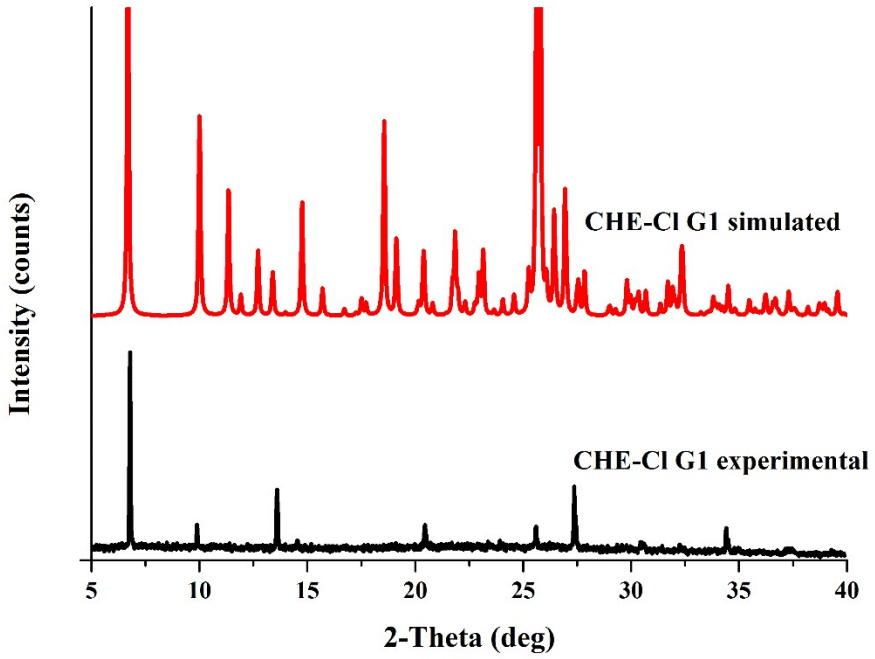
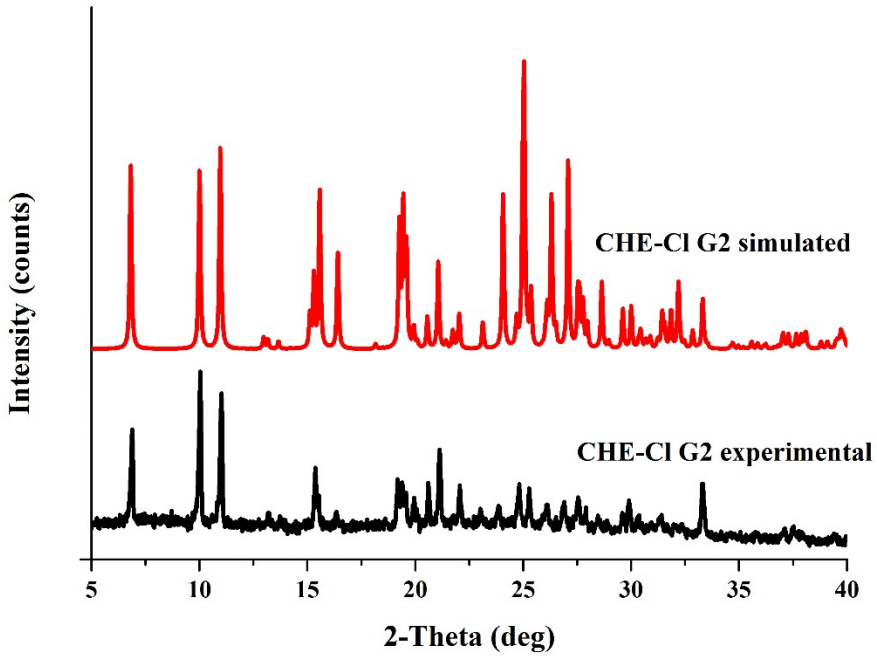
Electronic Supplementary Material (ESI) for CrystEngComm.

Hydrochromism Behavior among Solid Forms of Chelerythrine Hydrochloride

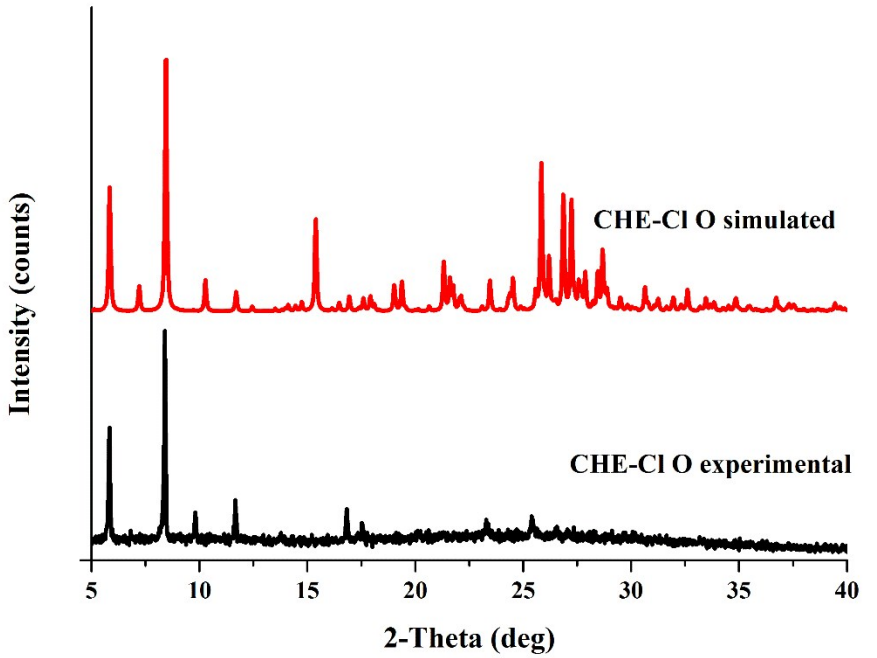
Supporting information



(a)



(b)



(c)

Fig. S1 Comparison between experimental and calculated XRPD of CHE-Cl (a) G1, (b) G2 and (c) O.

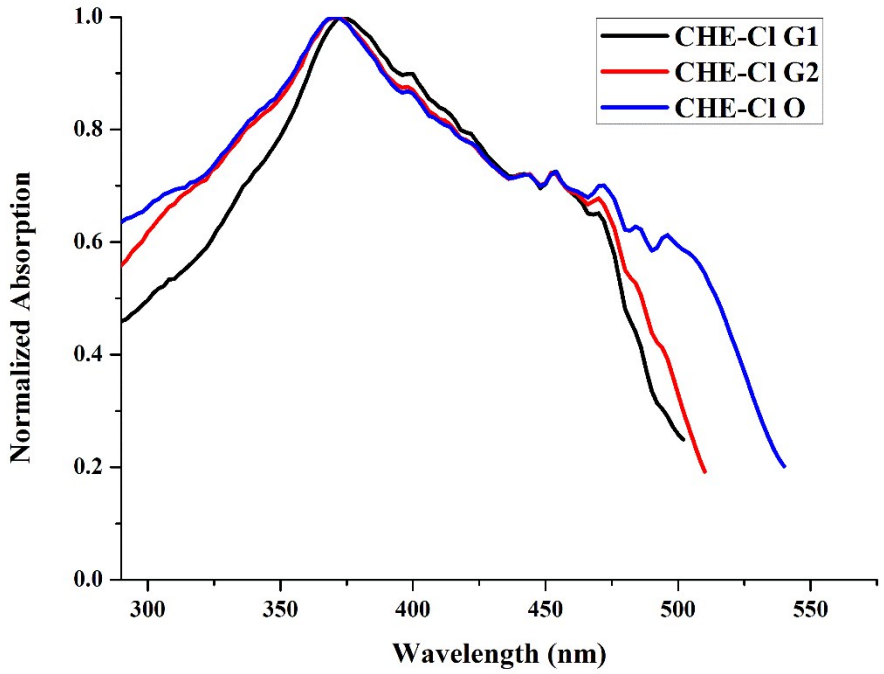


Fig. S2 Absorption spectra of CHE-Cl solid forms.

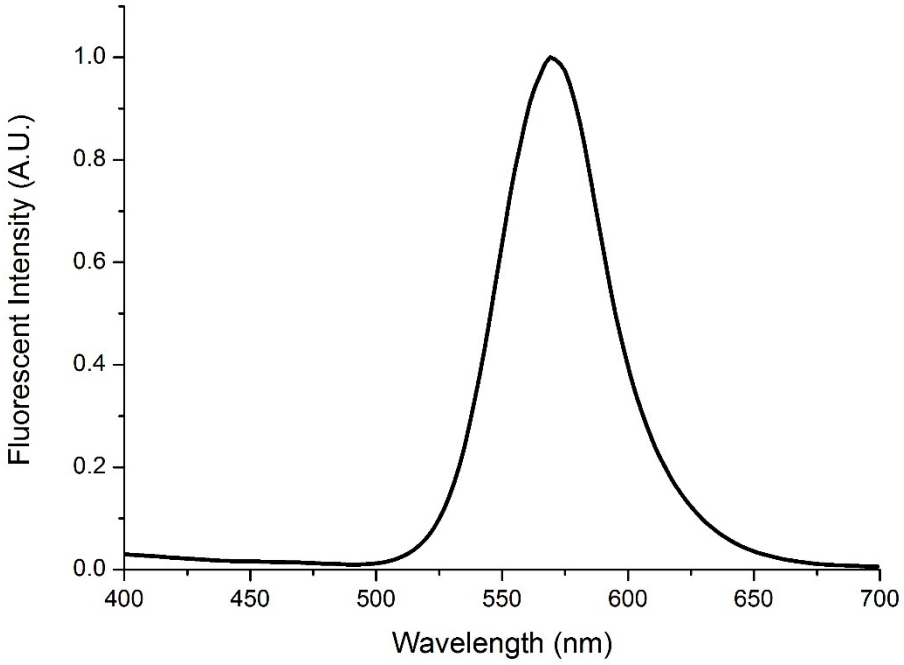


Fig.S3 Solid-state fluorescent emission spectrum of CHE-Cl raw material.

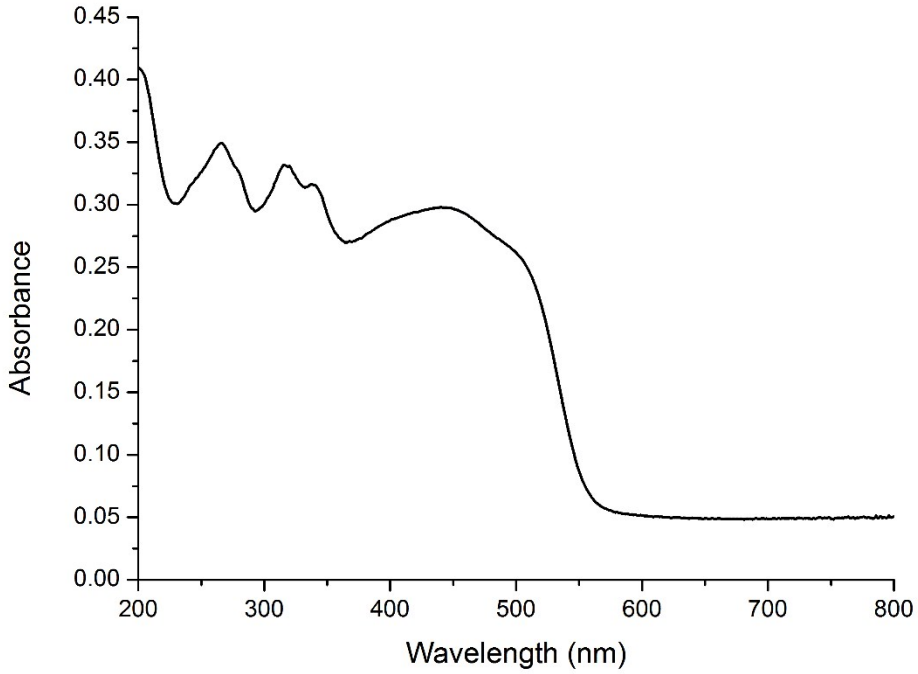
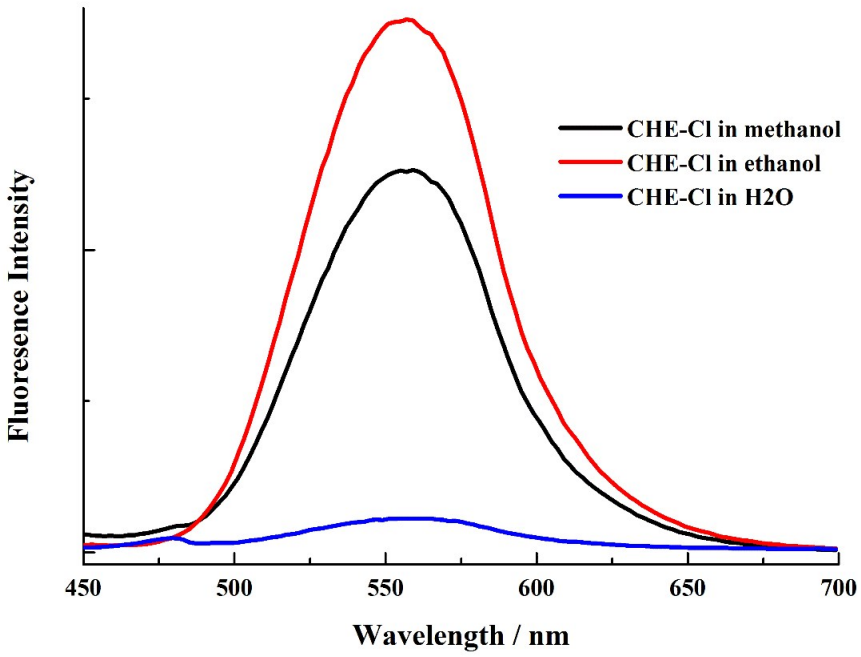


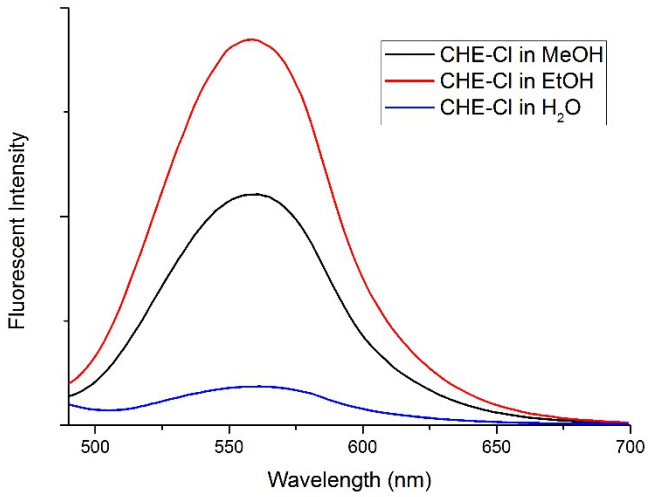
Fig.S4 Solid-state UV-vis absorption spectrum of CHE-Cl raw material.

Table S1. Quantum yields of solid forms of CHE-Cl.

	Quantum yield (%)
CHE-Cl G1	22.60
CHE-Cl G2	21.12
CHE-Cl O	13.99

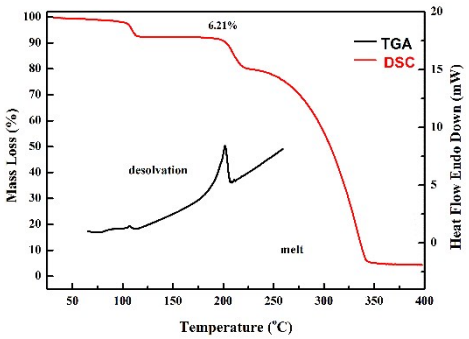


(a)

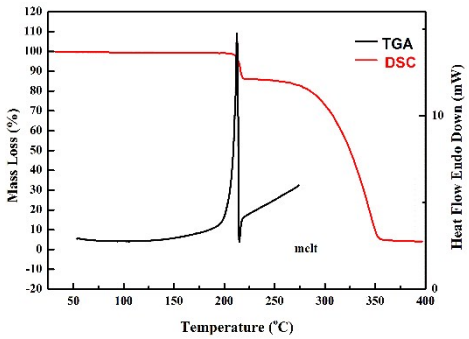


(b)

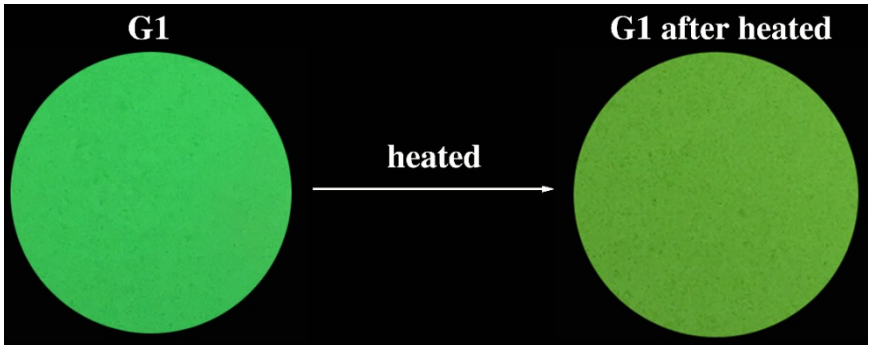
Fig. S5 Fluorescent spectra of CHE-Cl in different solvent with a concentration of (a) 0.1 (b) 0.01mg/mL.


6.21%
TGA
DSC
desolvation
melt
Mass Loss (%)
Heat Flow Endo Down (mW)
Temperature (°C)

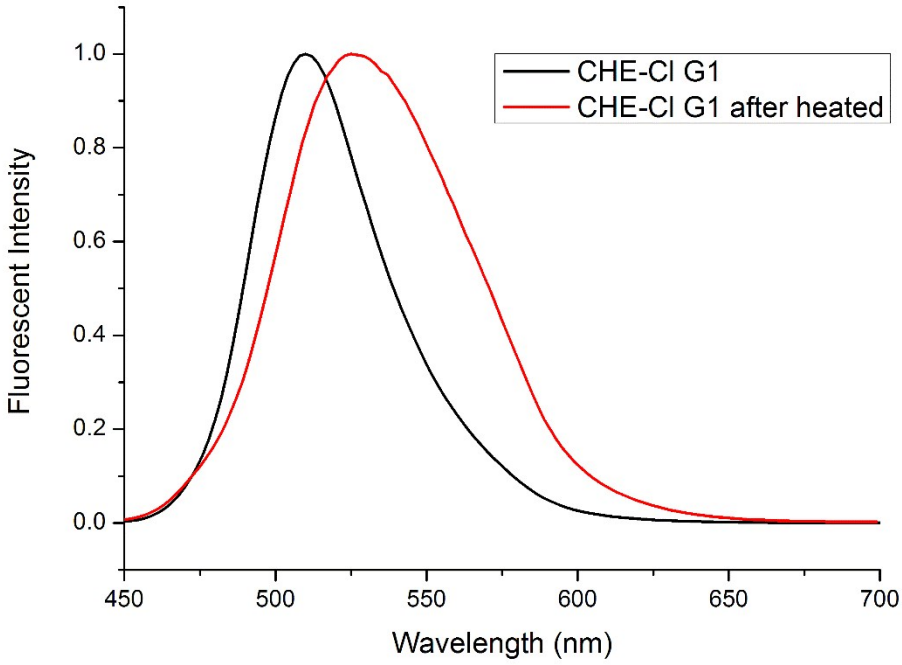
(a)


TGA
DSC
melt
Mass Loss (%)
Heat Flow Endo Down (mW)
Temperature (°C)

(b)


G1
G1 after heated
heated

(c)


CHE-Cl G1
CHE-Cl G1 after heated
Fluorescent Intensity
Wavelength (nm)

(d)

Fig. S6 (a) Thermal analysis of CHE-Cl G1, (b) Thermal analysis of CHE-Cl G2, (c) The fluorescent color (d) the fluorescent spectra of CHE-Cl G1 before and after 120 ^{o}C heated.

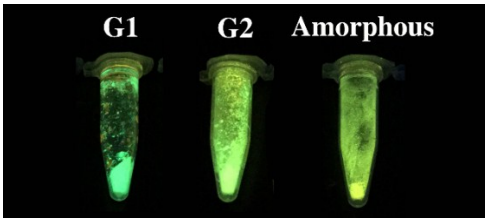
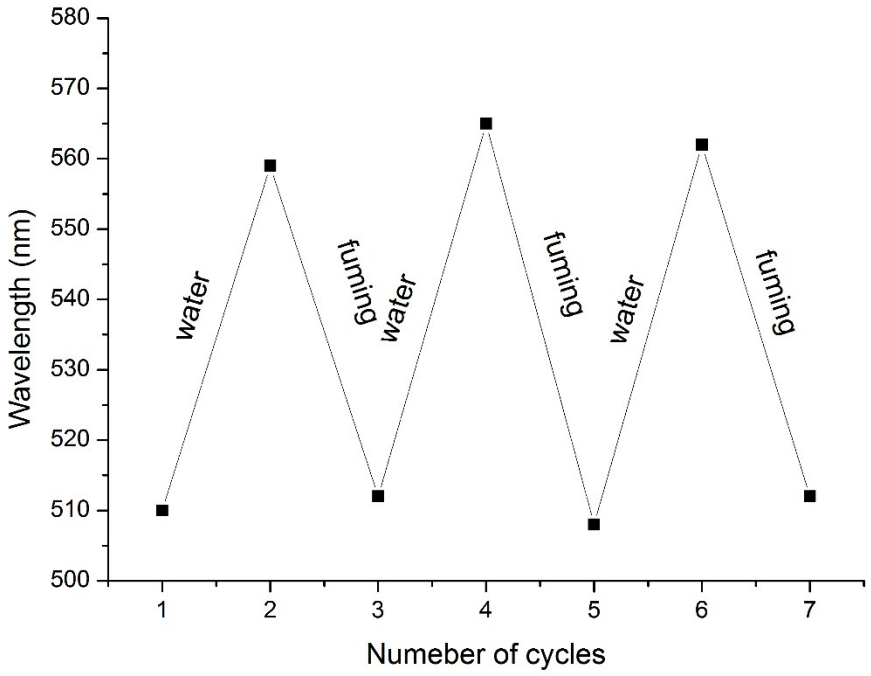
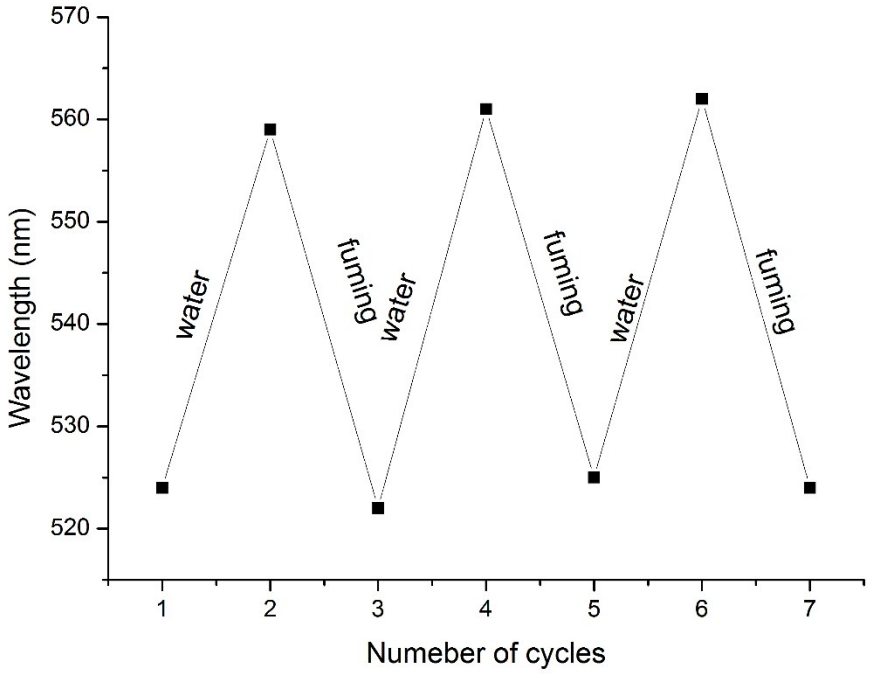


Fig. S7 The fluorescent color of CHE-Cl G1, G2 and amorphous powder (G1 or G2 after grinding).



(a)



(b)

Fig. S8 Repeated switching of solid-state fluorescence of (a) G1 and (b) G2 by repeated water dropping and fuming cycles.

Table S2. Unit Cell Comparison for the salts of CHE and its relevant solid forms.

	CHE-Cl G1	CHE-Cl G2	CHE-Cl O
Formula	$C_{21}H_{18}NO_4Cl$ CH_4O	$C_{21}H_{18}NO_4Cl$	$C_{21}H_{18}NO_4Cl$ $4.5H_2O$
Crystal system	monoclinic	monoclinic	orthorhombic
Space group	P 2_1/c	C 2/c	P 212121
Temperature (K)	170(2)	170(2)	170(2)
a (Å)	13.2953(4)	28.9199(9)	6.8891(2)
b (Å)	8.1752(3)	7.3899(2)	20.9101(7)
c (Å)	17.7914(6)	18.0028(6)	30.2189(11)
α (deg)	90	90	90
β (deg)	96.999(2)	116.427(2)	90

γ (deg)	90	90	90
Cell volume ($Å^3$)	1919.37(11)	3445.42(18)	4353.1(2)
Calc. density ($g\ cm^{-3}$)	1.439	1.480	1.419
Z	4	8	8
R_{int}	0.0313	0.0383	0.0919
$R_1(I > 2\sigma(I))$	0.0422	0.0406	0.0471
wR_2	0.1262	0.1051	0.0942
Goof (S)	0.9605	1.028	1.007
CCDC	1584746	1584747	1584748

Table S3. Unit Cell Comparison for the salts of CHE and its relevant solid forms.

Crystal form	Interactions	H···A/Å	D···A/Å	<D-H···A/°	Symmetry code
CHE-Cl G1	O5-H5A···Cl1	2.32	3.1110	157	
	C5-H5···Cl1	2.74	3.4428	131	1-x,-1/2+y,1/2-z
	C10-H10A···O2	2.57	3.3044	131	-x,-y,-z
	C12-H12A···Cl1	2.68	3.5774	152	1-x,-1/2+y,1/2-z
	C17-H17···Cl1	2.82	3.7714	177	1-x,1-y,-z
	C20-H20···Cl1	2.62	3.5585	168	1-x,1-y,-z
	C22-H22A···O4	2.50	3.4158	155	-x,-y,-z
CHE-Cl G2	C5-H5···Cl1	2.77	3.4548	131	1/2-x,-1/2+y,1/2-z
	C16-H16···Cl1	2.81	3.6138	146	x,1-y,-1/2+z
	C12-H12C···Cl1	2.76	3.6663	158	1/2-x,-1/2+y,1/2-z
	C21-H21···Cl1	2.80	3.4617	129	1/2-x,3/2-y,-z
CHE-Cl O	O9-H9C···O11	1.90	2.745	172	
	O9-H9D···O10	1.89	2.723	166	
	O12-H12D···O13	1.89	2.738	171	x+1, y, z
	O12-H12E···O9	1.91	2.751	170	
	O15-H15B···O16	1.94	2.798	170	
	O16-H16B···O17	1.93	2.775	171	
	O11-H11D···O7	1.99	2.812	162	

	O13-H13A···O3	2.00	2.848	171	
	O13-H13B···O14	1.84	2.685	171	
	O10-H10E···O12	2.00	2.754	144	x-1, y, z
	O14-H14B···O15	1.84	2.706	173	x-1, y, z