Electronic Supplementary Material (ESI) for CrystEngComm.
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Supplementary information

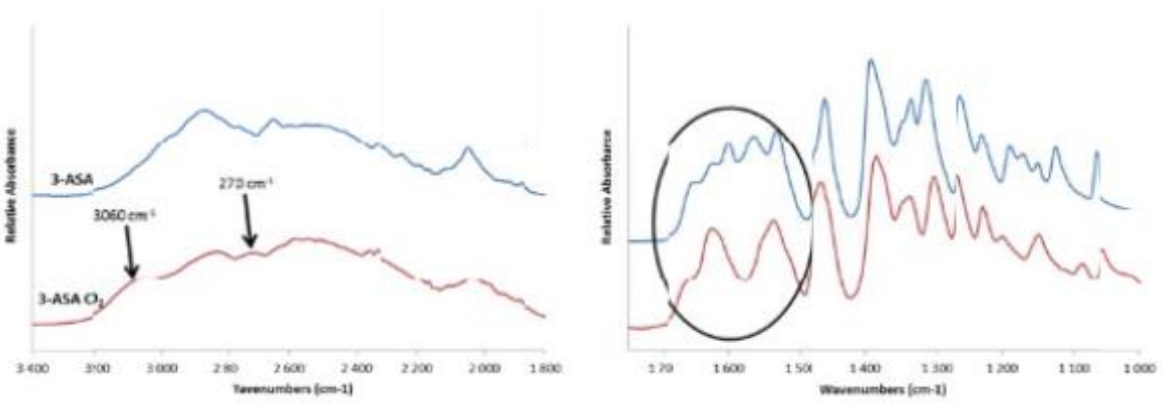


Fig. S1. ATR-FTI**R** spectra of raw 3-AS**A** and CO_2 recrystalliz**e**d 3-ASA. **M**ain differ**e**nces are highlig**h**ted.

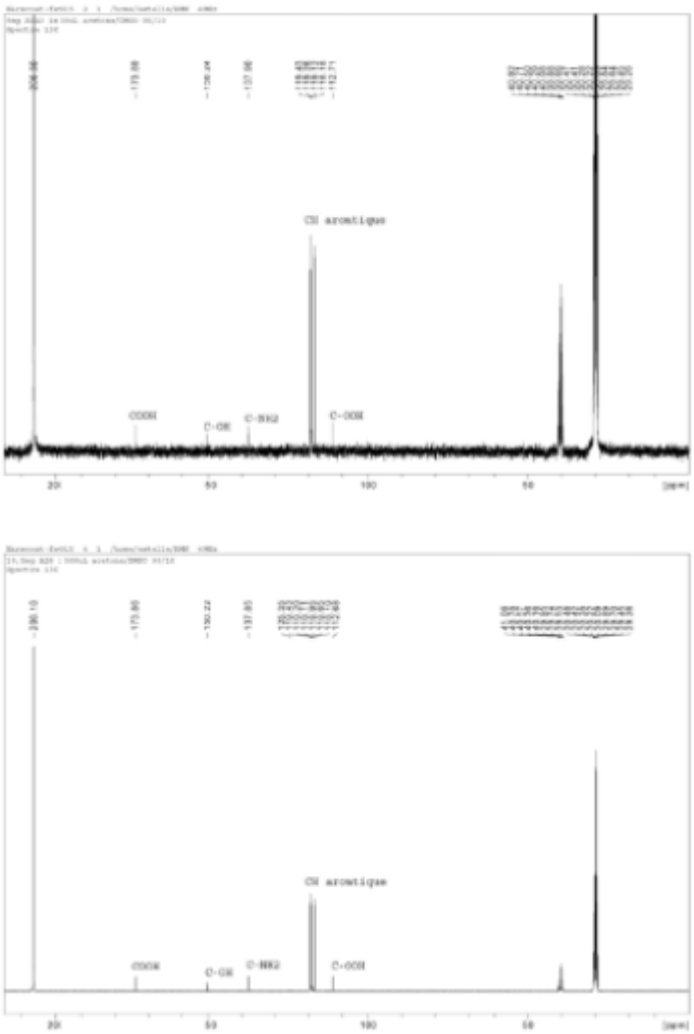
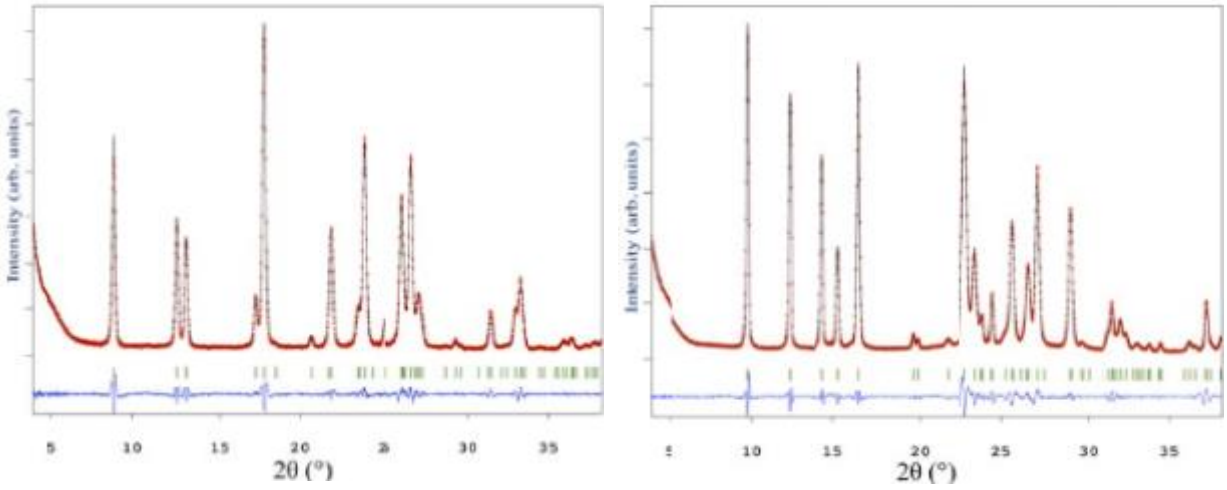


Fig. S2. Carbon N**M**R spectra of raw 3-ASA (top) and CO_2 recrystall**i**zed 3-ASA (bottom)



(a) (b)

Fig. S3. Profile ma**t**ching of ra**w** and CO_2 recrystallize**d** 3-ASA, o**p**en red circ**l**es corresp**o**nd to the experim**e**ntal PXR**D** pattern, bl**a**ck continu**o**us line represent the calculated pat**t**ern (LeBail method) from the refined **c**ell parameters, green **v**ertical lin**e**s are pred**i**cted Bragg positions **a**nd blue continu**o**us line is **t**he difference between experimen**t**al and calc**u**lated patt**er**ns. (a) ra**w** 3-ASA (backgr**o**und correct**e**d Rwp = 0.099) and (b**)** CO_2 recrys**t**allized 3-A**S**A (backgr**o**und correct**e**d Rwp = 0.088)

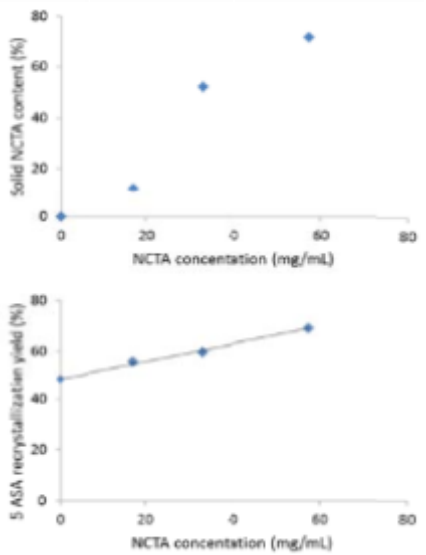


Fig. S4. Influence of NCTA coñcentrat**i**on on the product c**o**mposition (a:top) an**d** on the recrystal**l**ization of **5**-ASA (b:bo**t**tom). GAS **r**ecrystallizat**i**on from acetone:DMS**O** at 36°C a**n**d P_{final} of 11 MPa. Solution of 5-ASA (C=17 mg/mL) **a**nd NCTA (**0** to 57mg/**m**L).

Table S1. Crystal data and structure refinement for **1**

Empirical formula	$C_7H_7NO_3$
Formula weight g.mol^{-1}	153.14
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.2375(9)
b/Å	4.5168(5)
c/Å	14.7924(13)
β/°	107.394(8)
Volume/Å^3	652.73(11)
Z	4
ρ_{calc}g/cm^3	1.558
μ/mm^{-1}	1.053
F(000)	320.0
Crystal size/mm^3	0.05 × 0.02 × 0.02
Radiation	CuKα (λ = 1.54187)
2Θ range for data collection/°	13.096 to 135.462
Index ranges	$-11 \leq h \leq 12$, $-5 \leq k \leq 3$, $-16 \leq l \leq 17$
Reflections collected	3676
Independent reflections	1174 [R_{int} = 0.0524, R_{sigma} = 0.0778]
Data/restraints/parameters	1174/0/119
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0673, wR_2 = 0.1696
Final R indexes [all data]	R_1 = 0.0995, wR_2 = 0.2268
Largest diff. peak/hole / e Å^{-3}	0.41/-0.35

Table S2. Selected bond Lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C2	1.346(4)	C3	C7	1.487(4)
O2	C7	1.283(4)	C3	C4	1.401(5)
O3	C7	1.264(4)	C1	C6	1.383(5)
N1	C1	1.453(4)	C4	C5	1.377(5)
C2	C3	1.403(4)	C6	C5	1.390(5)
C2	C1	1.399(5)			

Table S3. Hydrogen Bonds for **1**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1	H1	O2	1.00(4)	1.68(4)	2.548(3)	143(3)
N1	H1A	O3[1]	1.02(4)	1.77(4)	2.784(4)	177(3)
N1	H1B	O3[2]	0.98(4)	1.77(4)	2.737(4)	169(3)
N1	H1C	O2[3]	0.88(4)	1.95(4)	2.826(4)	173(4)

[1]+X,3/2-Y,-1/2+Z; [2]+X,1/2-Y,-1/2+Z; [3]-X,1/2+Y,1/2-Z