*R(int)* = 0.0575]
Completeness	99.9 %(to θ = 27.48°)
GOF on F^2	1.046
Final *R* indices [*I*>2sigma(*I*)]	$^aR_1$ = 0.0491, wR_2 = 0.1052
R indices (all data)	$^aR_1$ = 0.0805, wR_2 = 0.1173
Largest diff. peak and hole(e. Å $^{-3}$)	0.151 and -0.221

$^a R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)]\}^{1/2}$

Table SII Selected distances (Å) and angles (°) of DAP

Bond length		Angle	
N(1)-C(7)	1.489(4)	C(7)-N(1)-C(6)	114.1(2)
N(1)-C(6)	1.538(3)	C(7)-N(1)-C(2)	112.4(2)
N(1)-C(2)	1.536(4)	C(6)-N(1)-C(2)	114.6(2)
N(1)-H(1D)	0.9100	C(7)-N(1)-H(1D)	104.8
Cl(1)-O(4)	1.402(2)	C(8)-C(7)-N(1)	116.0(3)
Cl(1)-O(1)	1.407(2)	O(4)-Cl(1)-O(1)	110.26(17)
Cl(1)-O(2)	1.417(3)	O(2)-Cl(1)-O(3)	108.87(14)
Cl(1)-O(3)	1.432(2)	C(7)-N(1)-C(6)	114.1(2)