Family of conglomerate forming systems composed of chlocyphos and alkyl-amine. Assessment of their resolution performances by using various modes of preferential crystallization.

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Supporting information

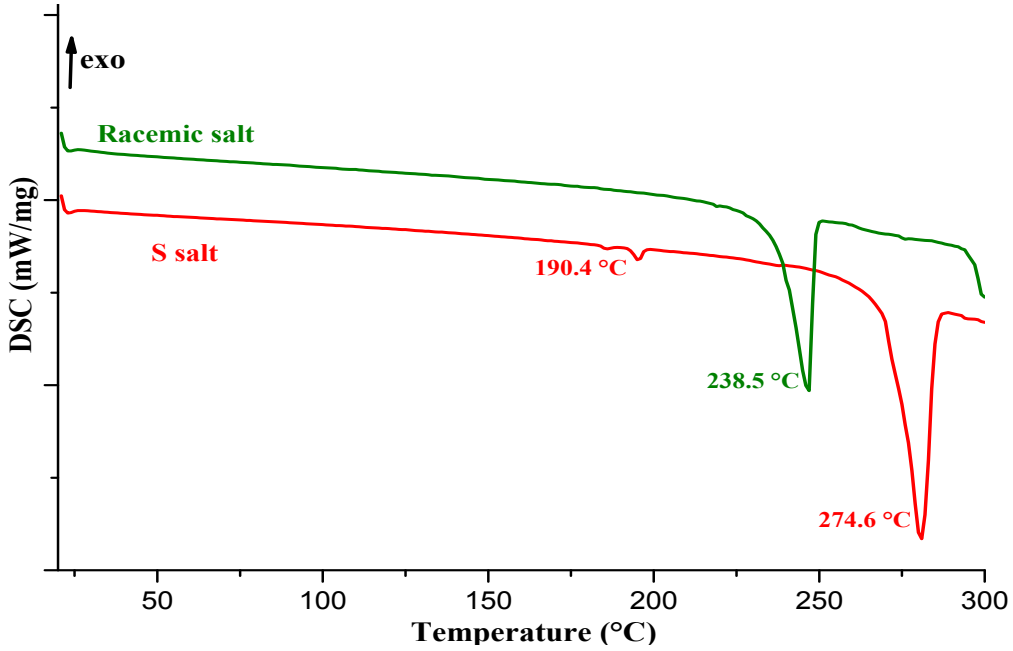


Figure S1: DSC curves of racemic (green) and S (red) ethylammonium chlocyphos salt

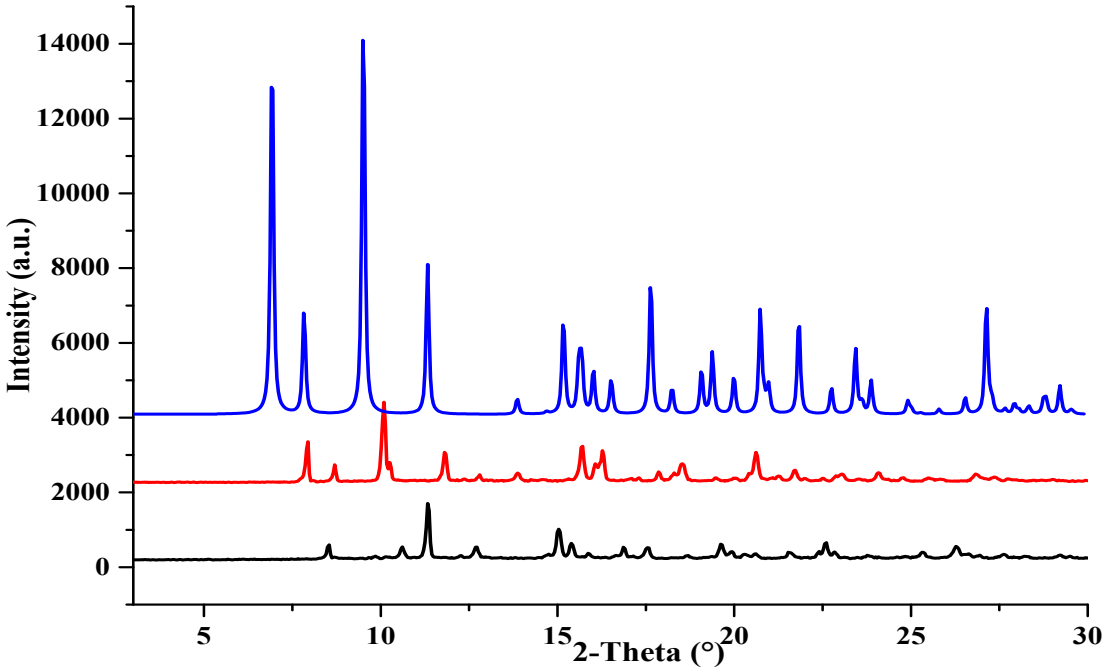


Figure S2: Calculated (blue for racemic) and experimental (black for racemic and red for S) XRPD patterns of propylammonium chlocyphos salt

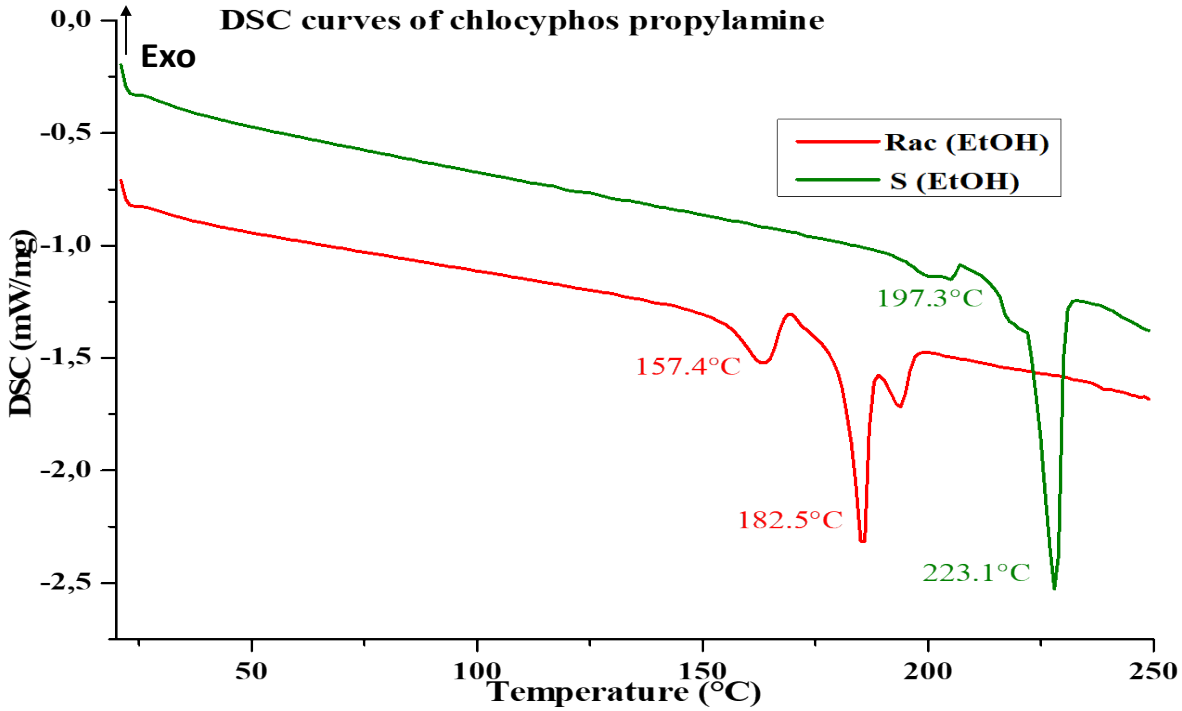
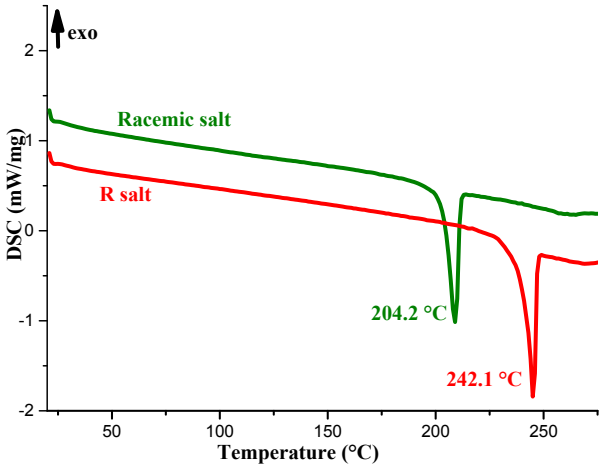


Figure S3: DSC curves of racemic (red) and S (green) propylammonium chlocyphos salt

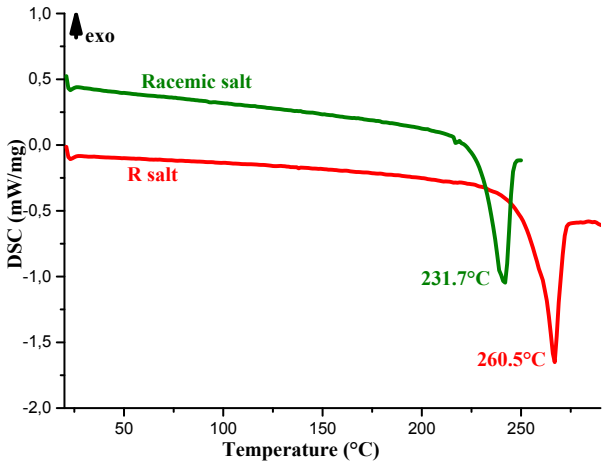
Table S1: Crystallographic data of racemic propylammonium chlocyphos salt

Chemical Formula	$[C_{11}H_{13}ClPO_4]$ $[C_3H_7NH_3]$
CSD number	CCDC 1912822
Molecular Weight / $g.mol^{-1}$	335.7
Crystal System	Monoclinic
Space Group	$P2_1$
Z, Z'	2,1
a / Å	11.427 (8)
b / Å	6.541 (5)
c / Å	12.924 (9)
α / °	90
β / °	100.02 (1)
γ / °	90
V / $Å^3$	951.4 (1)
d_{calc} / $g.cm^{-3}$	1.172 (1)
F (000) / e^-	356
Absorption coefficient μ (MoKα_1) / mm^{-1}	0.297
Absolute structure (Flack) parameter	0.3 (2)

(i) Chlocyphos butylamine



(ii) Chlocyphos isobutylamine



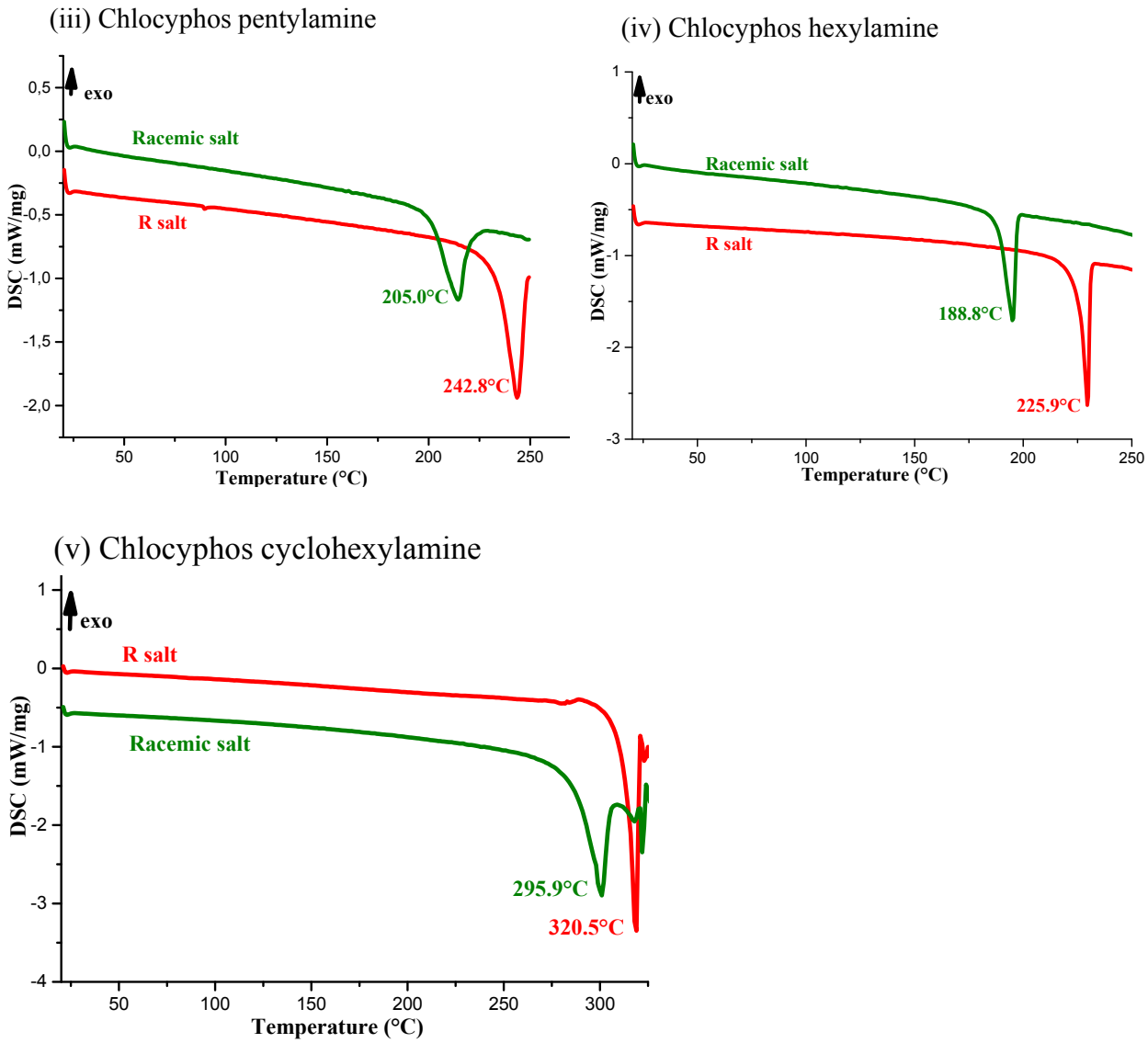
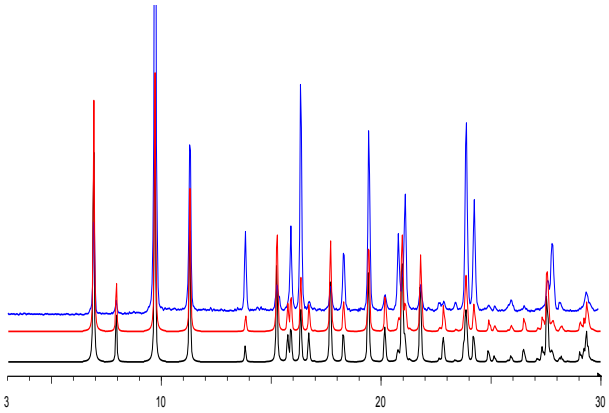
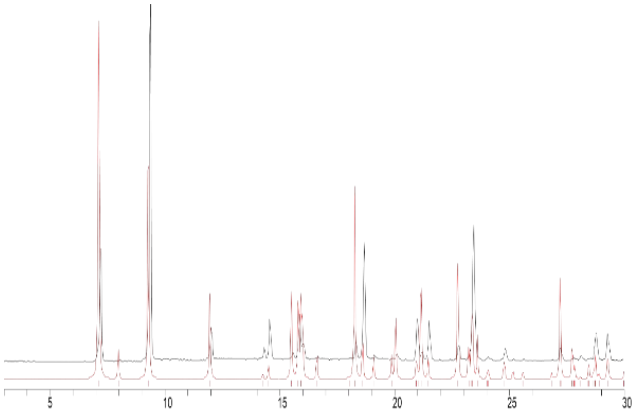


Figure S4: DSC curves of racemic (green) and R (red) of (i) butylammonium, (ii) isobutylammonium, (iii) pentylammonium, (iv) hexylammonium and (v) cyclohexylammonium chlocyphos salts

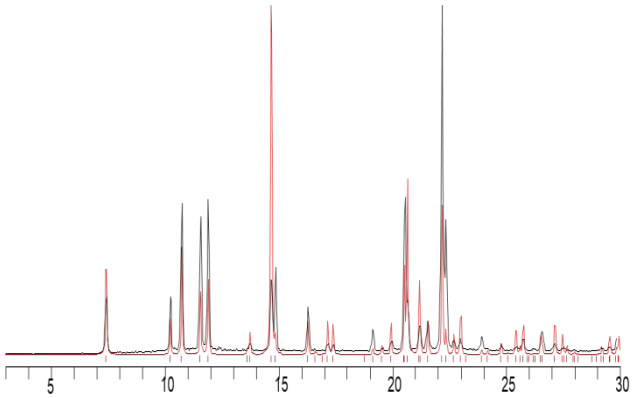
(i) chlocyphos butylamine



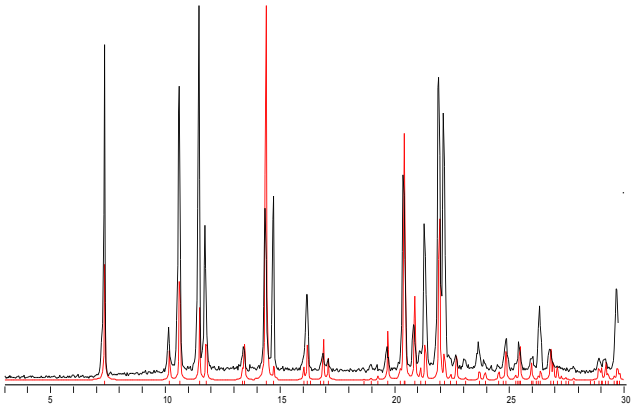
(ii) chlocyphos isobutylamine



(iii) chlocyphos pentylamine



(iv) chlocyphos hexylamine



(v) chlocyphos cyclohexylamine

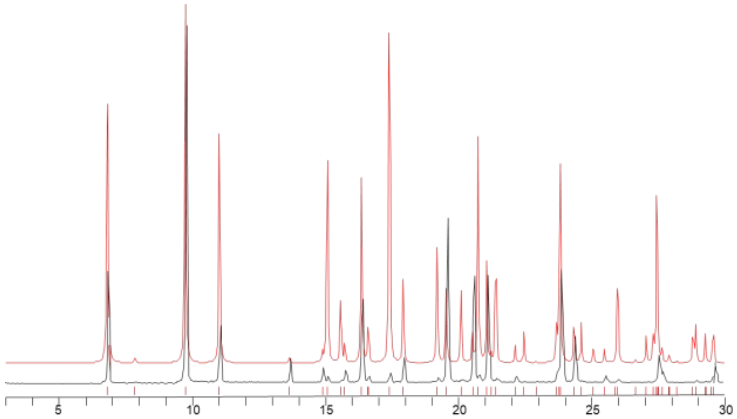
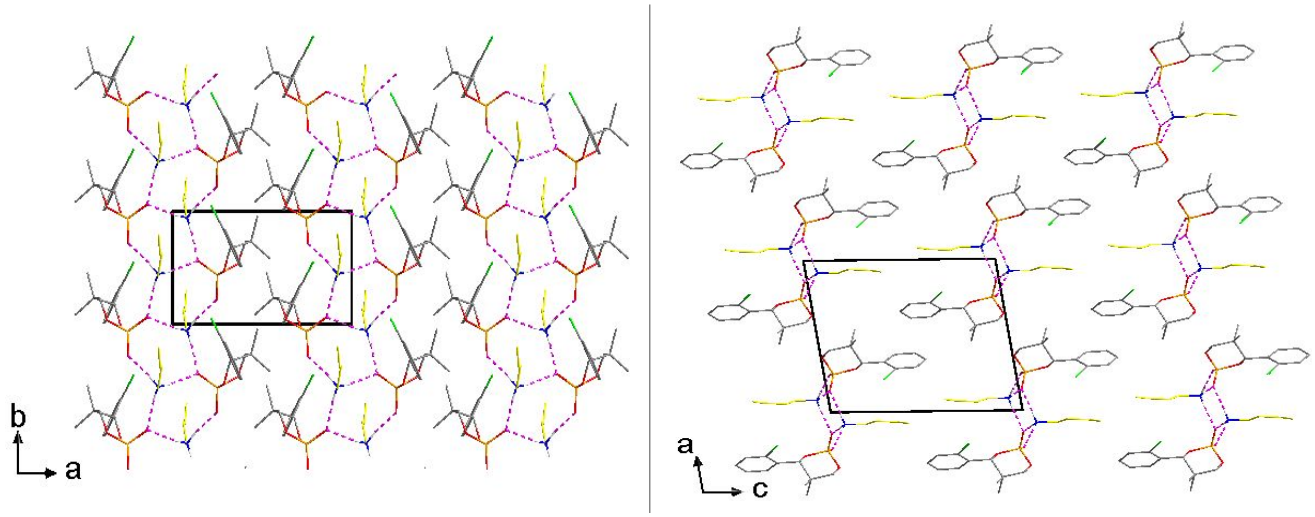
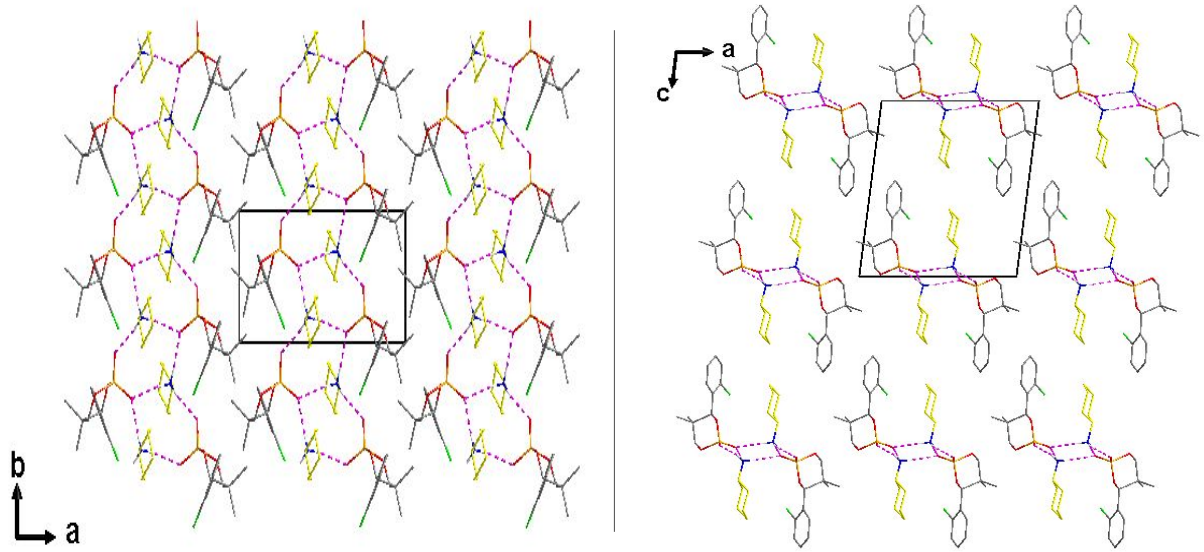


Figure S5: Calculated (red) and experimental (black for racemic, and blue for R) XRPD patterns of (i) butylammonium, (ii) isobutylammonium (iii) pentylammonium, (iv) hexylammonium and (v) cyclohexylammonium chlocyphos salts

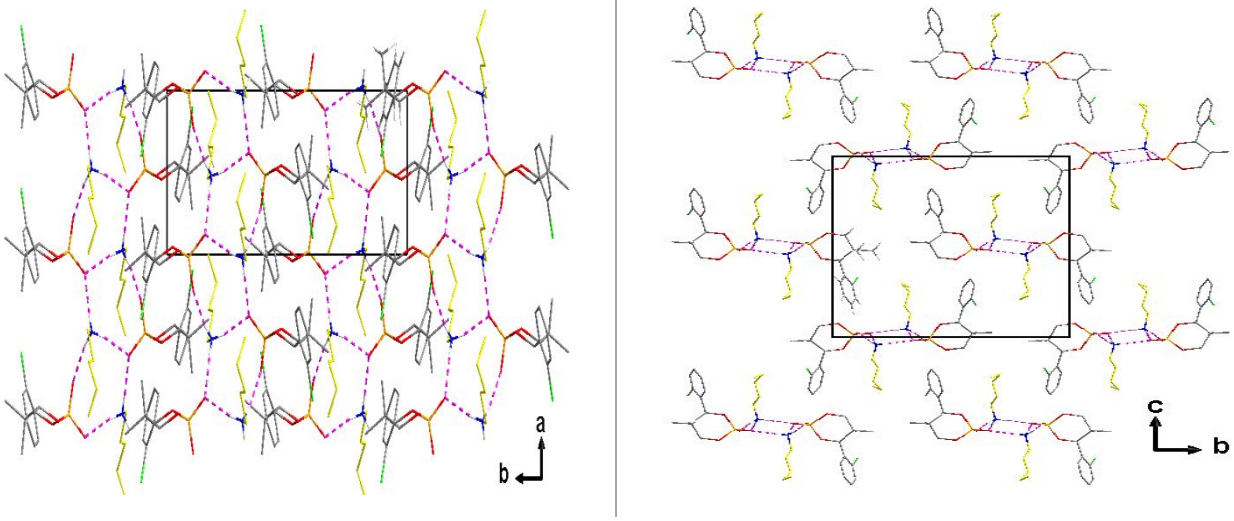
(i) chlocyphos butylamine



(ii) chlocyphos cyclohexylamine



(iii) Chlocyphos pentylamine



(iv) chlocyphos hexylamine

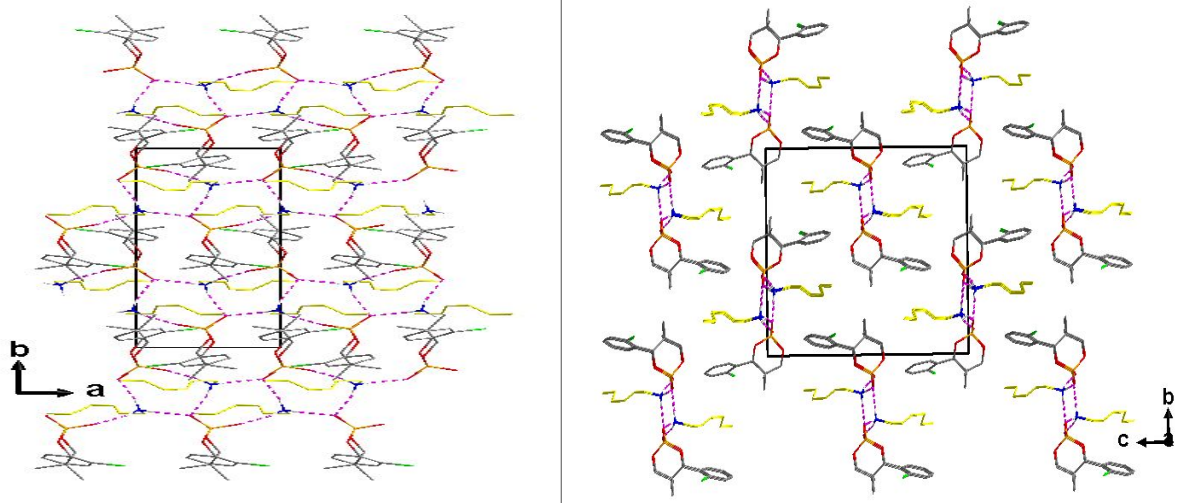


Figure S6: Double row periodic bond chains and the projection of the whole packing along c (left) and b or a (right) axes for (i) butylammonium, (ii) cyclohexylammonium ($P2_1$ space group), (iii) pentylammonium and (iv) hexylammonium chlocyphos salts ($P2_12_12_1$ space group). The black rectangles represent a unit cell.

Table S3: Initial conditions and results of SIPC mode at 25ml scale

(i) *Isobutylammonium chlocyphos salt*

$m_{\pm}$ (g)	m_{EtOH}(g)	m_{seeds} (g) / ee (%)	T_F (°C)
1.500	19.72	0.02 / ±100	5

N°	Time(min)	m_{total} (g)	m_{crops}(g)	OP (%)	m_{pure}(g)	Yield (%)	ee_f (% ee)
A	45	1.520	0.163	+64.81	0.106	5.75	3.41
B	42	1.520	0.143	+68.21	0.097	5.13	3.13
C	40	1.520	0.073	+90.43	0.066	3.07	2.15
D	38	1.520	0.156	-93.15	0.145	8.33	4.61
E	38	1.520	0.133	-83.84	0.111	6.07	3.55
F	38	1.520	0.122	-88.47	0.108	5.87	3.47
Mean	**38**	**1.520**	**0.137**	**±88.49**	**0.102**	**6.76**	**3.39**

Calculation: Mean value = runs (D+E+F)/3

(ii) *Hexylammonium chlocyphos salt*

$m_{\pm}$ (g)	m_{IPA} (g)	m_{seeds} (g) / ee (%)	T_F (°C)
2.335	19.65	0.05 / +100	5

N°	Time (min)	m_{total} (g)	m_{crops} (g)	OP (%)	m_{pure} (g)	Yield (%)	ee_f (% ee)
A	37.5	2.385	0.240	+82.95	0.199	6.38	4.09
B	38.5	2.385	0.257	+77.11	0.198	6.33	4.07
C	38.5	2.385	0.130	+80.61	0.105	2.35	2.20
D	37.5	2.365	0.116	+63.88	0.074	1.03	1.56
E	37.5	2.355	0.173	+68.64	0.119	2.95	2.48
F	37.5	2.355	0.091	+76.98	0.070	0.86	1.48
Mean	**37.8**	**2.372**	**0.168**	**+75.03**	**0.127**	**3.32**	**2.65**

Calculation: Mean value = runs (A+B+C+D+E+F)/6

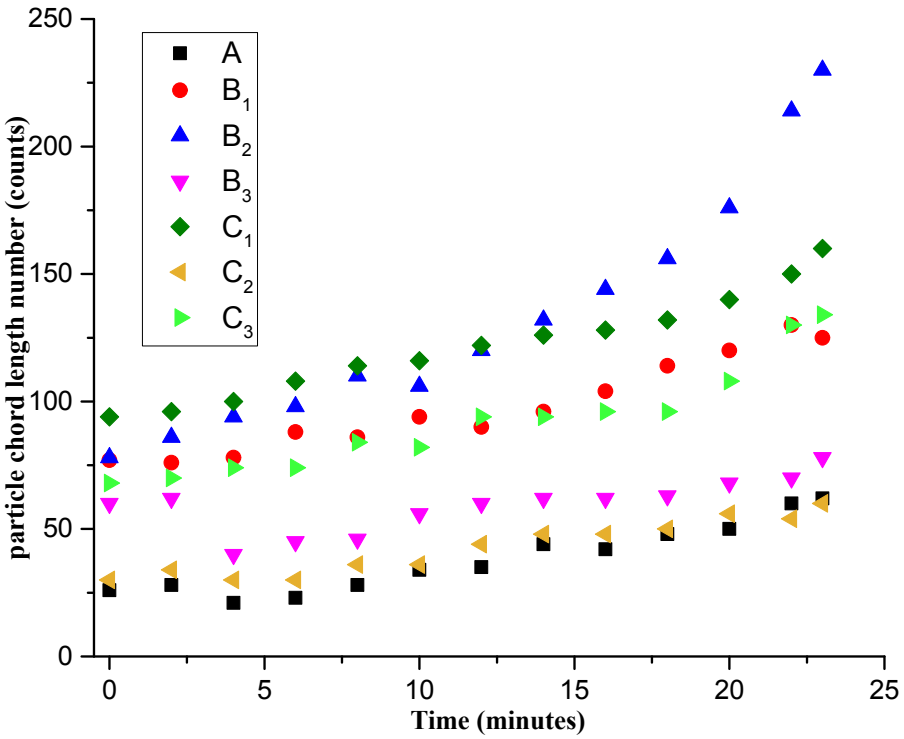


Figure S7: Particle chord length number versus time for AS3PC mode of hexylammonium chlocyphos salt