Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Room temperature synthesis of $CuInS_2$ nanocrystals

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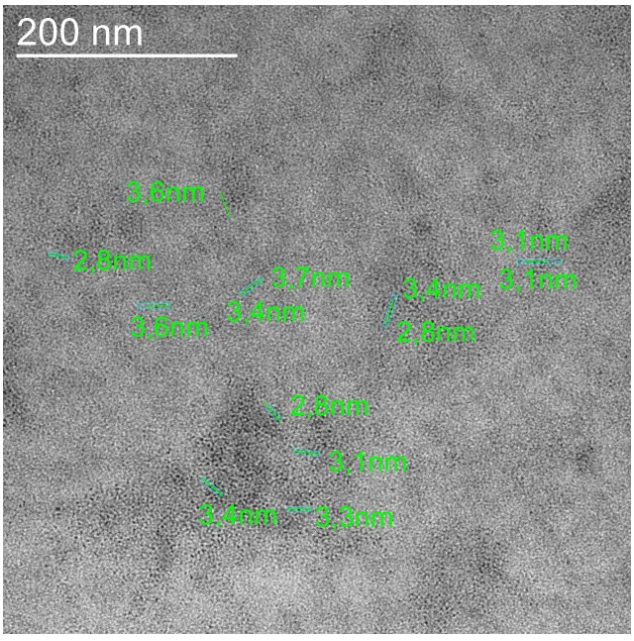

Fig. S1 TEM image of the synthesized $CuInS_2$ nanocrystals and corresponding particle sizes.

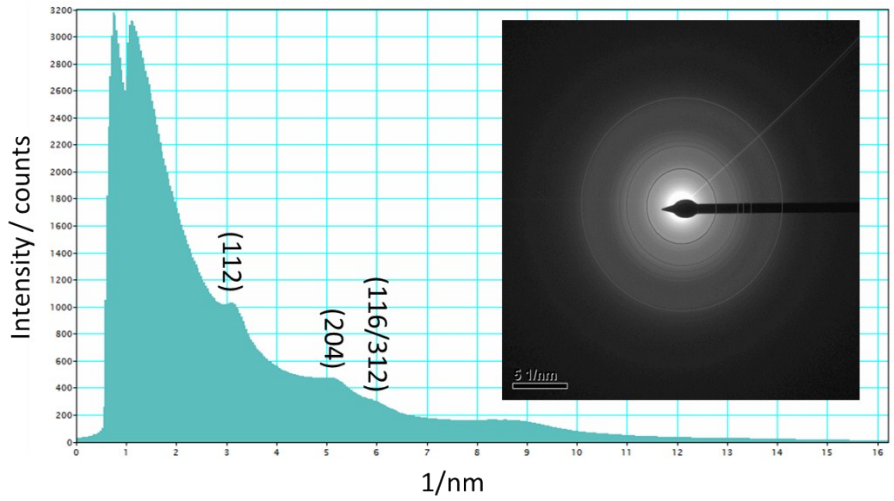

Fig. S2 SAED pattern and the corresponding radial intensity profile of the $CuInS_2$ nanocrystals.

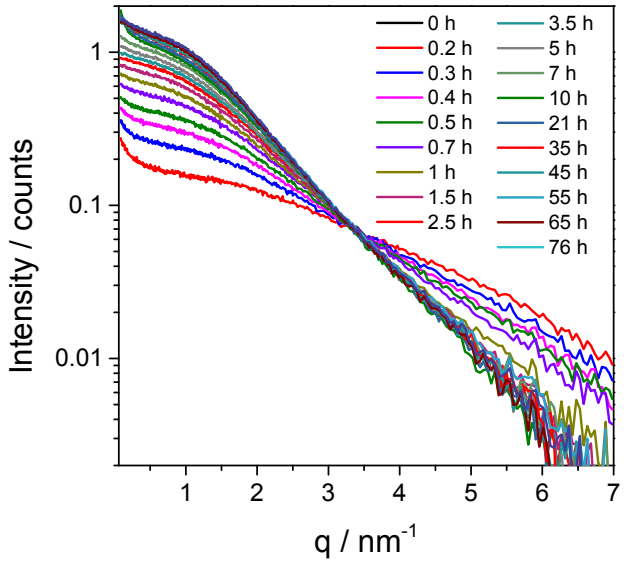

Fig. S3 SAXS data of a time resolved measurement during a synthesis performed directly in the measurement capillary.

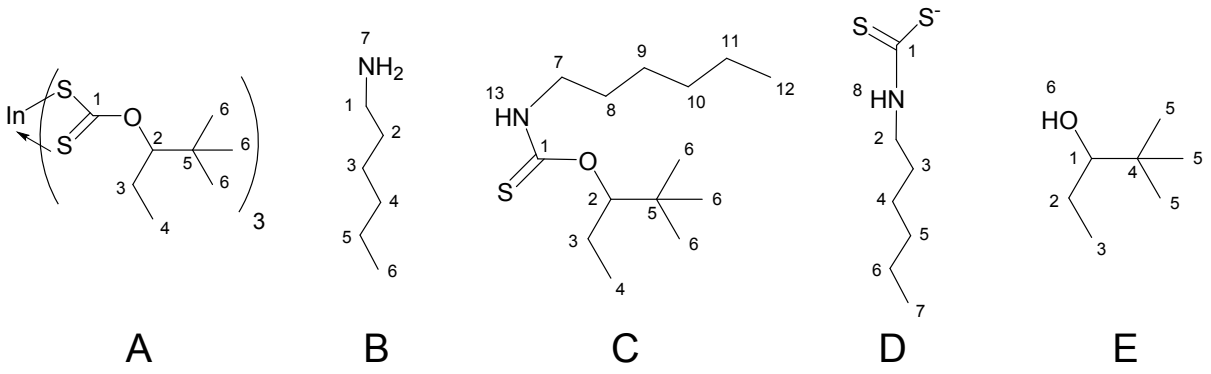

Fig. S4 Chemical structures auf educts (indium xanthate A, hexylamine B) and reaction products (thiocarbamate C, dithiocarbamate D, alcohol E) and labelling of the carbon/hydrogen atoms used in Tables S1 and S2.

Table S1 ^{1}H NMR spectroscopic data – indium xanthate/hexylamine model reaction

In xanthate (A) [ppm]	hexylamine (B) [ppm]	thiocarbamate isomers (C) [ppm]	dithiocarbamate (D) [ppm]	alcohol (E) [ppm]
A2: 4.75 (t ; 1H)	B1: 2.68 (t ; 2H)	C2: 5.36 (dd)	D2: 3.45 (t)	E1: 3.10 (dd; 1H)
A3: 1.76 (m ; 2H)	B2: 1.44 (m ; 2H)	C3: 1.72; 1.53	D3: 1.64	E2: 1.22 (m ; 1H)
A4: 1.02 (t ; 3H)	B3: 1.29 (br ; 2H)	C4: 0.98	D4: 1.30	1.56 (m ; 1H)
A6: 0.99 (s ; 9H)	B4: 1.29 (br ; 2H)	C6: 0.98; 0.92	D5: 1.30	E3: 0.99 (t ; 3H)
	B5: 1.29 (br ; 2H)	C7: 3.30; 3.58	D6: 1.30	E5: 0.87 (s ; 9H)
	B6: 0.89 (t ; 3H)	C8: 1.60; 1.50	D7: 0.90	E6: 1.51 (s ; 1H)
	B7: 1.07 (br ; 2H)	C9: 1.30	D8: 7.69 (br)	
		C10: 1.30		
		C11: 1.30		
		C12: 0.89		
		C13: 6.80; 6.30		

Table S2 ^{13}C NMR spectroscopic data – indium xanthate/hexylamine model reaction

In xanthate (A) [ppm]	hexylamine (B) [ppm]	thiocarbamate isomers (C) [ppm]	dithiocarbamate (D) [ppm]	alcohol (E) [ppm]
A1: 230.9	B1: 42.4	C1: 191.7; 190.9	D1: 205.2	E1: 81.8
A2: 103.2	B2: 34.0	C2: 90.7; 88.1	D2: 51.1	E2: 24.3
A3: 23.5	B3: 26.7	C3: 23.1; 23.3	D3: 27.8	E3: 11.6
A4: 11.1	B4: 31.8	C4: 11.0; 11.2		E4: 35.0
A5: 36.2	B5: 22.7	C5: 35.9; 35.4	other peaks are	E5: 25.8
A6: 26.1	B6: 14.1	C6: 26.2; 26.5	overlapping with	
		C7: 45.3; 43.1	C, B, and E	
		C8: 29.3; 28.7		
		C9: 26.5		
		C10: 31.5		
		C11: 22.6		
		C12: 14.0		

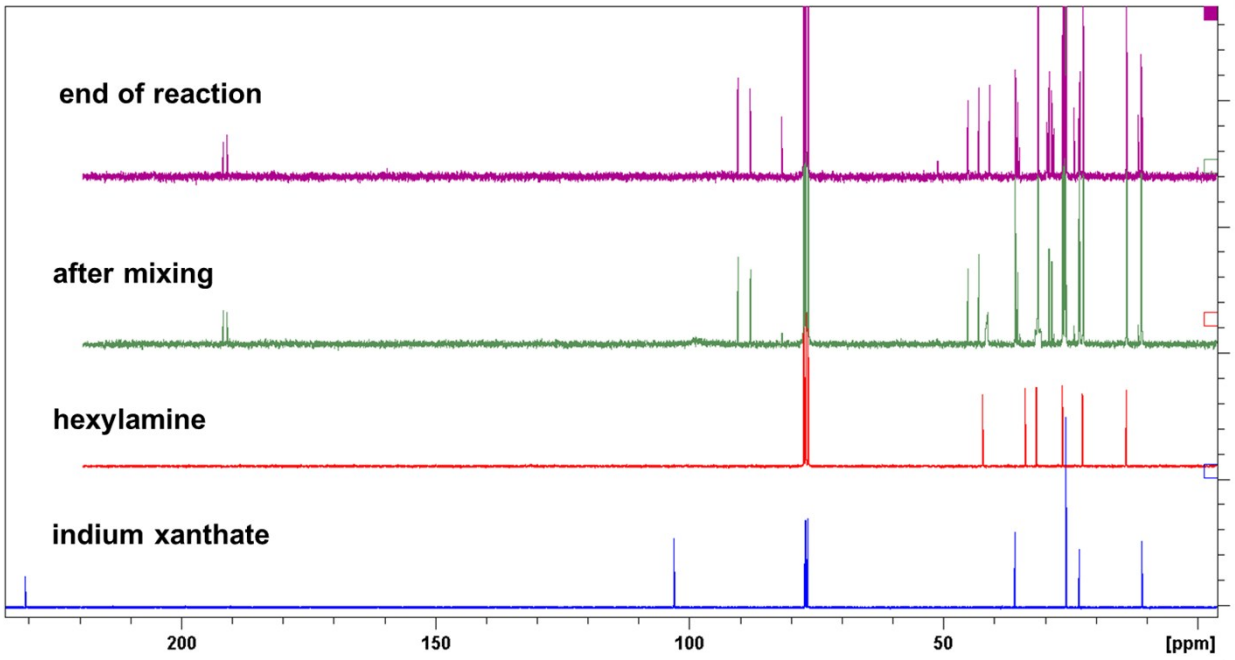

Fig. S5 ^{13}C NMR spectra of the pure educts indium xanthate and hexylamine, and spectra of the reaction shortly after mixing and at the end of the reaction (corresponding ^{1}H NMR spectra can be found in the main text of the article).

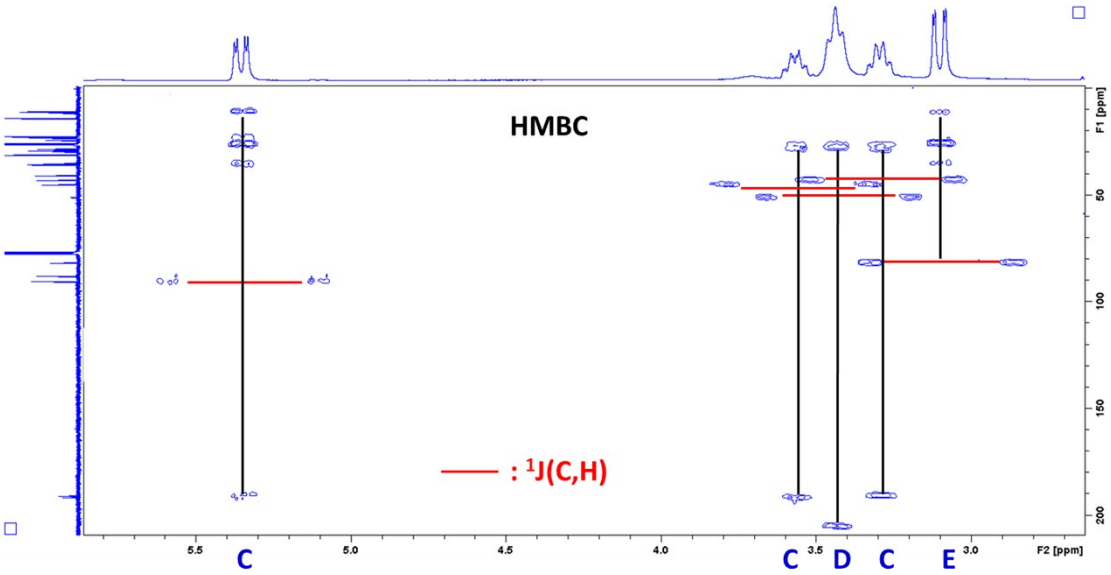

Fig. S6 Heteronuclear Multiple Bond Correlation (HMBC) NMR spectrum (^{13}C, ^{1}H) used for the identification of the reaction products by visualization of long-range couplings.

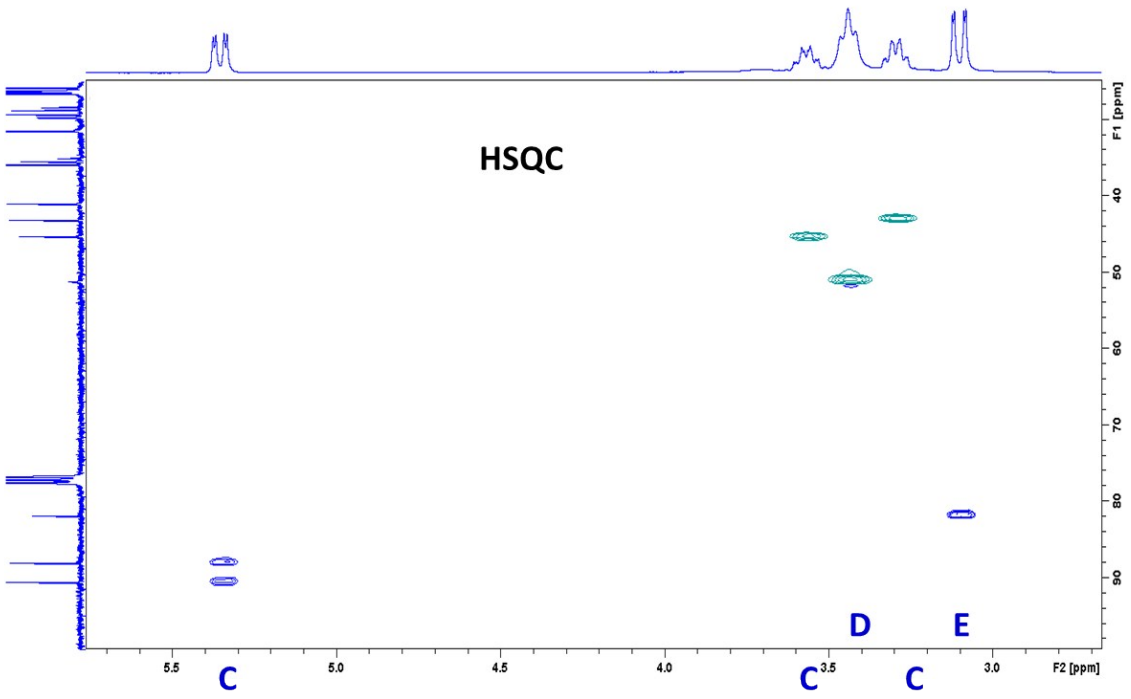

Fig. S7 Heteronuclear Single Quantum Coherence (HSQC) NMR spectrum (^{13}C, ^{1}H) used for the identification of the reaction products by visualization of direct ^{1}H-^{13}C coupling.

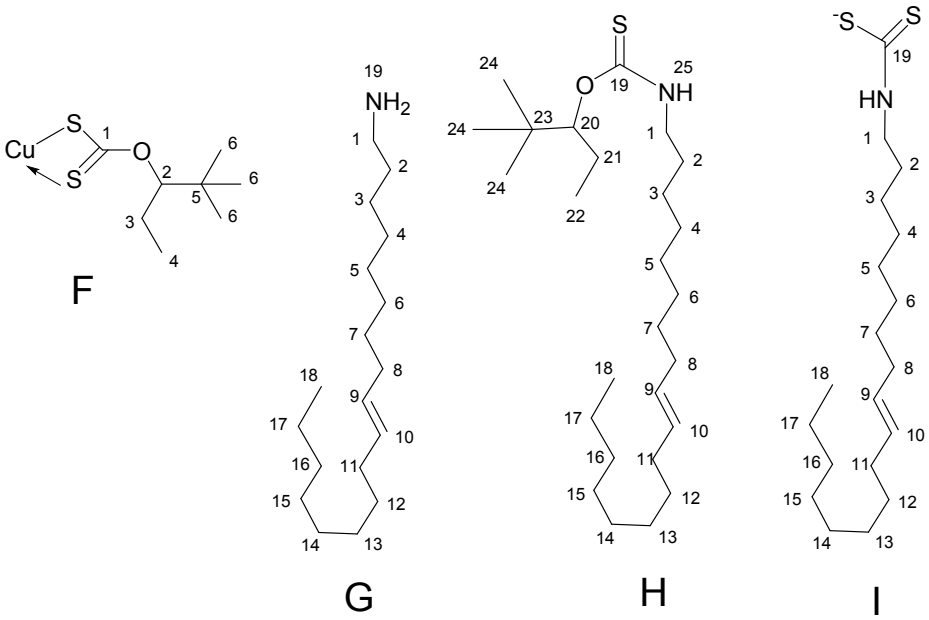

Fig. S8 Chemical structures of educts (copper xanthate F, oleylamine G) and reaction products (thiocarbamate H, dithiocarbamate I, alcohol E) and labelling of the carbon/hydrogen atoms used in Tables S3 and S4.

Table S3 ^{1}H NMR spectroscopic data - Cu/In xanthates - oleylamine

Cu xanthate (F) [ppm]	Cu/In xanthate* (A/F) [ppm]	oleylamine (G) [ppm]	thiocarbamate isomers (H) [ppm]	dithiocarbamate (I) [ppm]
F2: 5.24 (t ; 1H)	AF2: 5.04 (t ; 1H)	G1: 2.64 (t ; 2H)	H25: 6.78; 6.28	H1: 3.46
F3: 1.73 (m ; 2H)	AF3: 1.72 (m; 2H)	G2: 1.40 (m, 2H)	H1: 3.27; 3.55	
F4: 0.93 (t ; 3H)	AF4,6: 1.00 – 0.95 (bs : 12 H)	G3,4,5,6,7,12,13,14,15, 16,17: 1.35-1,15 (m, 22H)	H20: ~5.36 (**)	
F6: 0.95 (s ; 9H)		G8/11: 1.99 (m ; 4H)	all other peaks are overlapping with peaks stemming from oleylamine G, dithiocarbamate I, and alcohol E	all other peaks are overlapping with peaks stemming from oleylamine G, thiocarbamate H and alcohol E
		G9/10: 5.32 (m ;2H)		
		G18: 0.85 (t ; 3H)		
		G19: 1.03 (bs ; 2H)		

***** peaks observed during reaction (reaction time 10 min)

** peak overlaid by oleylamine G9/10 protons

Table S4 ^{13}C NMR spectroscopic data - Cu/In xanthates – oleylamine

Cu xanthate (F) [ppm]	Cu/In xanthate* (A/F) [ppm]	oleylamine** (G) [ppm]	thiocarbamate isomers (H) [ppm]	dithiocarbamate (I) [ppm]
F1: 230.4	AF1: 230 (b)	G1: 41.9	C19: 191.8 ; 191.0	C19: 206 (br)
F2: 98.9	AF2: 98 (b)	G2: 33.2	C20: 90.5 ; 88.9	C1: 51.5
		G9/10: 130.0,	C1: 45.3 ; 43.1	
F3: 23.5	AF3: 23	129.8		
F4: 11.3	AF4: 11	G17: 22.6		
F5: 36.6	AF5: 36.5	G18: 14.0	all other peaks are overlapping with G, I and F	all other peaks are overlapping with G, H and F
		G3-8, G11-16: 31.9, 29.8, 29.75, 29.72, 29.67, 29.58, 29.46, 29.33, 29.31, 29.25, 27.27,		
F6: 26.2	AF6: 26	26.11		

***** peaks observed during the reaction (reaction time 10 min)

****** main peaks, additional small peaks by small amounts of isomers and byproducts

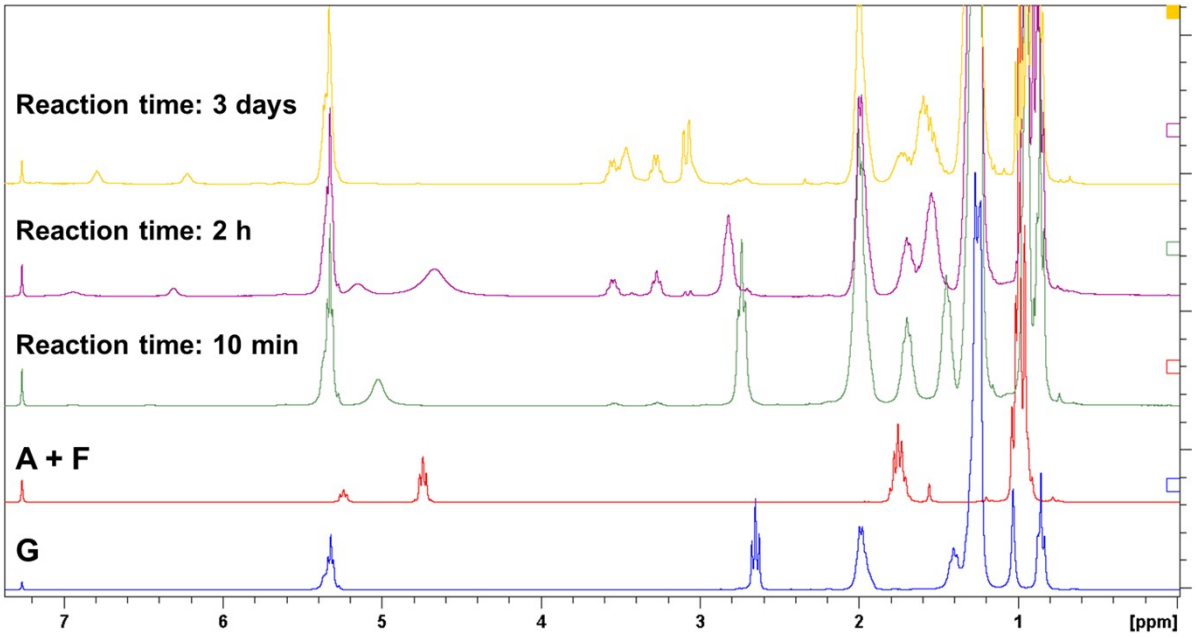

Fig. S9 ^{1}H NMR spectra of oleylamine (G), a mixture of indium and copper xanthate (A + F) and of the reaction mixture comprising of the metal xanthates and oleylamine after different reaction times.

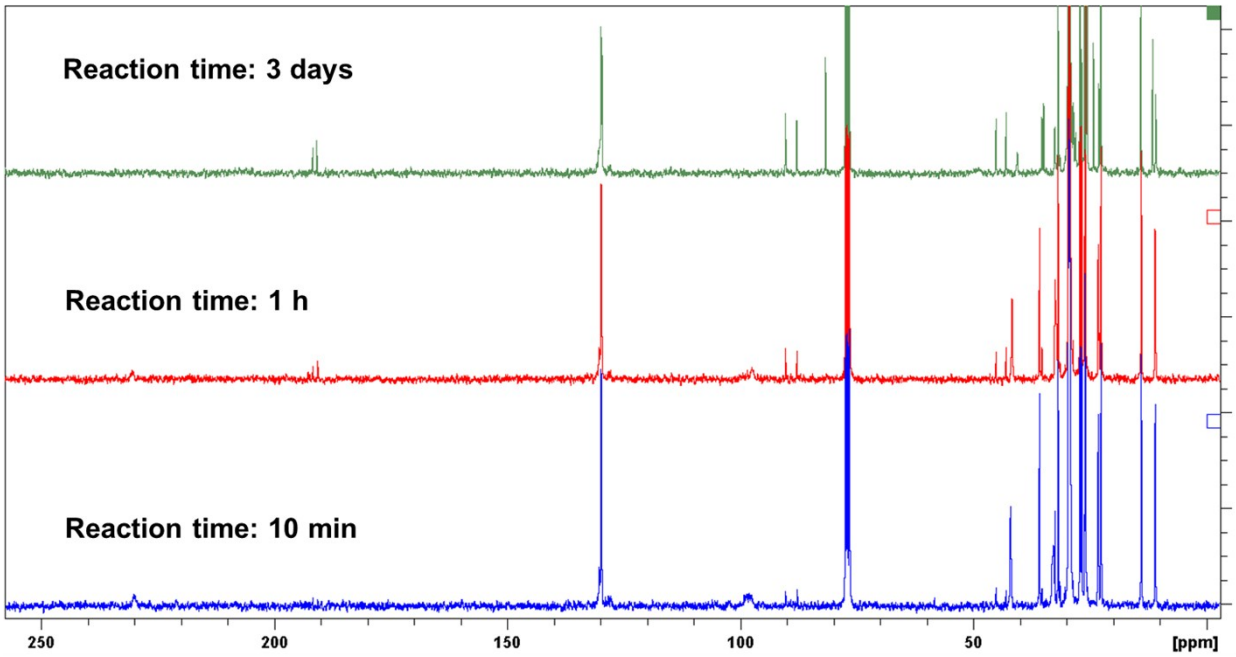

Fig. S10 ^{13}C NMR spectra of the reaction mixture (metal xanthates and oleylamine) after different reaction times.