Supplementary information

Boosting PVC Reactivity through Iodination for CO_2-Derived Functionalization

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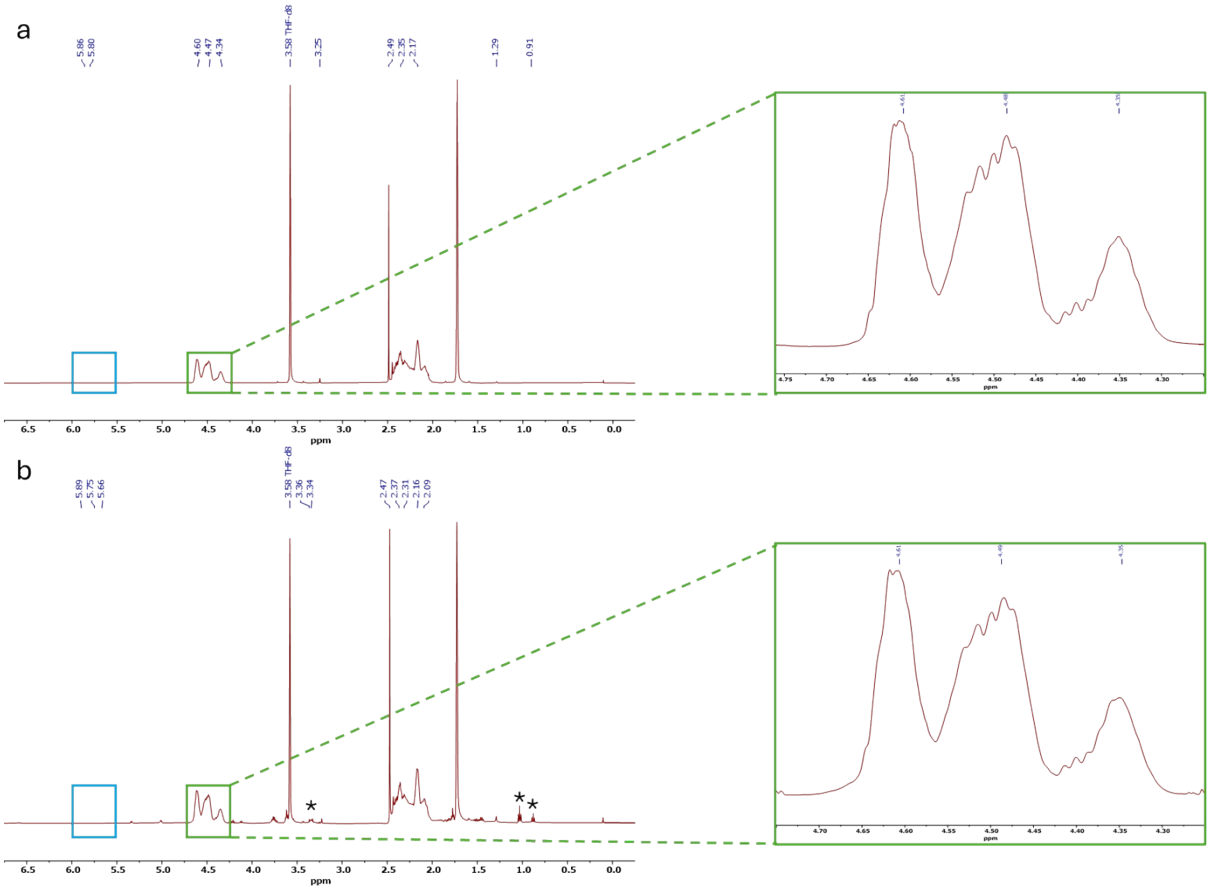
Table des matières

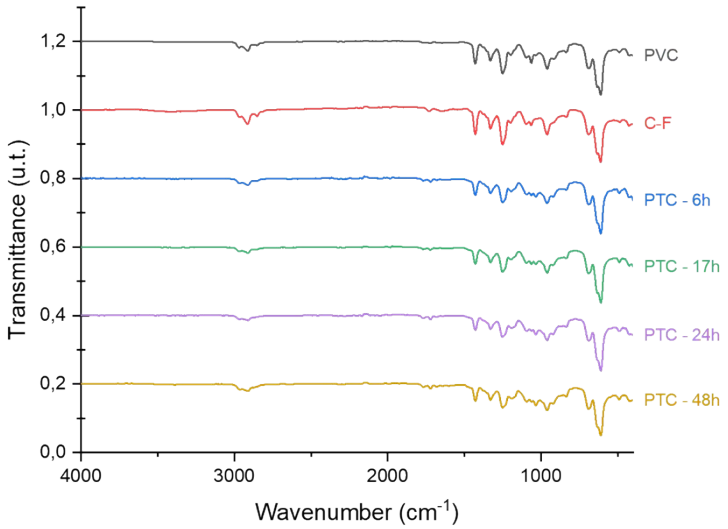
1. PVC iodination

a. Nuclear Magnetic Resonance



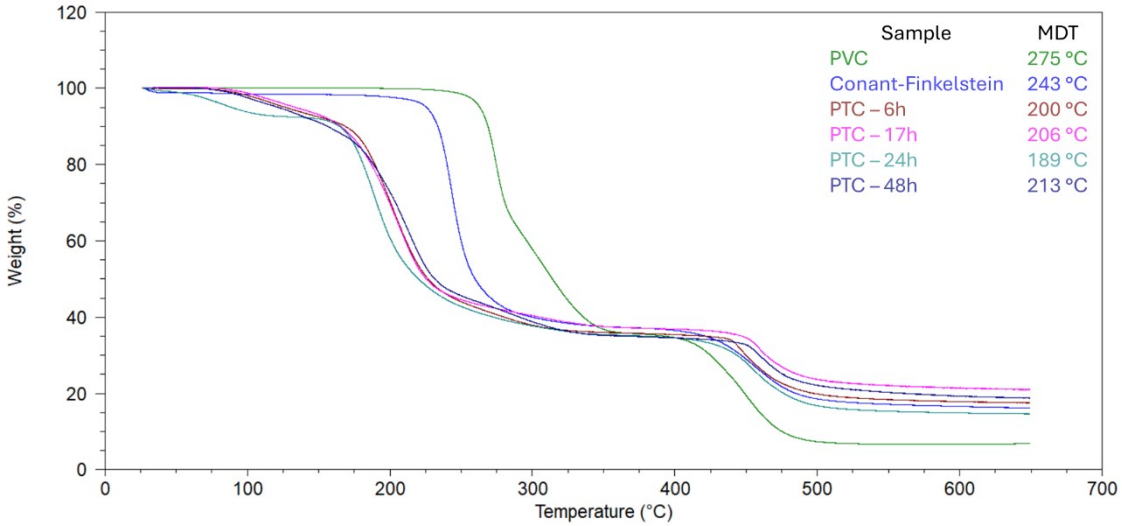
Supplementary Figure S1 – ^{1}H NMR spectra of a) PVC and b) PVC iodinated via phase-transfer catalysis for 24h. The remaining TBAB in b) is designated by asterisks (*).

b. Fourier Transform Infrared Spectroscopy



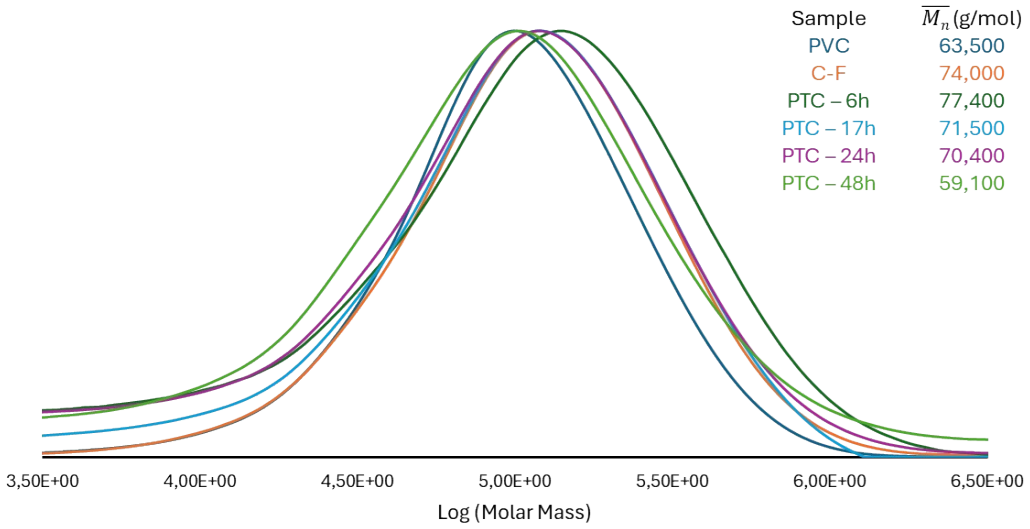
Supplementary Figure S2 – FT-IR of PVC and modified PVC samples iodinated via the Conant-Finkelstein reaction (C-F) or phase transfer catalysis (PTC) for 6, 17, 24, or 48 hours.

c. Thermogravimetric Analysis



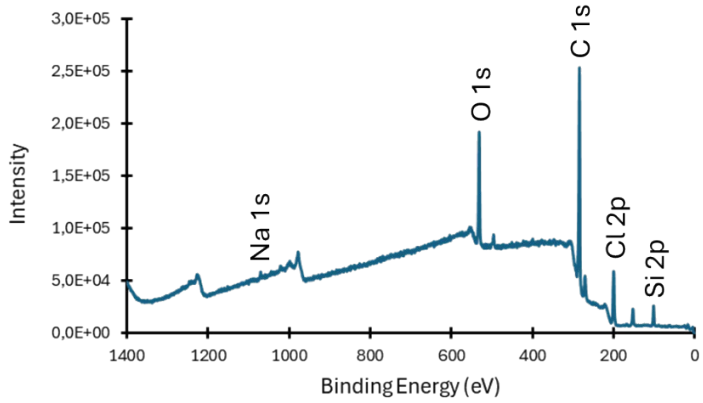
Supplementary Figure S3 – TGA of PVC and modified PVC samples iodinated via the Conant-Finkelstein reaction (C-F) or phase transfer catalysis (PTC) for 6, 17, 24, or 48 hours.

d. Size Exclusion Chromatography

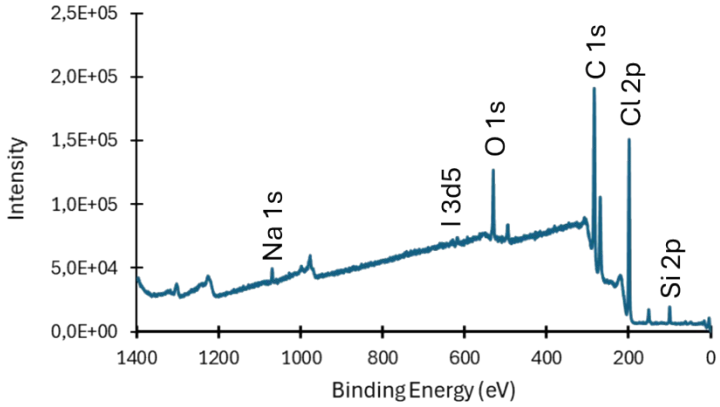


Supplementary Figure S4 – SEC traces of PVC and modified PVC samples iodinated via the Conant-Finkelstein reaction (C-F) or phase transfer catalysis (PTC) for 6, 17, 24, or 48 hours.

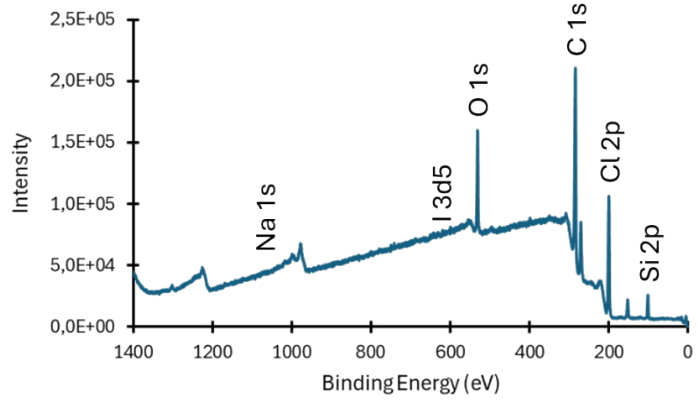
e. X-ray Photoelectron Spectroscopy



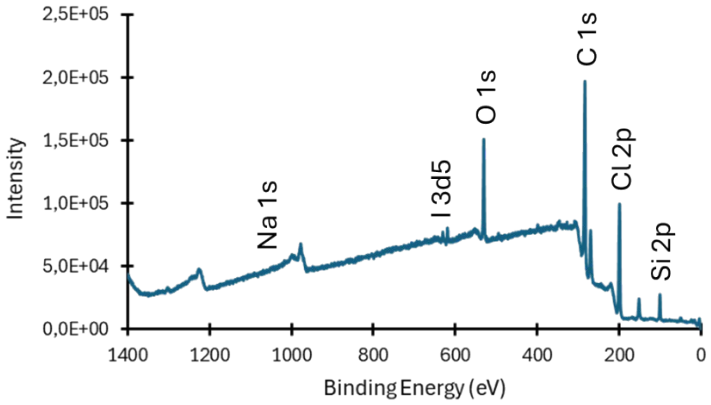
Supplementary Figure S5 – XPS spectrum of PVC.



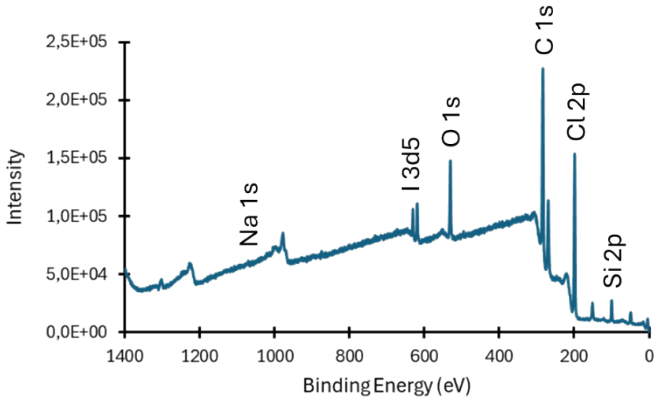
Supplementary Figure S6 – XPS spectrum of PVC iodinated via the Conant-Finkelstein reaction.



Supplementary Figure S7 – XPS spectrum of PVC iodinated via phase transfer catalysis for 6 hours.

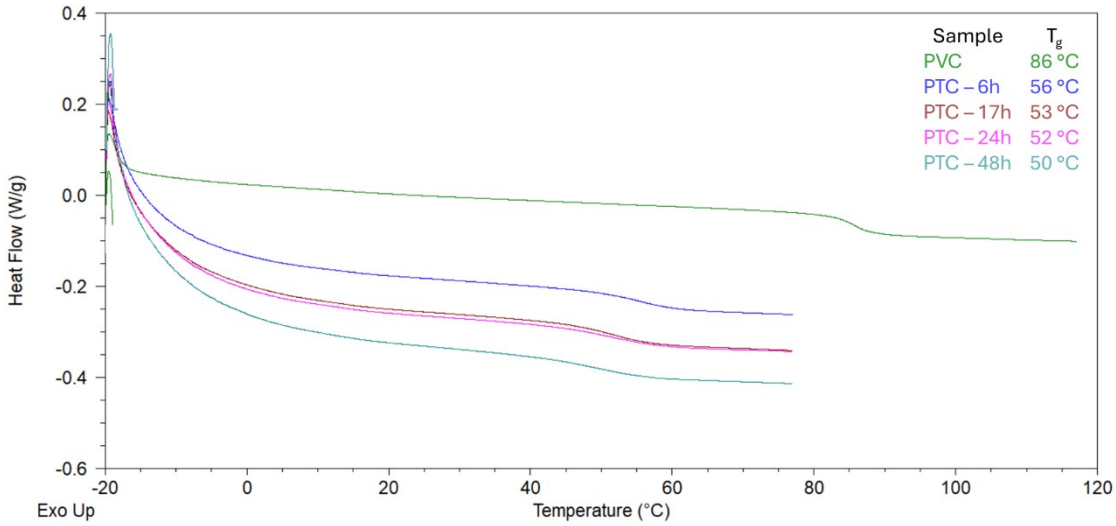


Supplementary Figure S8 – XPS spectrum of PVC iodinated via phase transfer catalysis for 17 hours.



Supplementary Figure S9 – XPS spectrum of PVC iodinated via phase transfer catalysis for 24 hours.

f. Differential Scanning Calorimetry



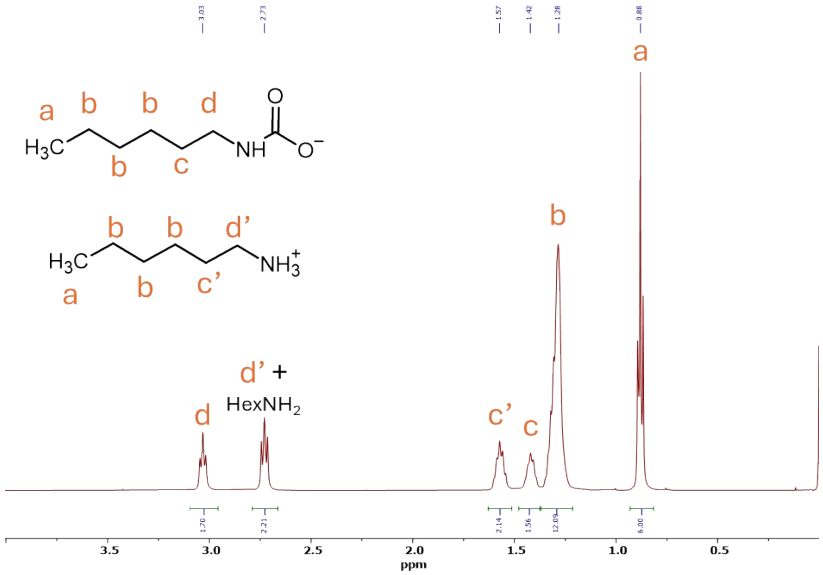
Supplementary Figure S10 – DSC of PVC and modified PVC samples iodinated via phase transfer catalysis (PTC) for 6, 17, 24, or 48 hours.

g. **Supplementary Table S1 –** Summary of physicochemical and thermal properties of pristine and iodinated PVC samples.

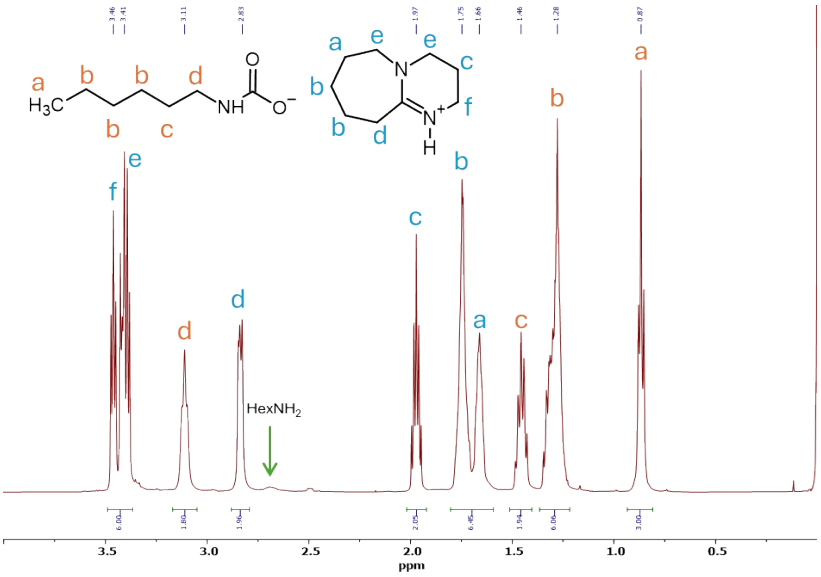
	Method	*t (h)*	*MDT (°C)*	*$\bar{M}_n$ (g/mol)*	*C 1s (at%)*	*Cl 2p (at%)*	*I 3d5 (at%)*	*Na 1s (at%)*	*T_g (°C)*	*Contact angle (°)*
1	PVC	0	275	63,500	73.52	6.53	0	0.49	86	85.6 ± 1.7
2	C-F	24	243	74,000	67.30	19.23	0.10	1.52	/	/
3	PTC	6	200	77,400	69.78	12.48	0.05	0.25	56	86.8 ± 1.1
4	PTC	17	206	71,500	70.29	12.14	0.18	0	53	85.5 ± 2.3
5	PTC	24	189	70,400	69.87	15.79	0.48	0.16	52	85.9 ± 1.6
6	PTC	48	213	59,100	67.47	17.37	0.84	0.23	50	83.4 ± 4.3

2. CO_2BAM characterization

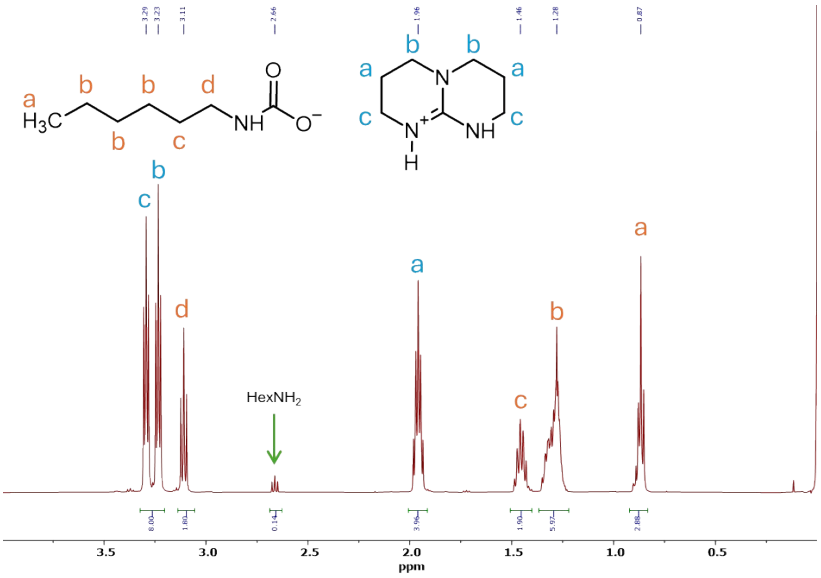
a. Nuclear Magnetic Resonance



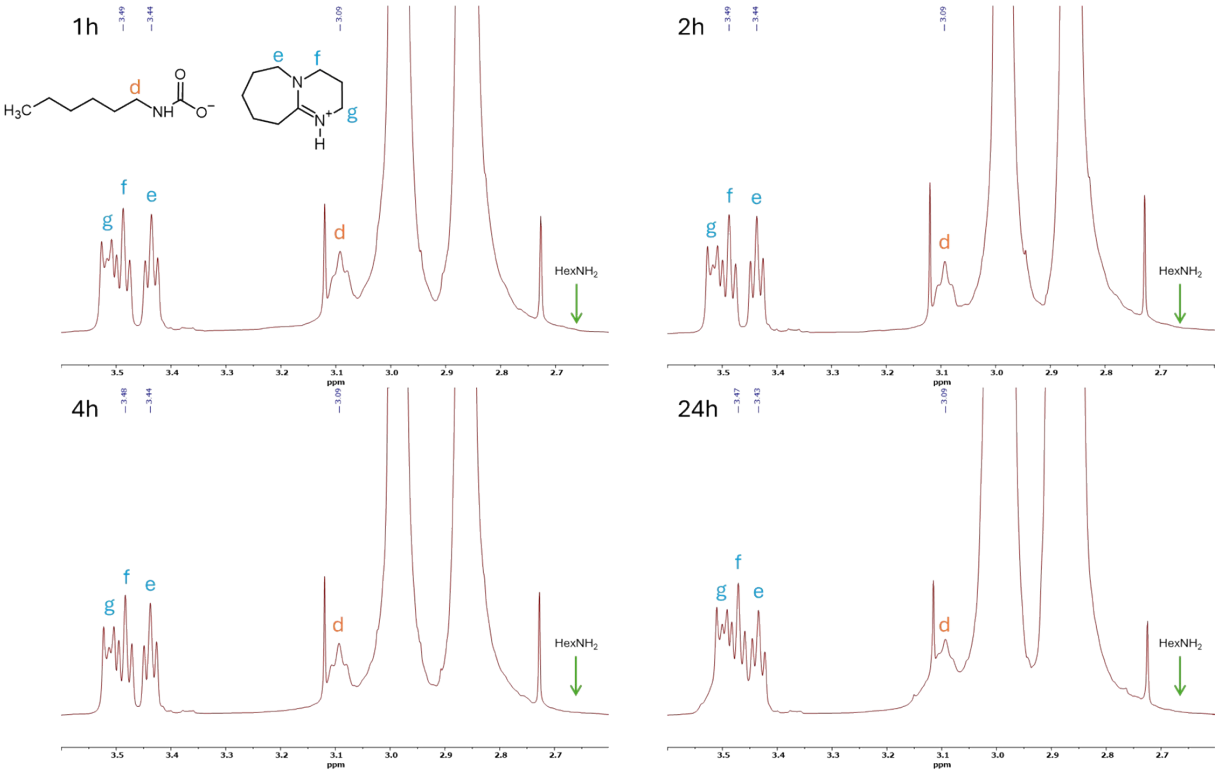
Supplementary Figure S11 – ^{1}H NMR spectrum of the amine only-based CO_2BAM.



Supplementary Figure S12 – ^{1}H NMR spectrum of the hexylamine and DBU-based CO_2BAM.

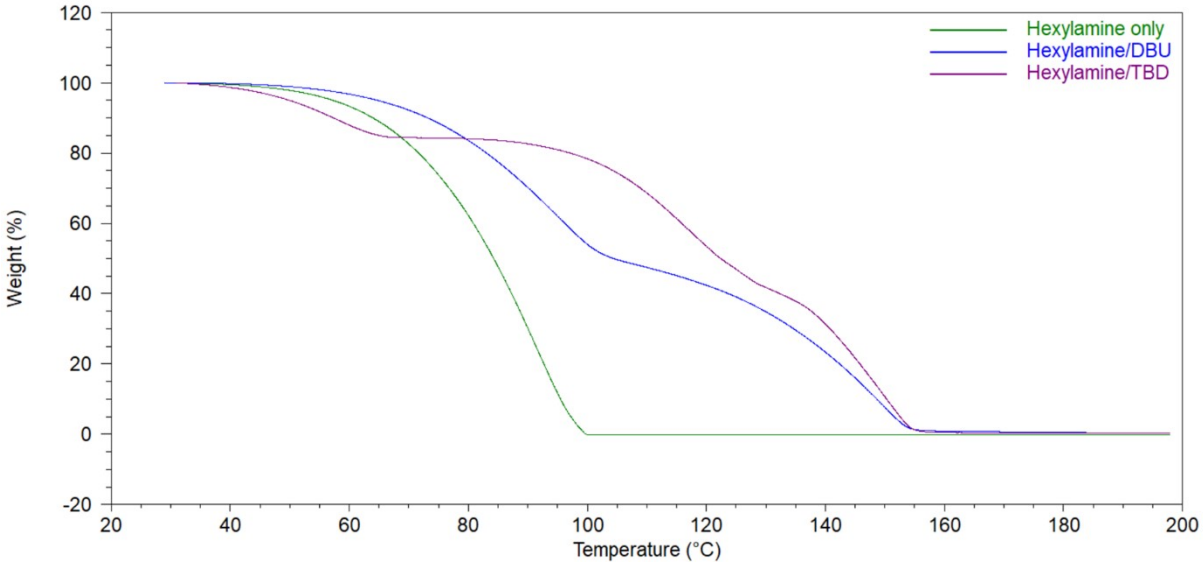


Supplementary Figure S13 – ^{1}H NMR spectrum of the hexylamine and TBD-based CO_2BAM.



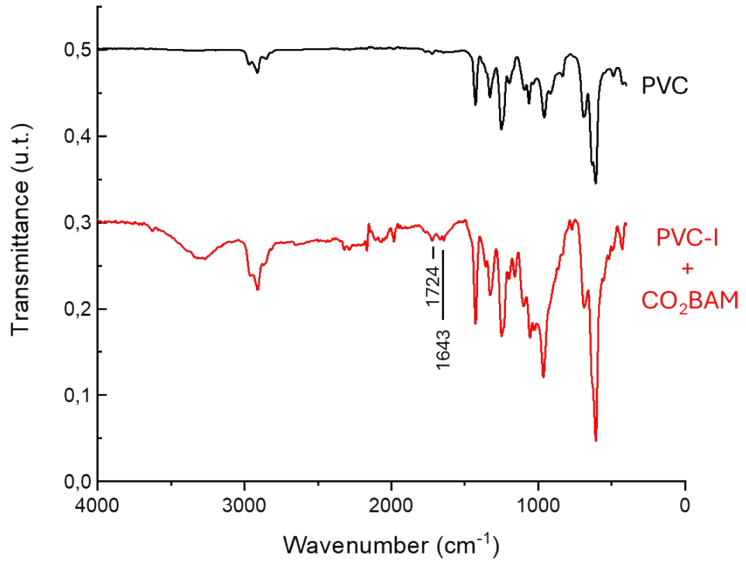
Supplementary Figure S14 – Stability of DBU-based CO_2BAM of 1-hexylamine in solution in DMF studied by ^{1}H NMR spectroscopy. The green arrow indicates where free hexylamine should appear in case of CO_2BAM degradation.

b. Thermogravimetric Analysis

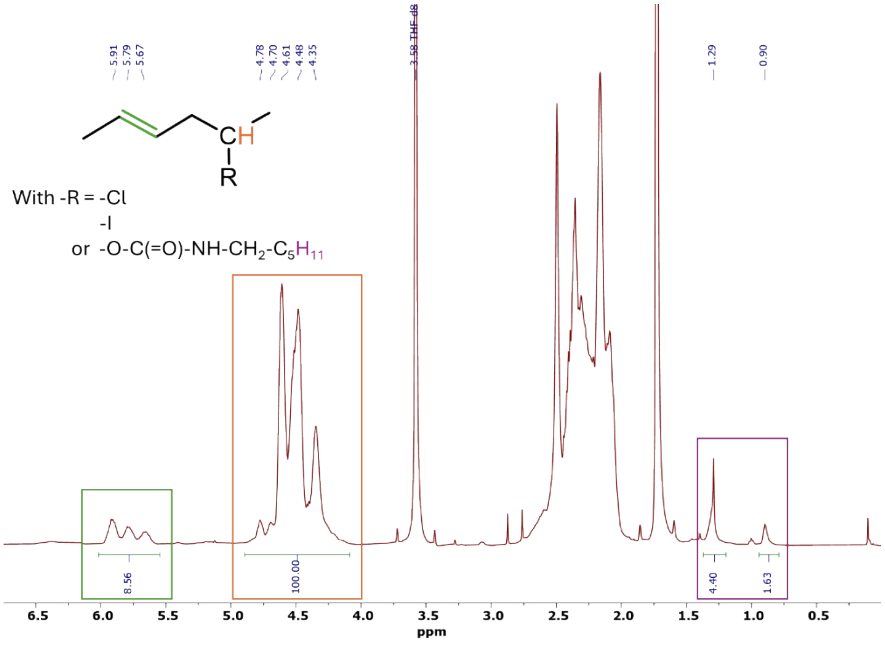


Supplementary Figure S15 – TGA thermograms of pristine 1-hexylamine, and hexylamine/DBU and hexylamine/TBD-based CO_2BAMs.

3. Reaction between iodinated PVC and DBU-based CO_2BAM – Product characterization



Supplementary Figure S16 – FT-IR spectra of pristine PVC and the product of reaction between PVC-I and the DBU-based CO_2BAM of 1-hexylamine.



Supplementary Figure S17 - ^{1}H NMR spectrum of the reaction product between PVC-I and the DBU-based CO_2BAM of 1-hexylamine.