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Supporting information for article:

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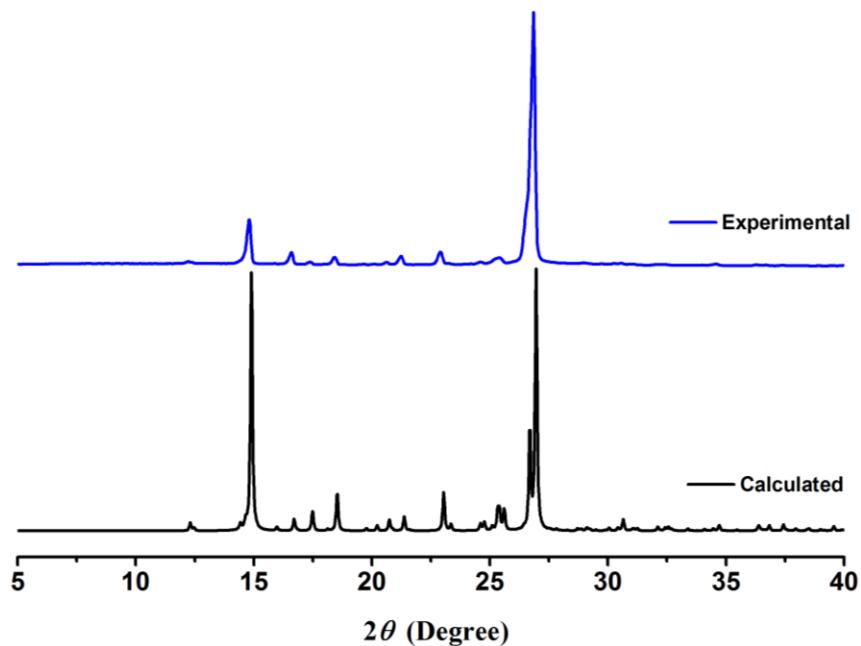
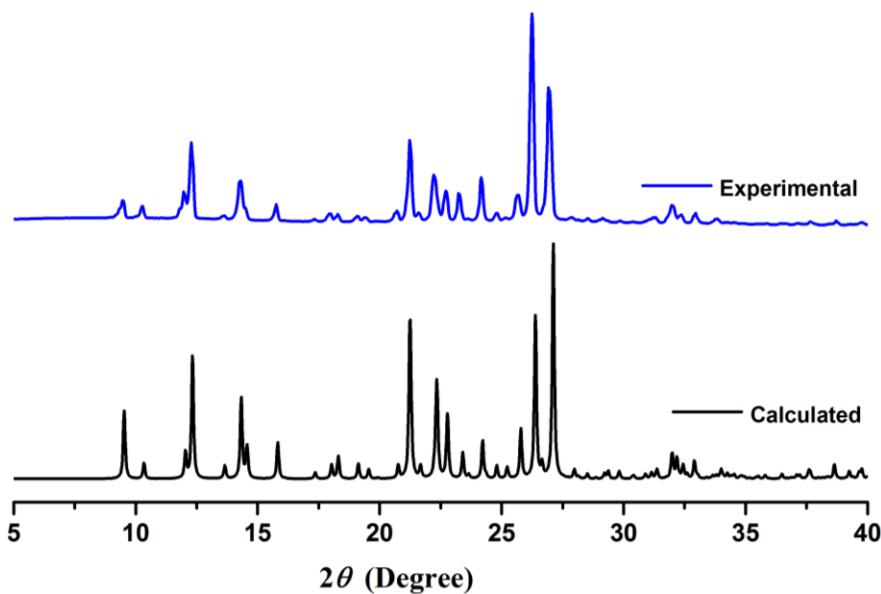
Lalit Rajput, Manas Banik, Jayasubba Reddy Yarava, Sumy Joseph, Manoj Kumar Pandey, Yusuke Nishiyama and Gautam R. Desiraju

Exploring the salt-cocrystal continuum with solid-state NMR using natural abundance samples: implications for crystal engineering

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S1. PXRD of SA1, SA2, CO1, and CNT1.**Figure S1** PXRD of SA1.**Figure S2** PXRD of SA2.

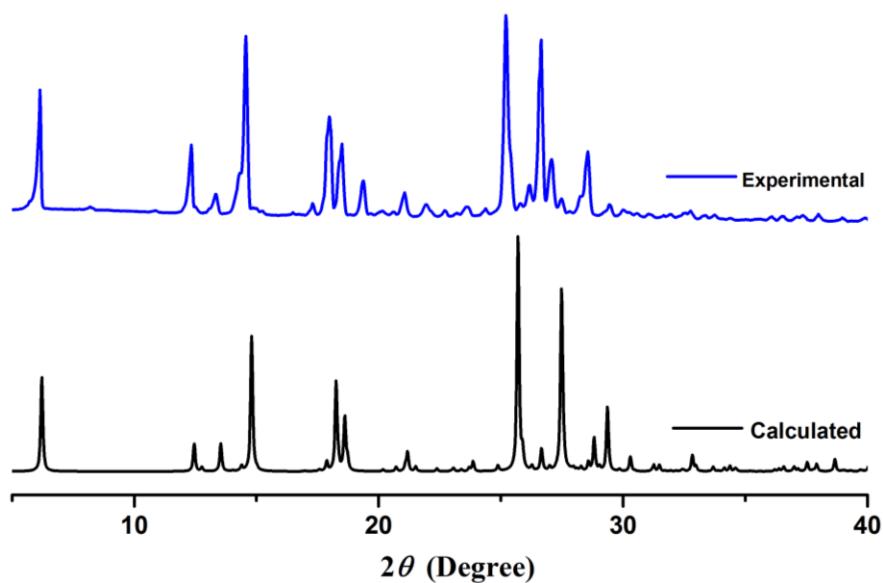


Figure S3 PXRD of CO1.

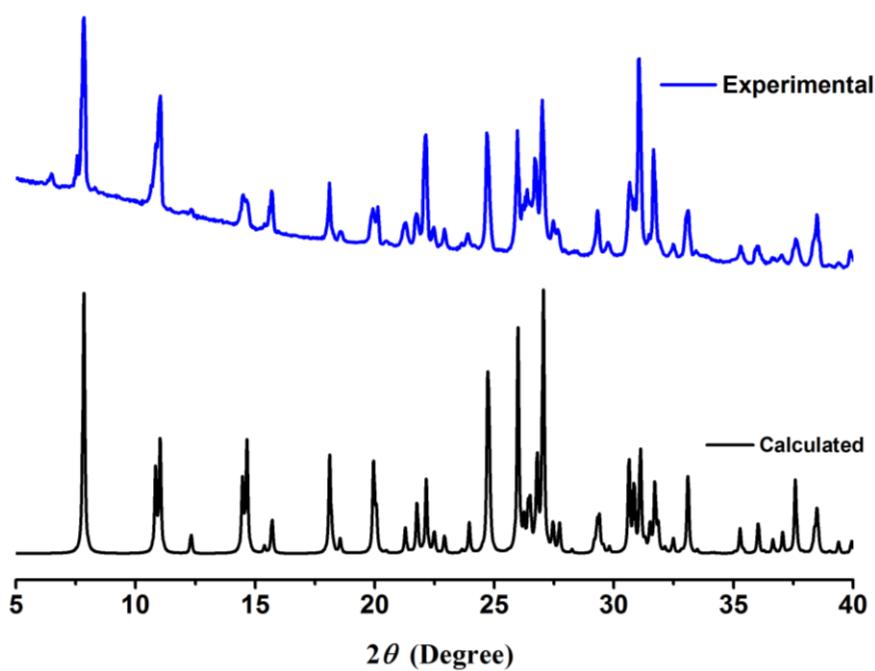
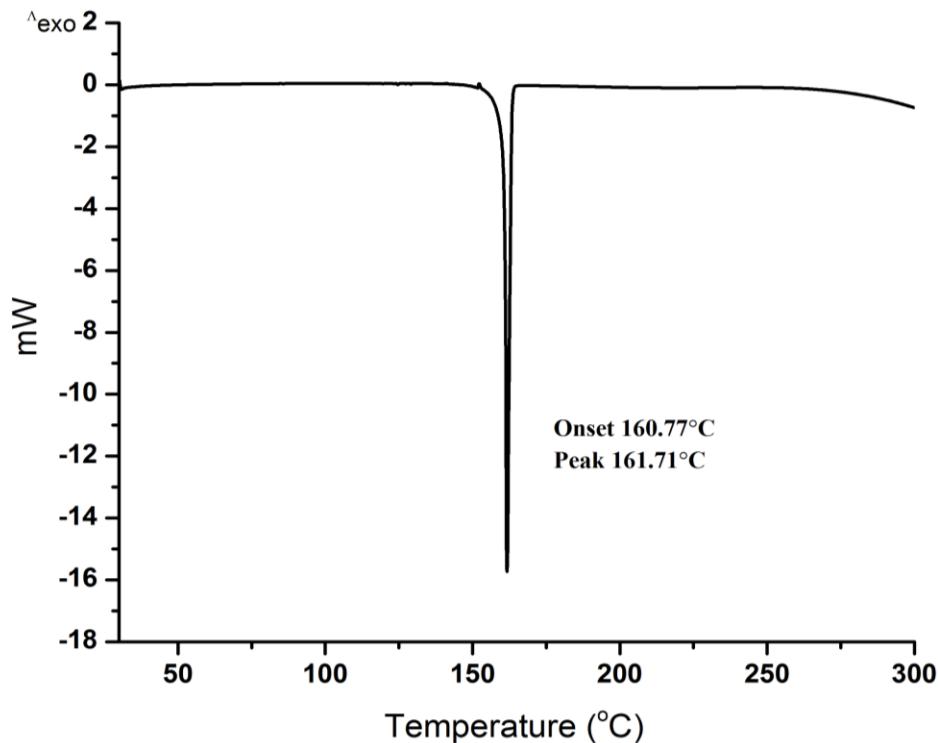
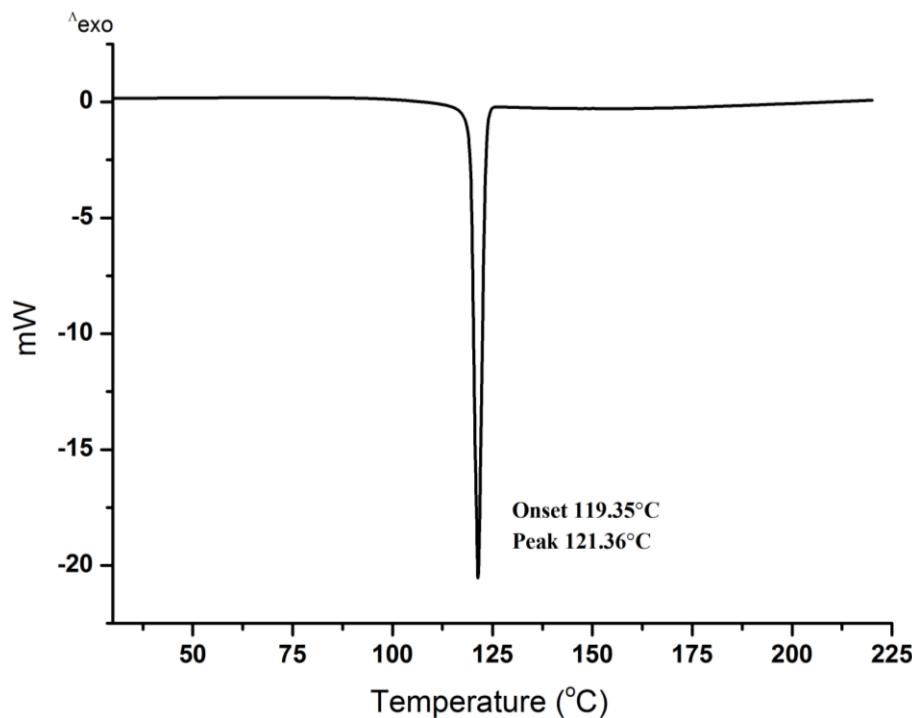


Figure S4 PXRD of CNT1.

S2. DSC of SA1, SA2, CO1, and CNT1.**Figure S5** DSC of SA1.**Figure S6** DSC of SA2.

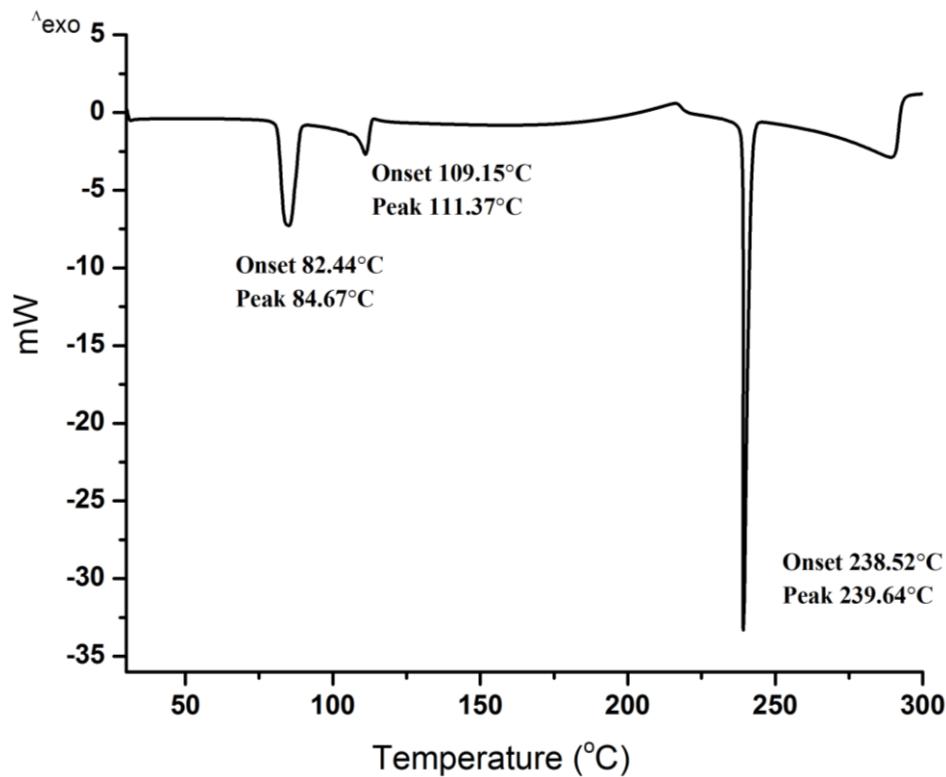


Figure S7 DSC of CO1.

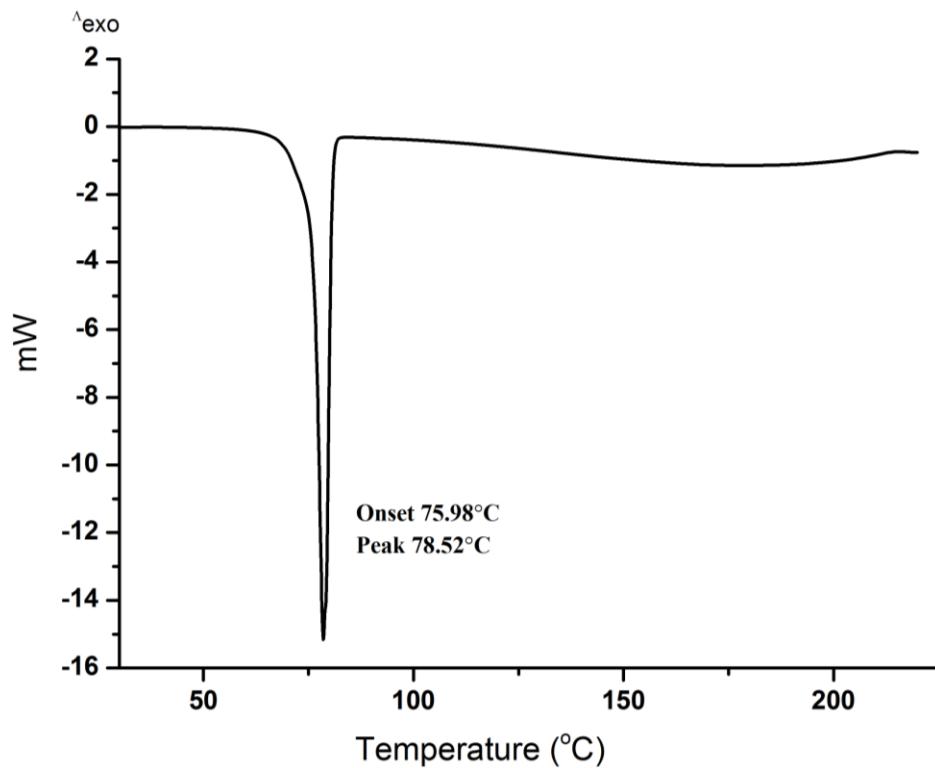


Figure S8 DSC of CNT1.

S3. FTIR of SA1, SA2, CO1, and CNT1

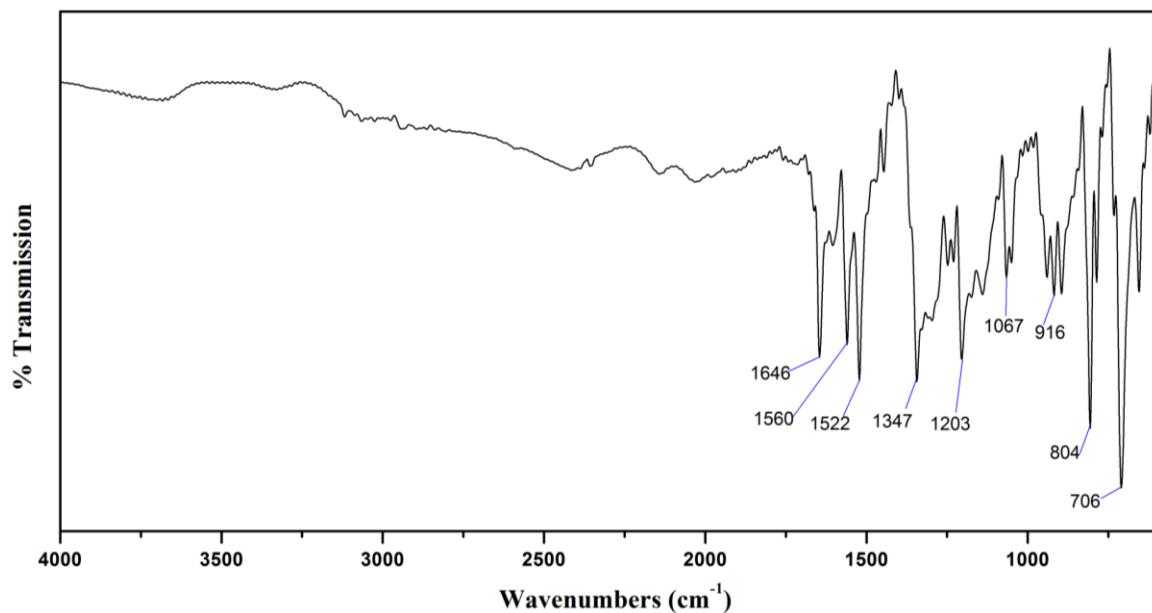


Figure S9 FTIR of SA1.

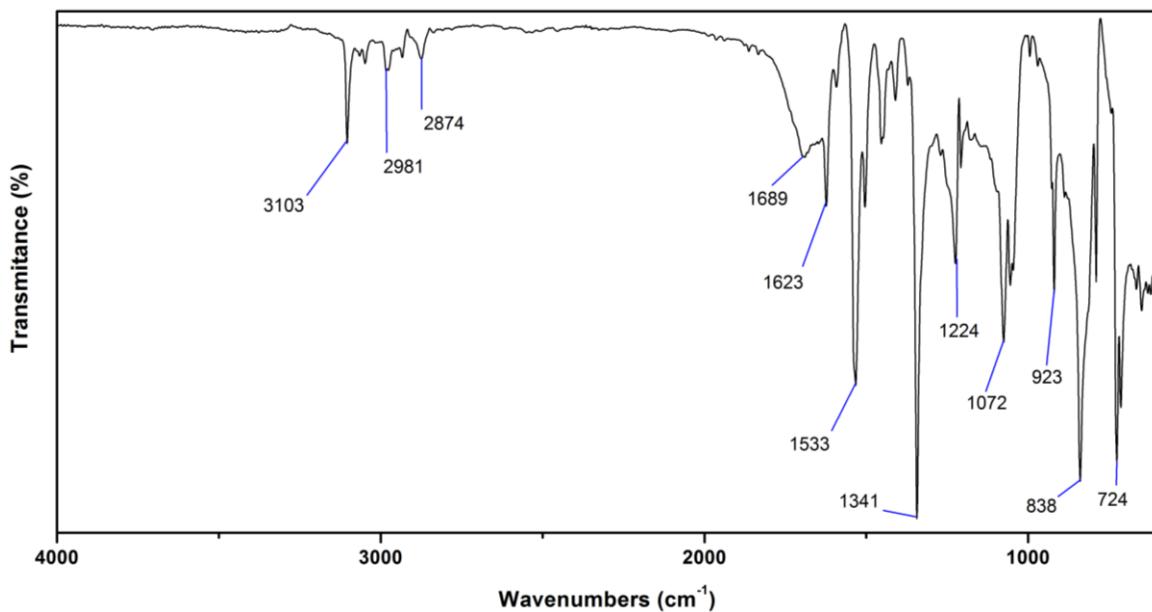


Figure S10 FTIR of SA2.

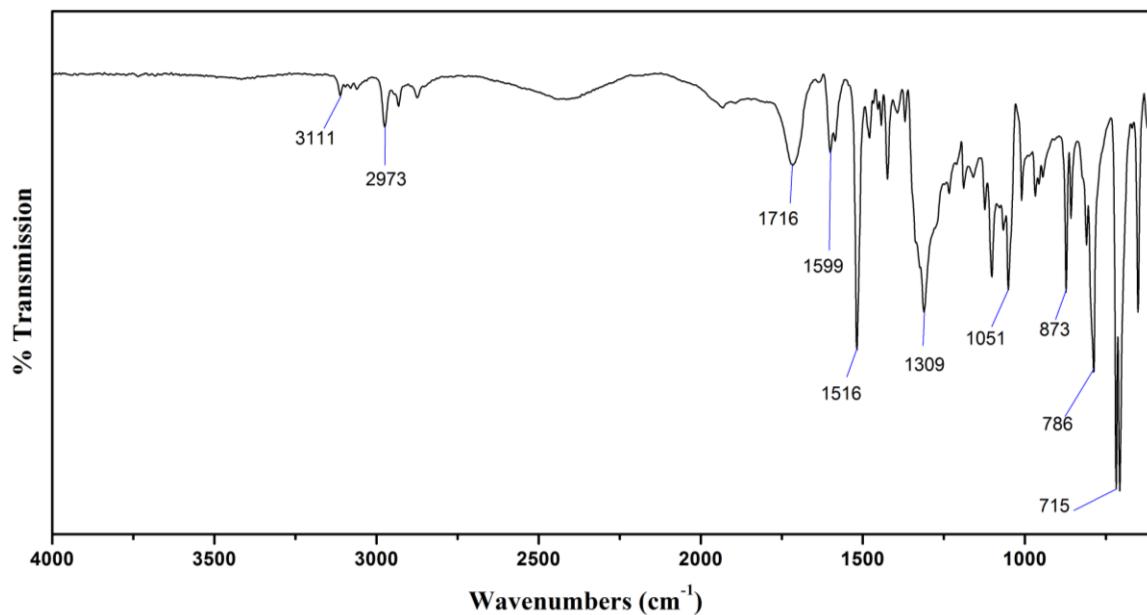


Figure S11 FTIR of CO1.

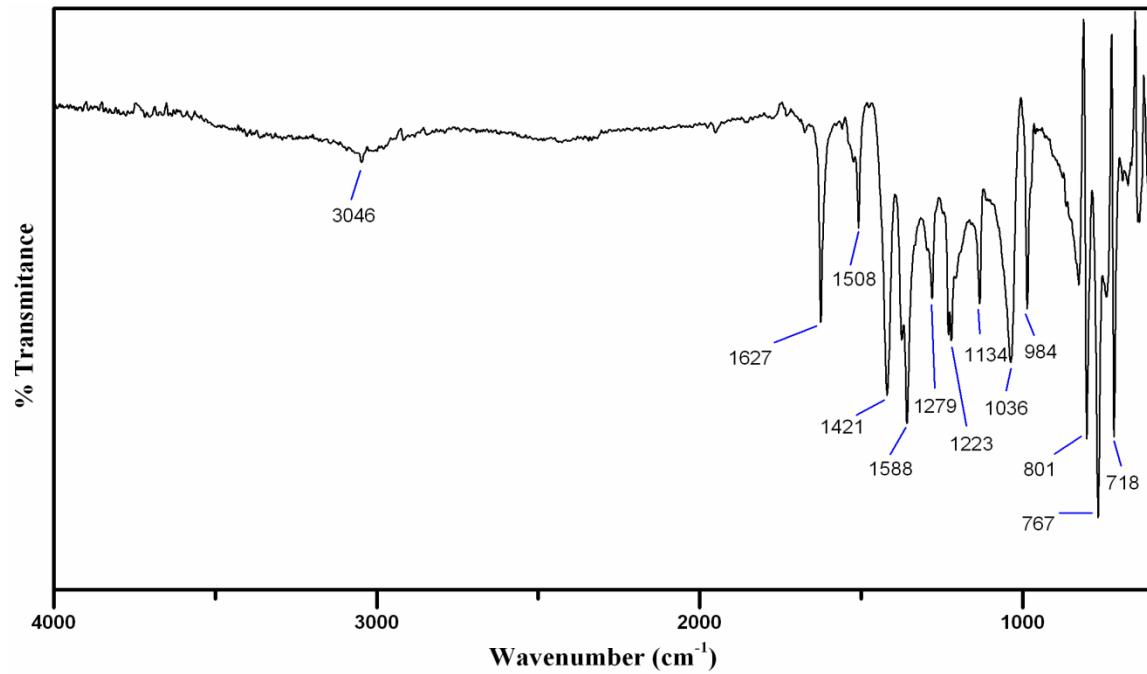


Figure S12 FTIR of CNT1.

S4. Hydrogen bonding parameters of SA1, SA2, CO1, and CNT1

Table S1 Hydrogen bond geometrical parameters (Rigaku) of **SA1, SA2, CO1, and CNT1**.

Compound	Interaction	D–H/ Å	H···A/ Å	D···A/ Å	∠D–H···A/ °	Symmetry
SA1(RT)	N(1)–H(1N)···O(2)	1.01(3)	1.60(3)	2.611(3)	176(2)	$1/2-x, 1/2+y, 1/2-z$
	C(1)–H(1)···O(1)	0.98(2)	2.46(2)	3.214(3)	133.1(2)	$1/2-x, 1/2+y, 1/2-z$
SA1(LT)	N(1)–H(1N)···O(2)	0.99(2)	1.62(2)	2.613(2)	177.3(2)	$1/2-x, -1/2+y, 1/2-z$
	C(1)–H(1)···O(1)	0.982(1)	2.478(1)	3.212(2)	131.3(1)	$1/2-x, -1/2+y, 1/2-z$
SA2(RT)	N(1)–H(1N)···O(1)	1.20(3)	1.35(3)	2.556(3)	178(3)	$-1+x, 1/2-y, 1/2+z$
	C(1)–H(1)···O(2)	0.93(2)	2.51(3)	3.197(4)	131(2)	$-1+x, 1/2-y, 1/2+z$
SA2(LT)	N(1)–H(1N)···O(1)	1.18(3)	1.37(3)	2.545(2)	179(3)	$x, 1/2-y, 1/2+z$
	C(1)–H(1)···O(2)	0.940(2)	2.443(2)	3.160(3)	133.1(1)	$x, 1/2-y, 1/2+z$
CO1(RT)	O(1)–H(1A)···N(1)	1.10(4)	1.54(4)	2.629(3)	171(3)	$1+x, y, z$
	C(1)–H(1)···O(2)	0.93(3)	2.41(3)	3.172(3)	140(2)	$-1+x, y, z$
CO1(LT)	O(1)–H(1A)···N(1)	1.06(3)	1.57(3)	2.620(3)	173(2)	$x, y, 1+z$
	C(1)–H(1)···O(2)	0.975(1)	2.374(2)	3.144(3)	135.4(1)	$x, y, -1+z$
CNT1(RT)	N(1)–H(1N)···O(1)	0.99(9)	1.66(1)	2.550(5)	148(9)	
CNT1(LT)	N(1)–H(1)···O(1)	1.17(6)	1.36(6)	2.525(4)	175(6)	

Table S2 Hydrogen bond geometrical parameters of **SA1**, **SA2**, **CO1**, and **CNT1** (O–H, N–H and C–H distances are neutron normalized).

Compound	Interaction	D–H/ Å	H···A/ Å	D···A/ Å	∠D–H···A/ °	Symmetry
SA1(RT)	N(1)–H(1N)···O(2)	1.01	1.60	2.611(3)	176	$1/2-x, 1/2+y, 1/2-z$
	C(1)–H(1)···O(1)	1.08	2.39	3.214(3)	131	$1/2-x, 1/2+y, 1/2-z$
SA1(LT)	N(1)–H(1N)···O(2)	1.01	1.60	2.613(2)	177	$1/2-x, -1/2+y, 1/2-z$
	C(1)–H(1)···O(1)	1.08	2.41	3.212(2)	130	$1/2-x, -1/2+y, 1/2-z$
SA2(RT)	N(1)–H(1N)···O(1)	1.01	1.55	2.556(3)	178	$-1+x, 1/2-y, 1/2+z$
	C(1)–H(1)···O(2)	1.08	2.42	3.197(4)	128	$-1+x, 1/2-y, 1/2+z$
SA2(LT)	N(1)–H(1N)···O(1)	1.01	1.54	2.545(2)	179	$x, 1/2-y, 1/2+z$
	C(1)–H(1)···O(2)	1.08	2.35	3.160(3)	131	$x, 1/2-y, 1/2+z$
CO1(RT)	O(1)–H(1A)···N(1)	0.98	1.65	2.629(3)	172	$1+x, y, z$
	C(1)–H(1)···O(2)	1.08	2.29	3.172(3)	137	$-1+x, y, z$
CO1(LT)	O(1)–H(1A)···N(1)	0.98	1.64	2.620(3)	173	$x, y, 1+z$
	C(1)–H(1)···O(2)	1.08	2.30	3.144(3)	134	$x, y, -1+z$
CNT1(RT)	N(1)–H(1N)···O(1)	1.01	1.64	2.550(5)	148	
CNT1(LT)	N(1)–H(1N)···O(1)	1.01	1.52	2.525(4)	176	

Table S3 Hydrogen bond geometrical parameters (Bruker) of **CNT1**.

Compound	Interaction	D–H/ Å	H···A/ Å	D···A/ Å	∠D–H···A/ °	Symmetry
CNT1(RT)	O(1)–H(1)···N(1)	0.91(5)	1.65(5)	2.548(4)	170(5)	$-1+x, y, z$
CNT1(LT)	O(1)–H(1)···N(1)	1.13(5)	1.40(5)	2.523(4)	175(5)	

Table S4 Hydrogen bond geometrical parameters (Bruker) of **CNT1** (O–H, N–H and C–H distances are neutron normalized).

Compound	Interaction	D–H/Å	H···A/Å	D···A/Å	∠D–H···A/°	Symmetry
CNT1(RT)	O(1)–H(1)···N(1)	0.98	1.58	2.548(4)	169	-1+x,y,z
CNT1(LT)	N(1)–H(1)···O(1)	0.98	1.54	2.523(4)	175	

S5. ORTEP diagram for SA1, SA2, CO1, and CNT1 (Rigaku)

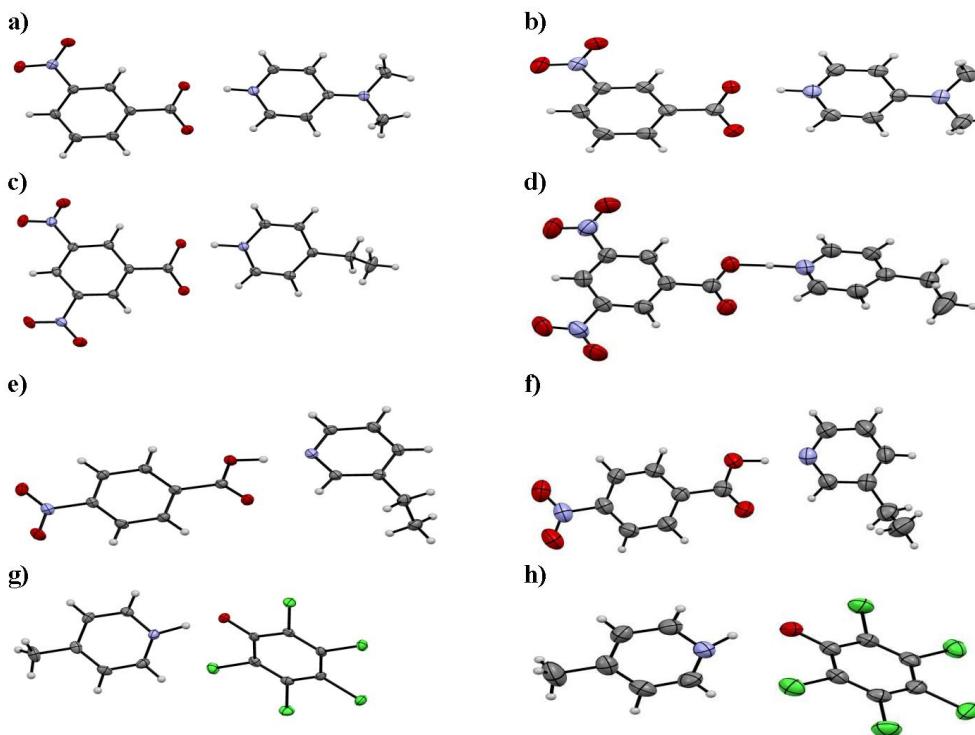


Figure S13 a) **SA1** at -163 °C, b) **SA1** at 25 °C, c) **SA2** at -163 °C, d) **SA2** at 25 °C, e) **CO1** at -163 °C, f) **CO1** at 25 °C, g) **CNT1** at -163 °C, h) **CNT1** at 25 °C.

S6. Calculated invCP-VC spectra of CO1

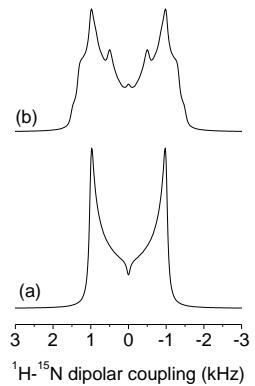


Figure S14 Calculated invCP-VC spectra of **CO1** (a) include only nearest $^1\text{H}-^{15}\text{N}$ interactions and (b) include three $^1\text{H}-^{15}\text{N}$ interactions.

S7. ssNMR 1D spectra of SA1, SA2, CO1, and CNT1

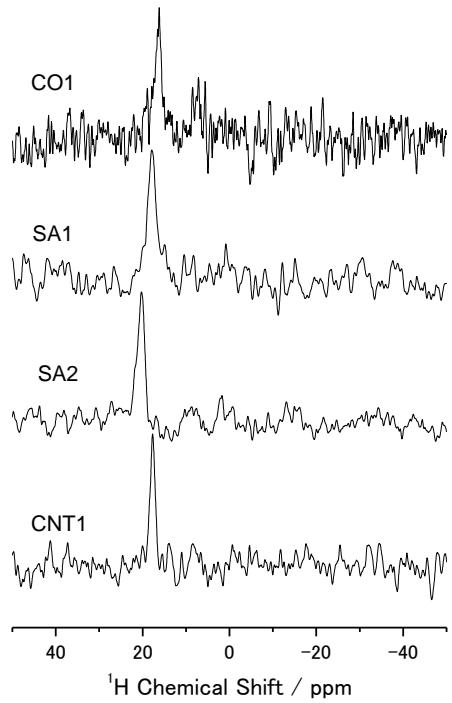


Figure S15 $^1\text{H} \rightarrow ^{15}\text{N} \rightarrow ^1\text{H}$ filtered 1H NMR spectra of **CO1**, **SA1**, **SA2**, and **CNT1**. The spectra are obtained by summing the CP-VC spectra with a contact time $< 300 \mu\text{s}$ to remove the remote magnetization transfer.