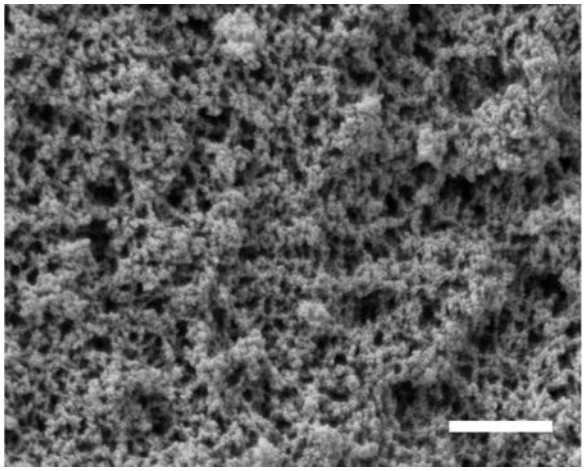
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Spatial Tuning of Adsorption Enthalpies by Exploiting Spectator Group Effects in Organosilica Carbon Capture Materials

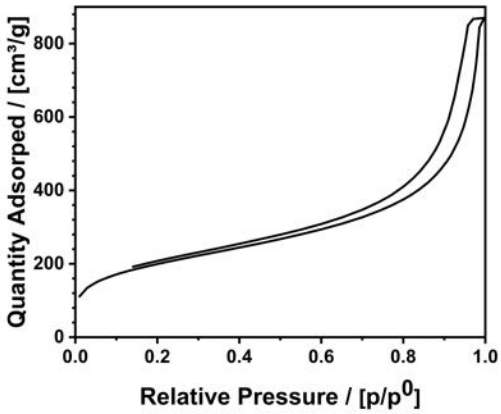
Mario Evers,[a] Karin Hauser[b], Wolfgang G. Hinze,[b] Nele Klinkenberg,[b] Yasar Krysiak,[a] Daniel Mombers,[a,‡] Sebastian Polarz[a,‡,*]

SUPPORTING INFORMATION

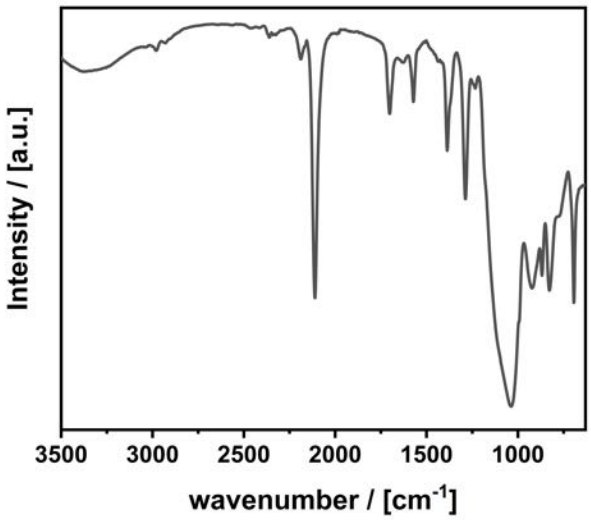
Fig. S1. Analytical Data for AzSil.



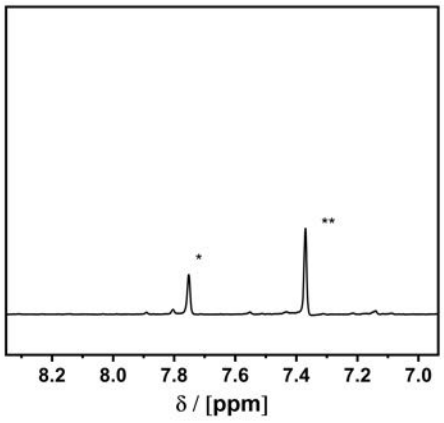
(a) SEM micrograph; scalebar = 1μm.



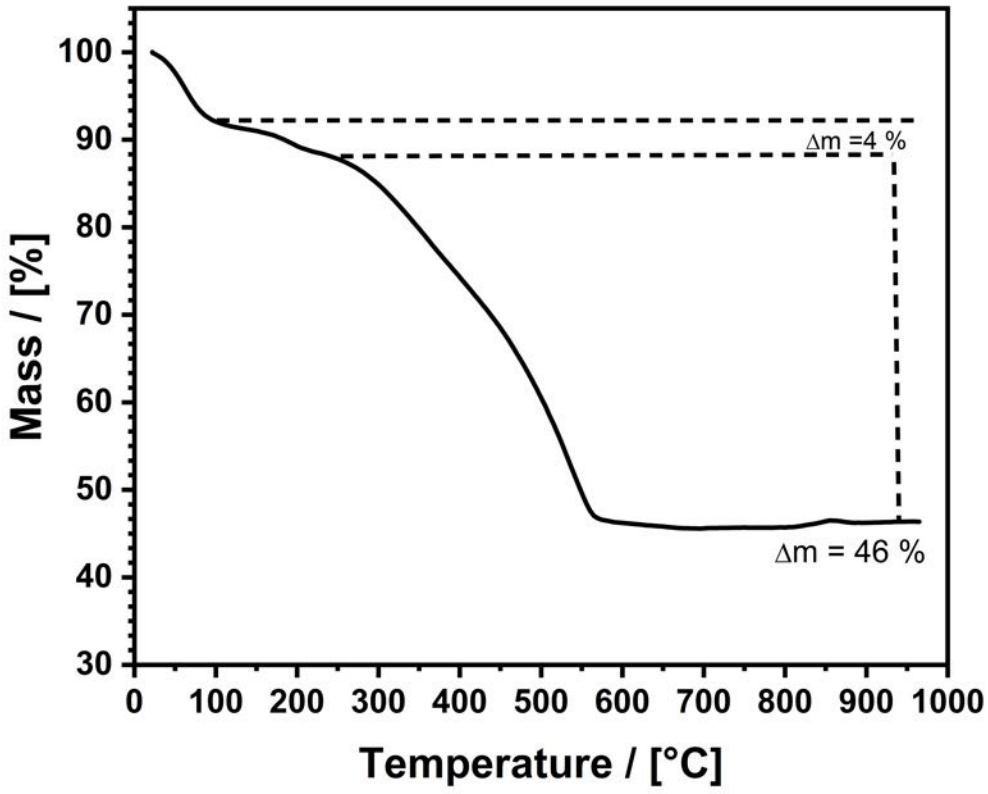
(b) N_2 physisorption isotherm; A_{BET} = 694 m^2/g.



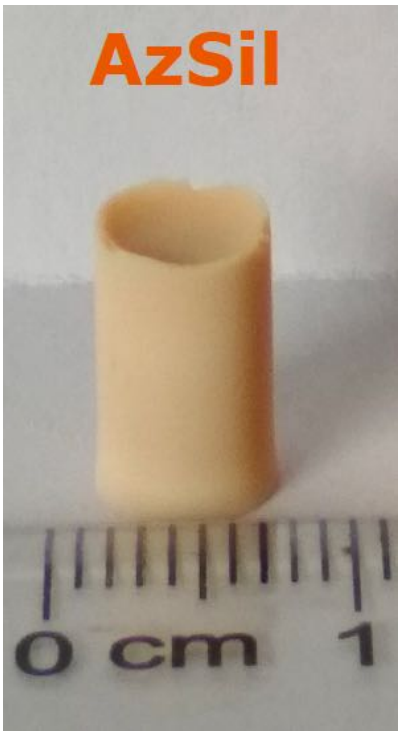
(c) FT-IR spectrum. ν (cm^{-1}) = 1044 (Si-O), 1316 (C(sp3)-C(sp3)), 1466 (C(sp3)C(sp3)), 2100 (N_3) 2851, 2920 (C-H), 3300 (OH).



(d) ^{1}H-NMR of dissolved material; (*) : 7.35 (m, 2H, o-arom. CH), (**) : 7.75 (m, 1H, p-arom. CH).

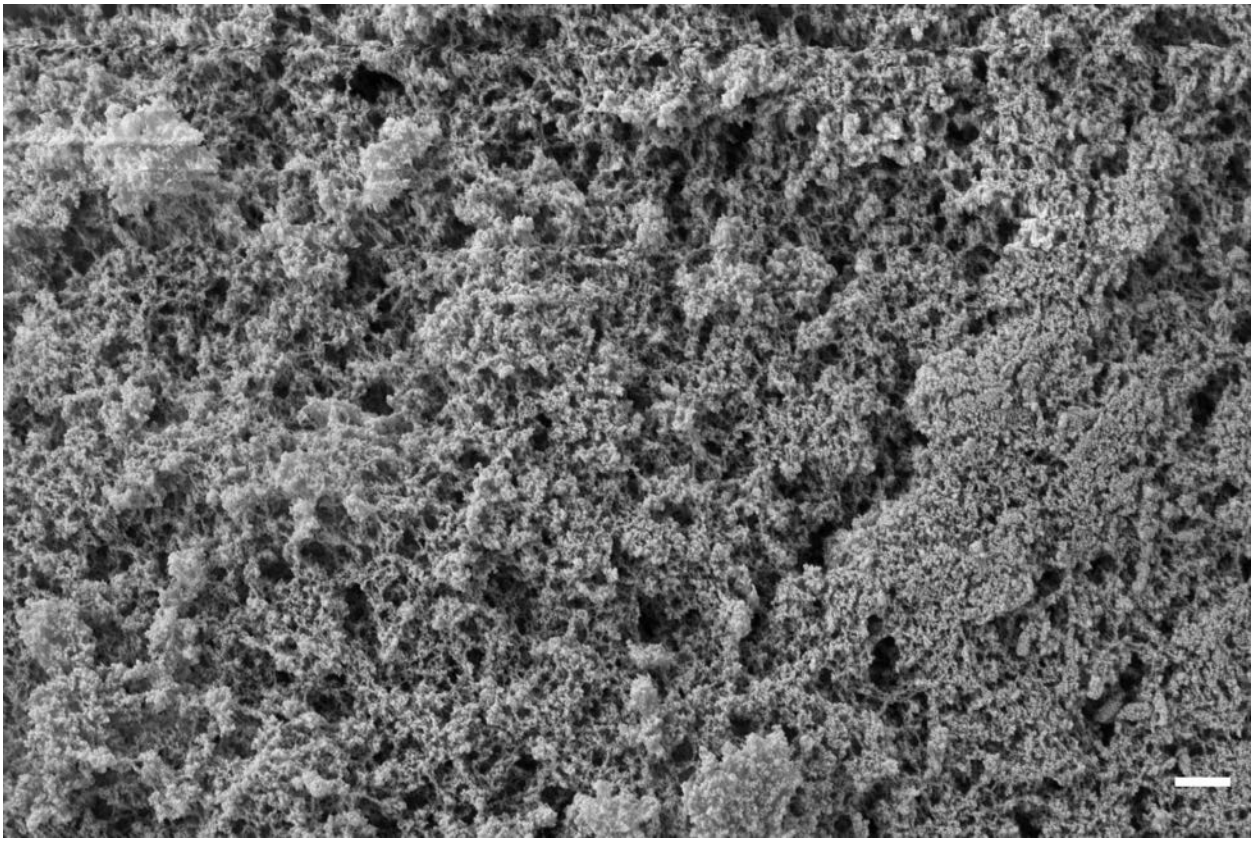

Mass / [%]
Temperature / [°C]
Δm =4 %
Δm = 46 %
100
90
80
70
60
50
40
30
0
100
200
300
400
500
600
700
800
900
1000

(e) TGA in air.

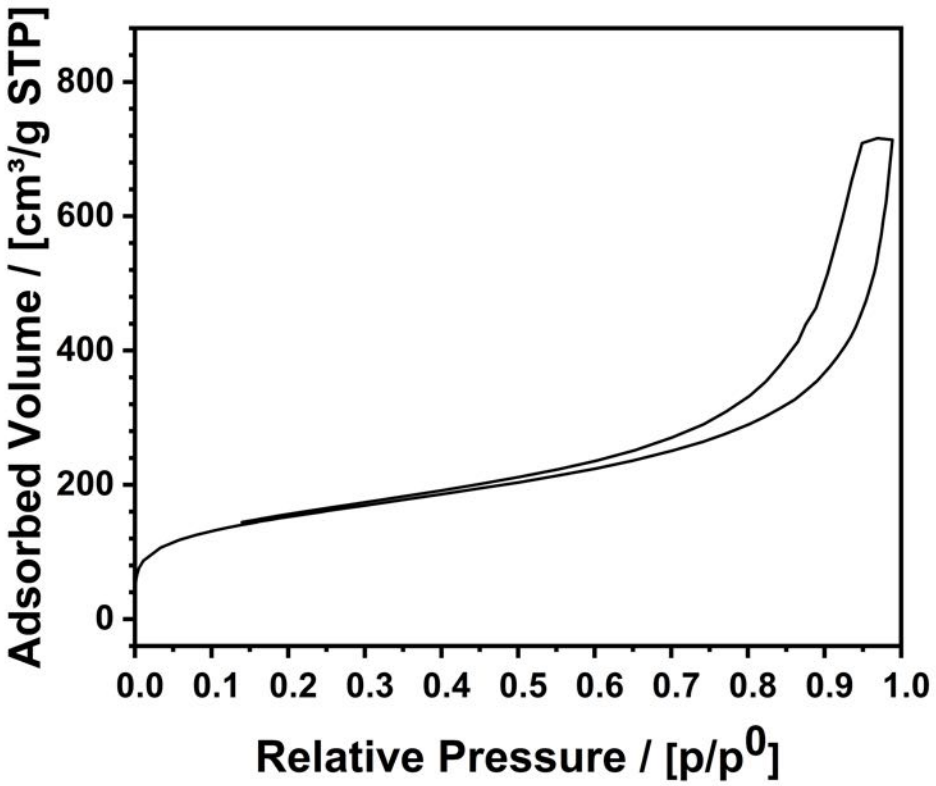


(f) Photographic image of monolithic aerogel obtained after supercritical drying.

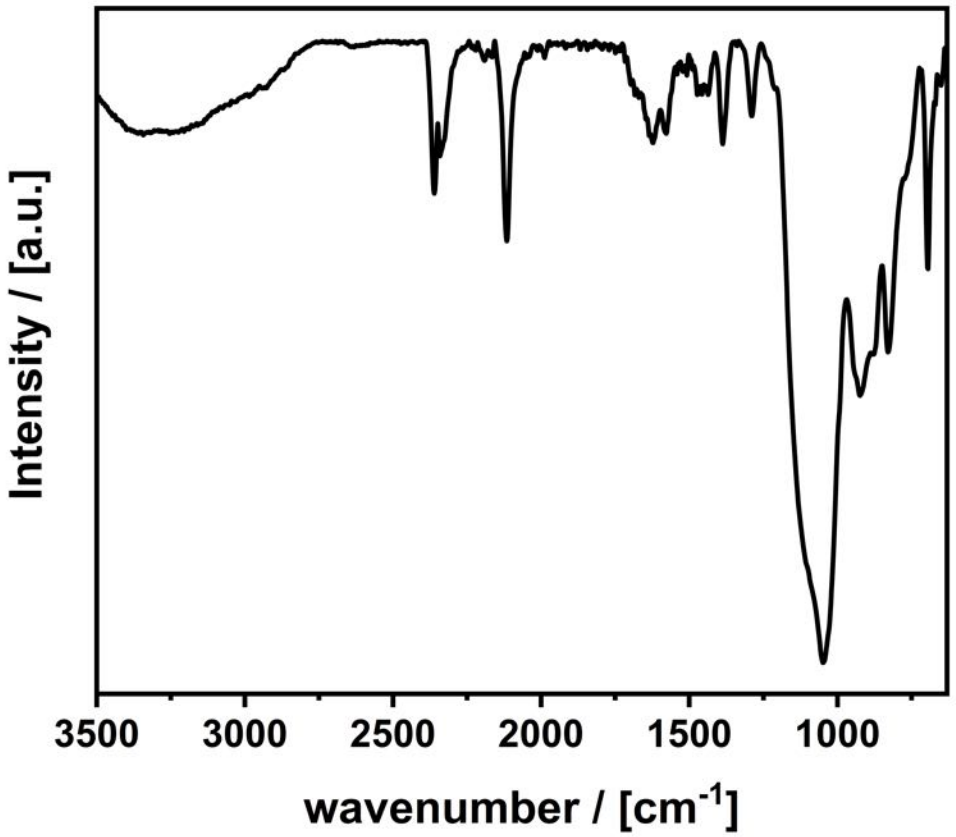
Fig. S2. Analytical Data for AmSil.



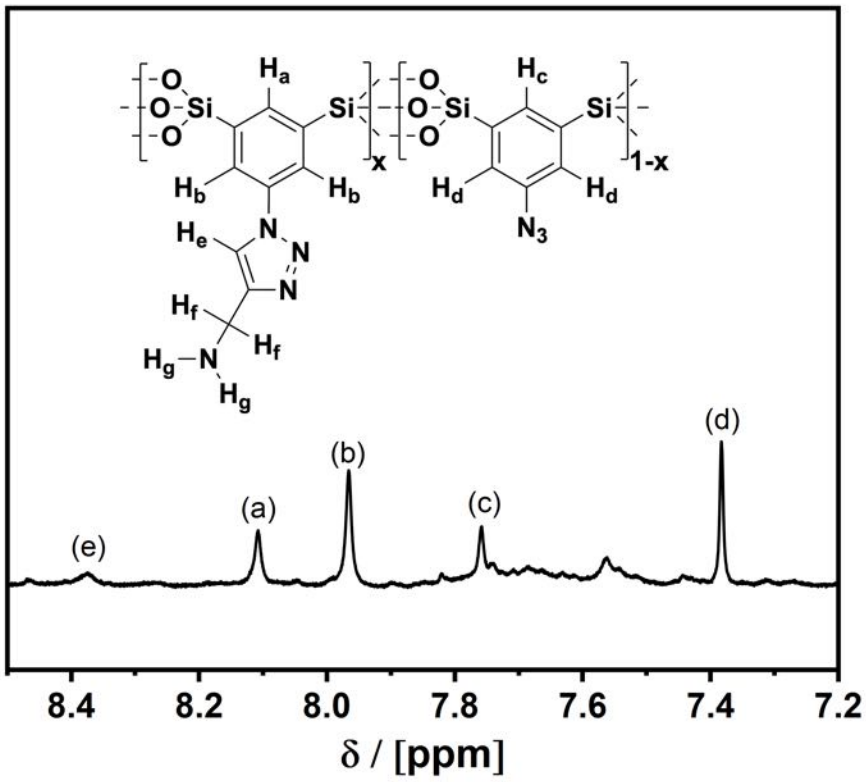
(a) SEM micrograph; scalebar = 1μm.



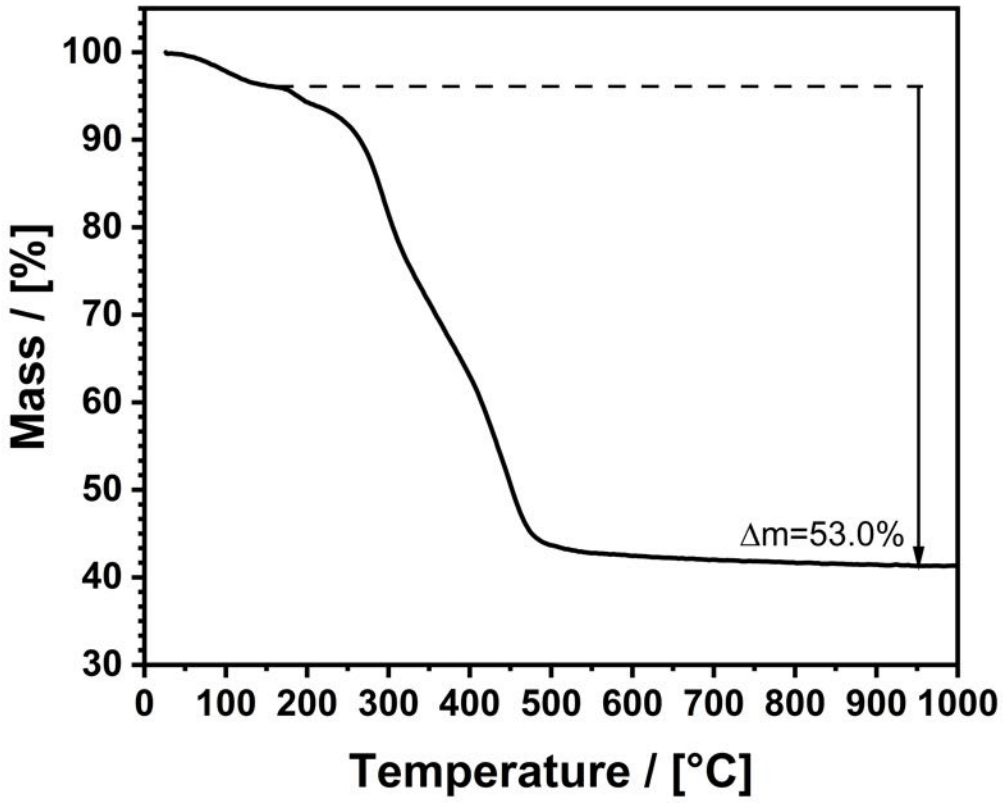
(b) N_2 physisorption isotherm; A_{BET} = 527 m^2/g.



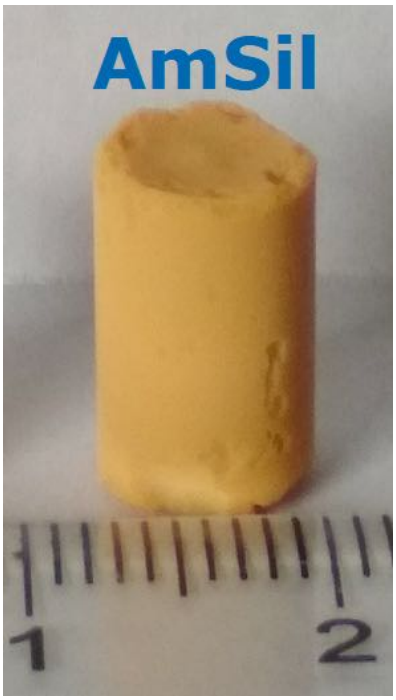
(c) FT-IR spectrum. ν (cm^{-1}) = 1044 (Si-O), 1316 (C(sp3)-C(sp3)), 1466 (C(sp3)C(sp3)), 2100 (N_3) 2851, 2920 (C-H), 3300 (OH).



(d) ^{1}H-NMR of dissolved material; (*) : 7.35 (m, 2H, o-arom. CH), (**) : 7.75 (m, 1H, p-arom. CH).

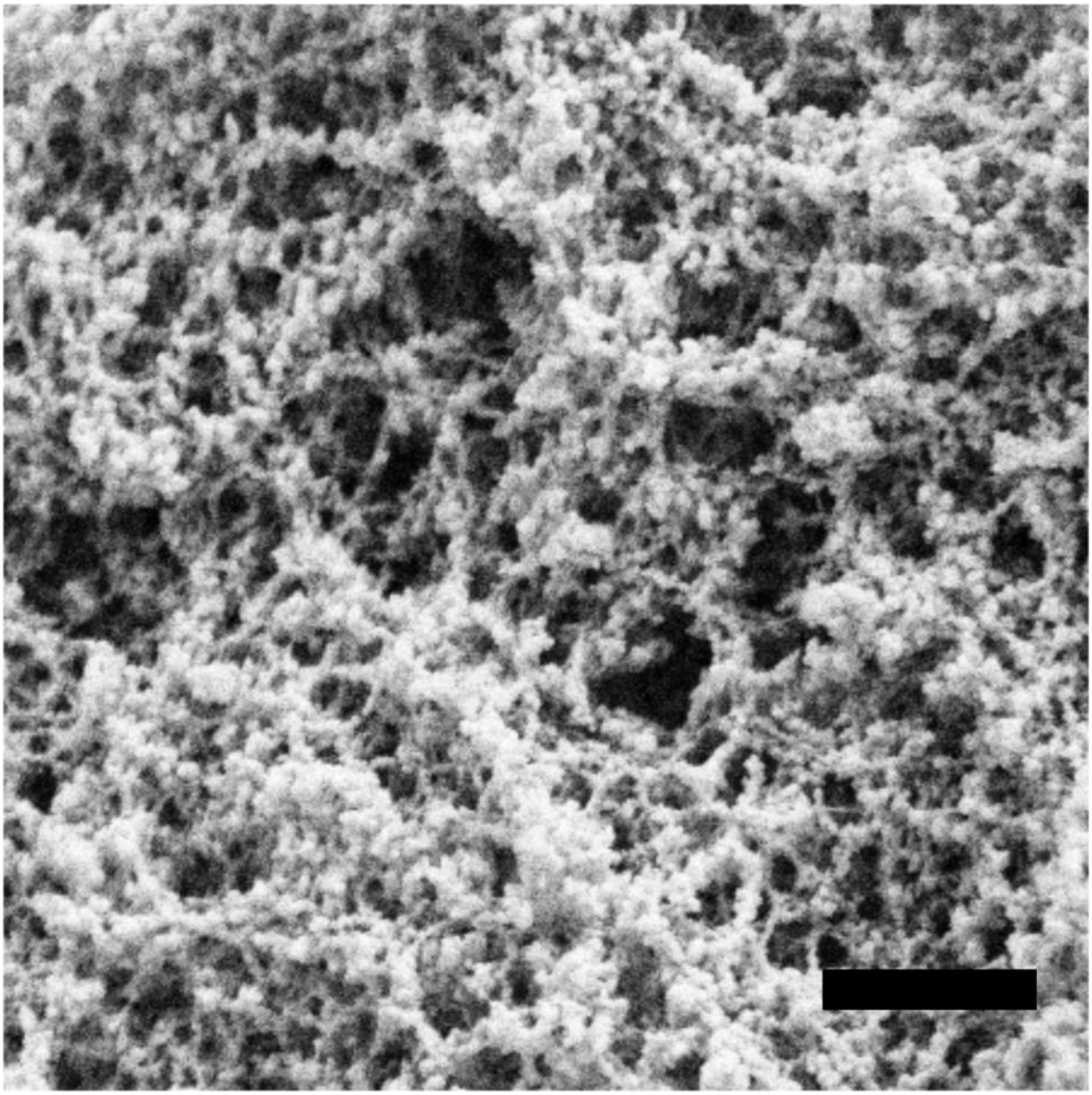

100
90
80
70
60
50
40
30
Mass / [%]
0
100
200
300
400
500
600
700
800
900
1000
Temperature / [°C]
Δm=53.0%

(e) TGA in air.

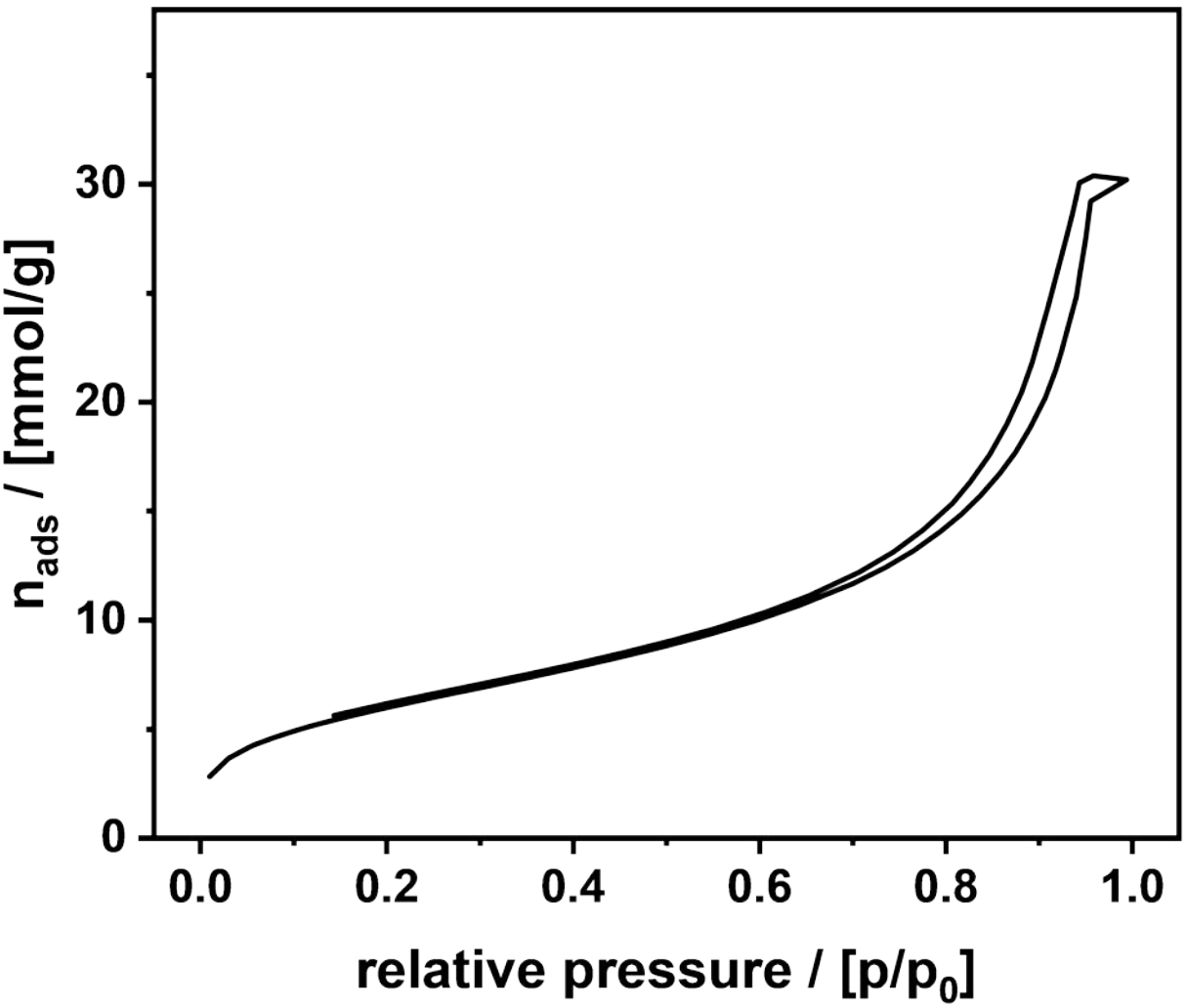


(f) Photographic image of monolithic aerogel obtained after supercritical drying.

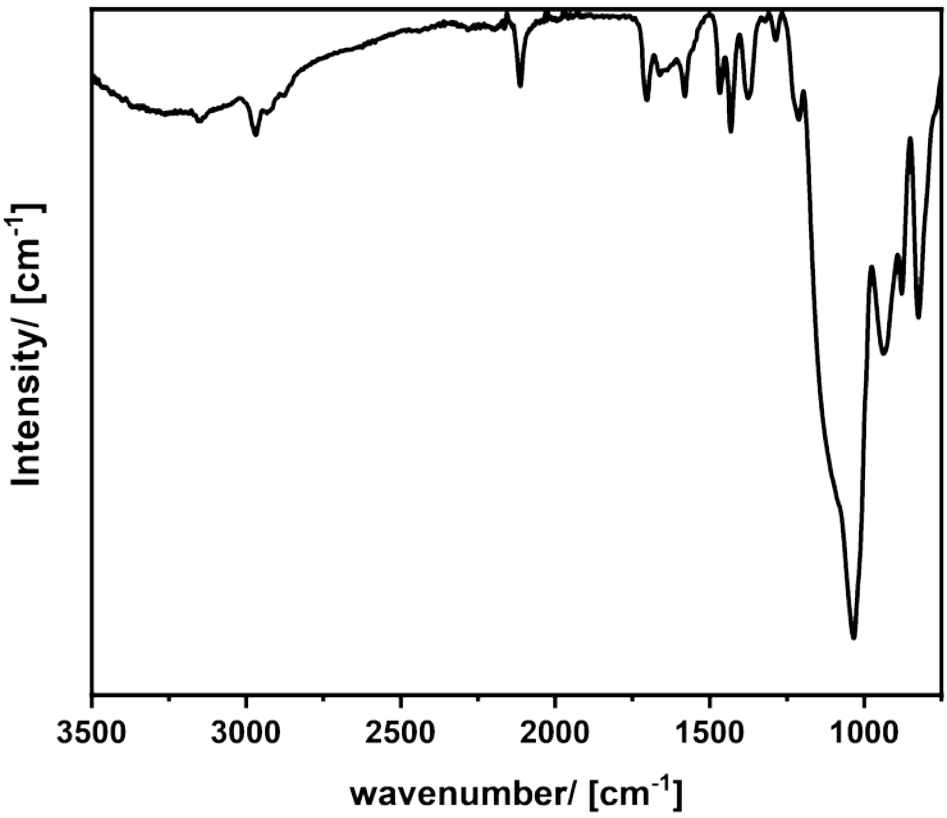
Fig. S3. Analytical Data for AmSP(a)Sil.



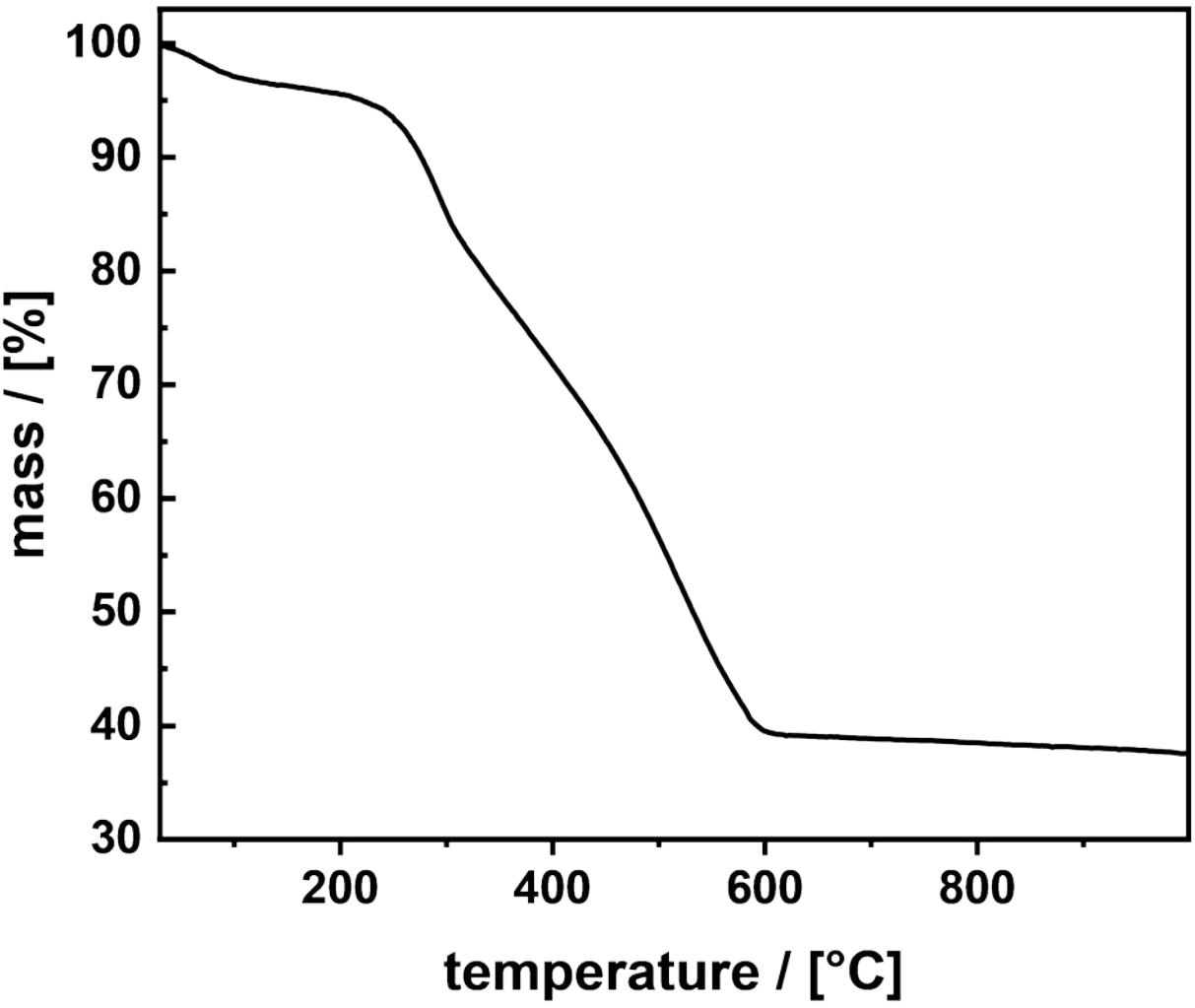
(a) SEM micrograph; scalebar = 1μm.



(b) N_2 physisorption isotherm; A_{BET} = 505 m^2/g.

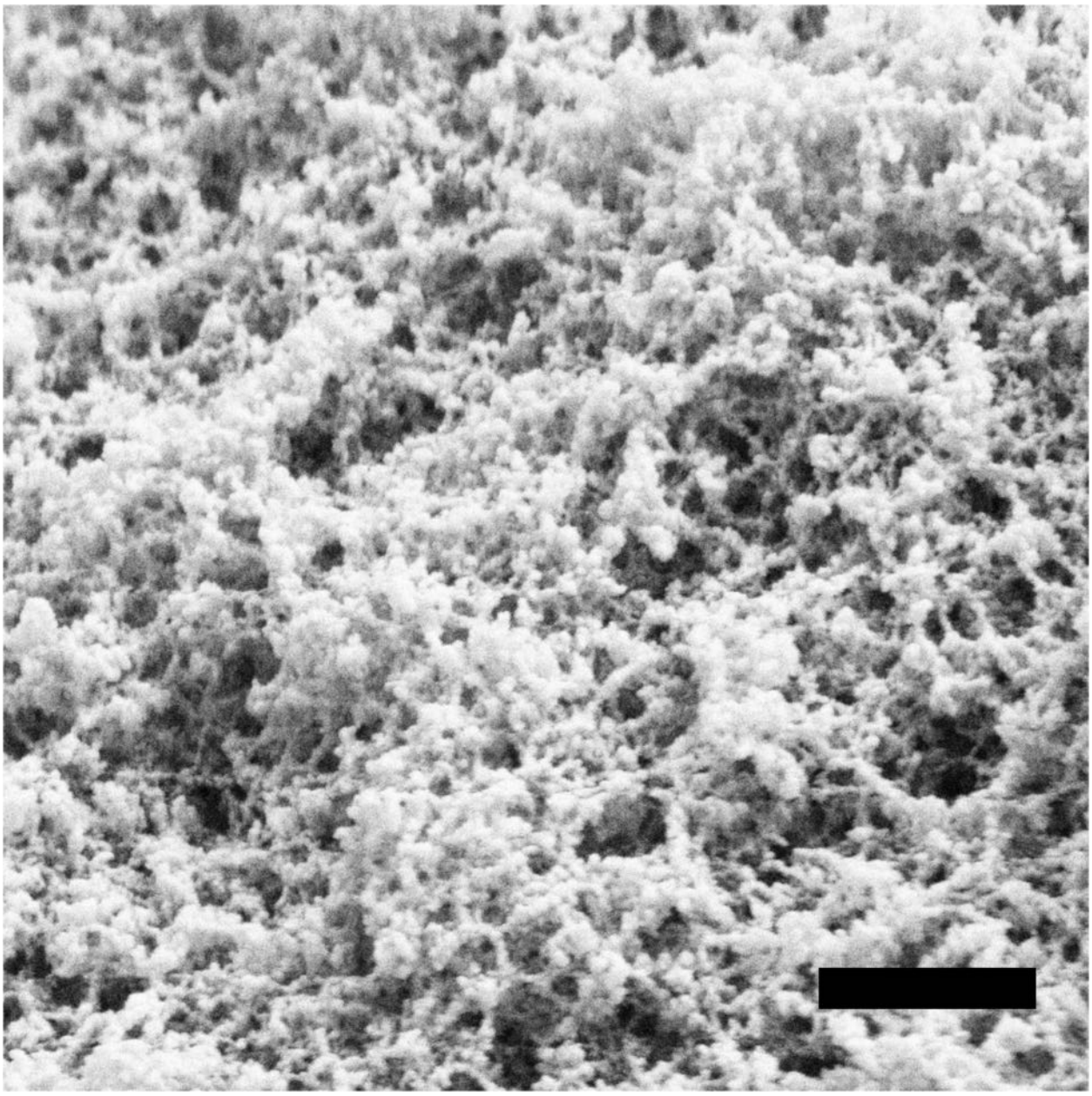


(c) FT-IR spectrum.

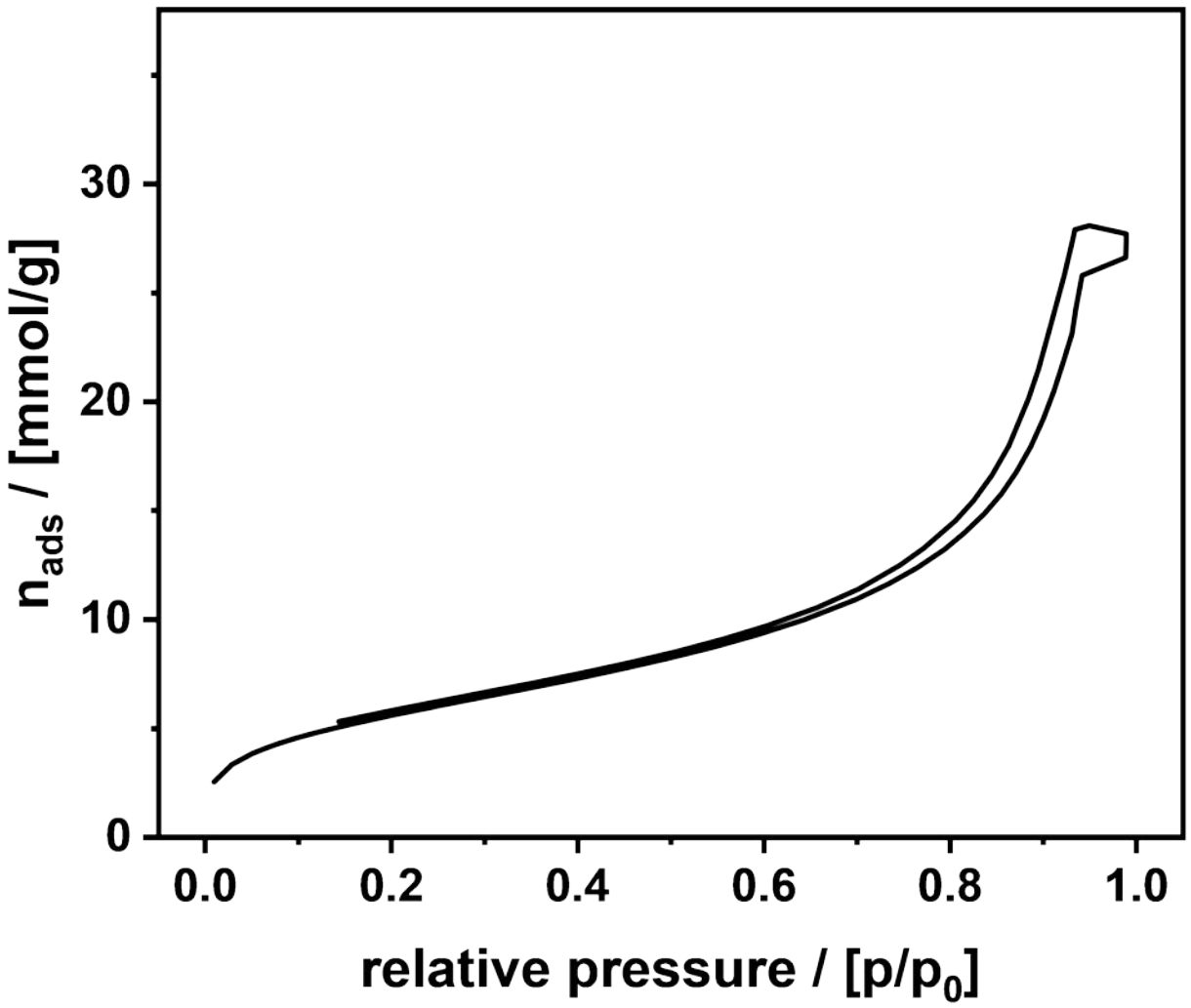


(d) TGA in air.

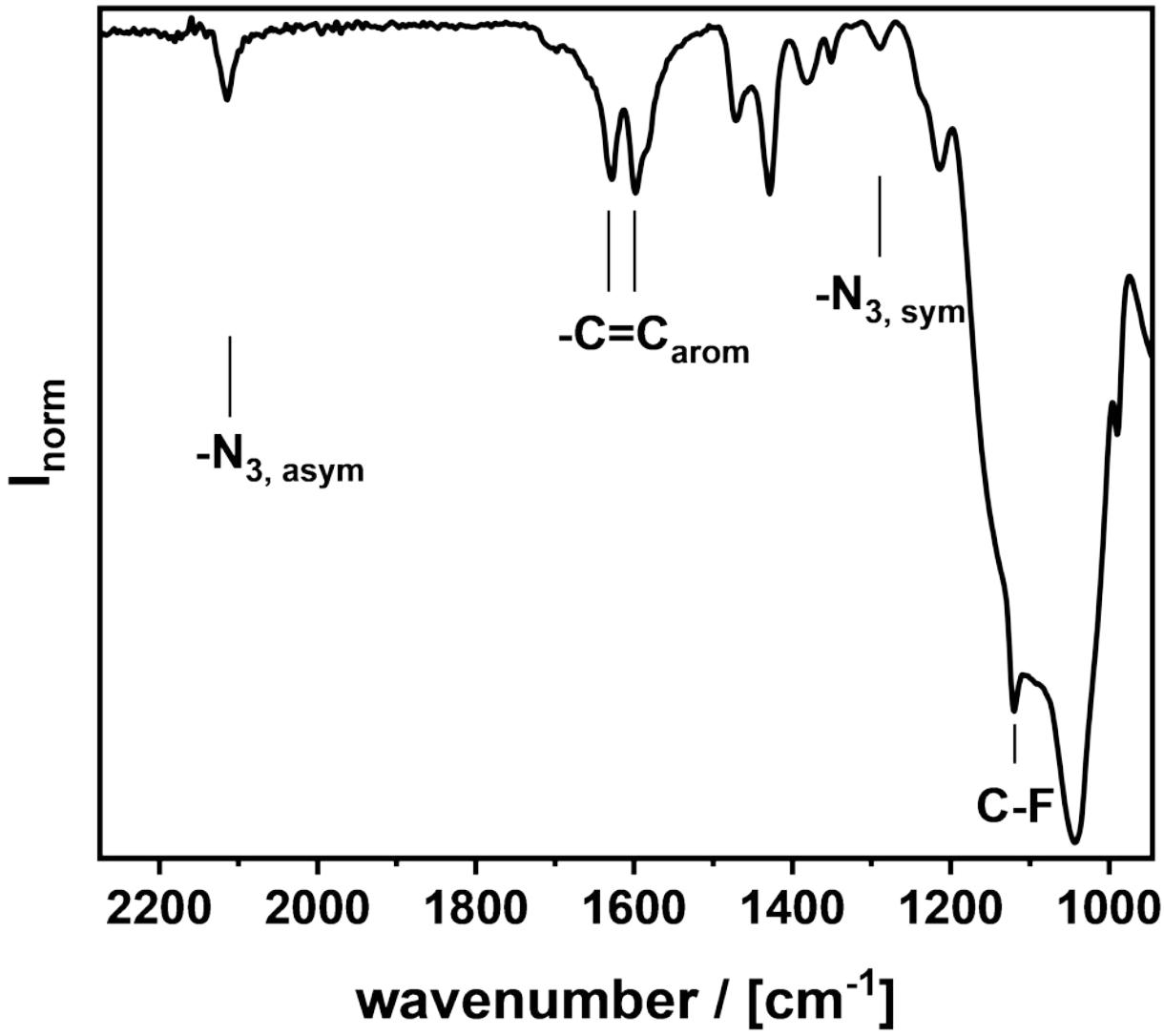
Fig. S4. Analytical Data for AmSP(b)Sil.



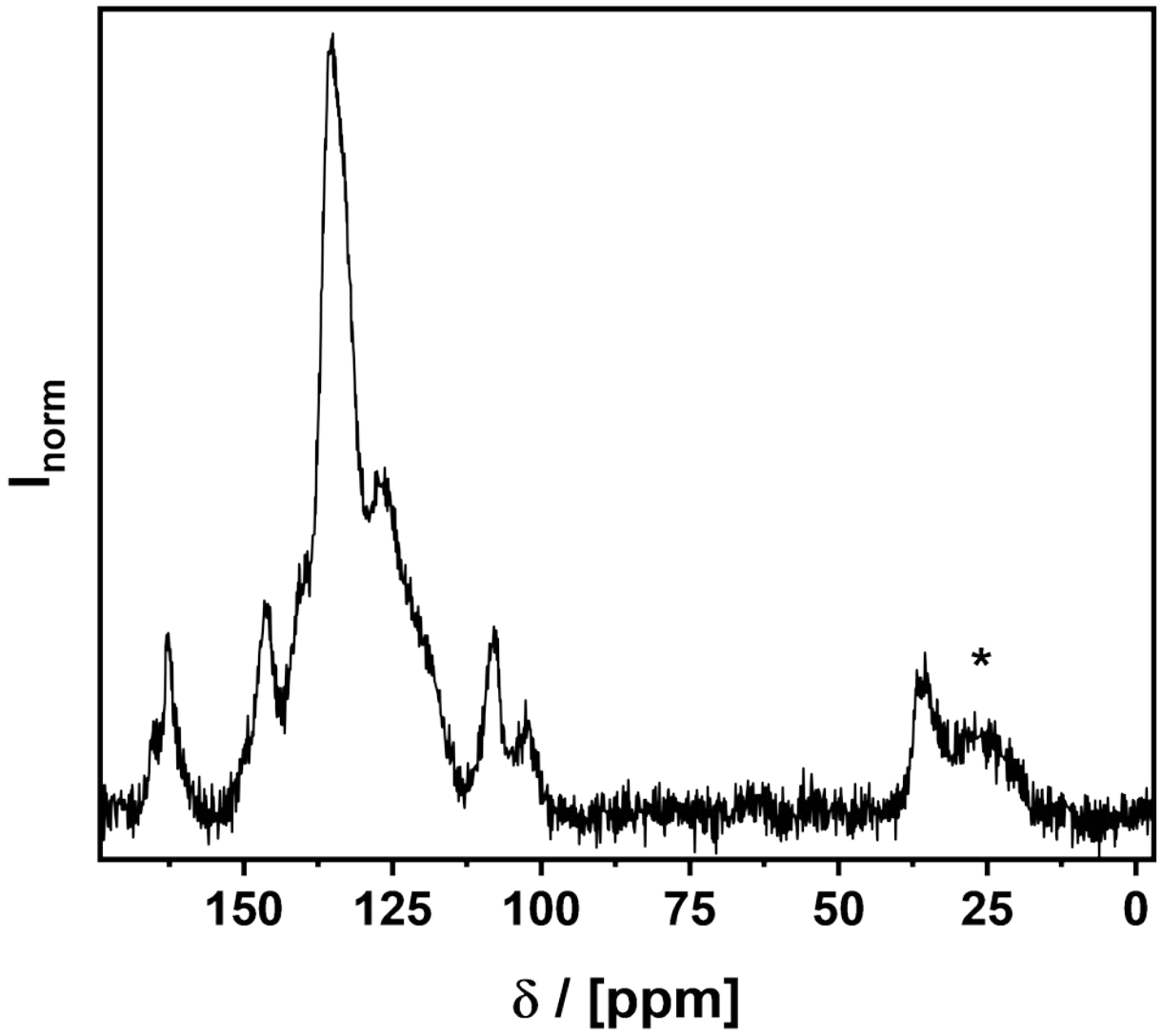
(a) SEM micrograph; scalebar = 1μm.



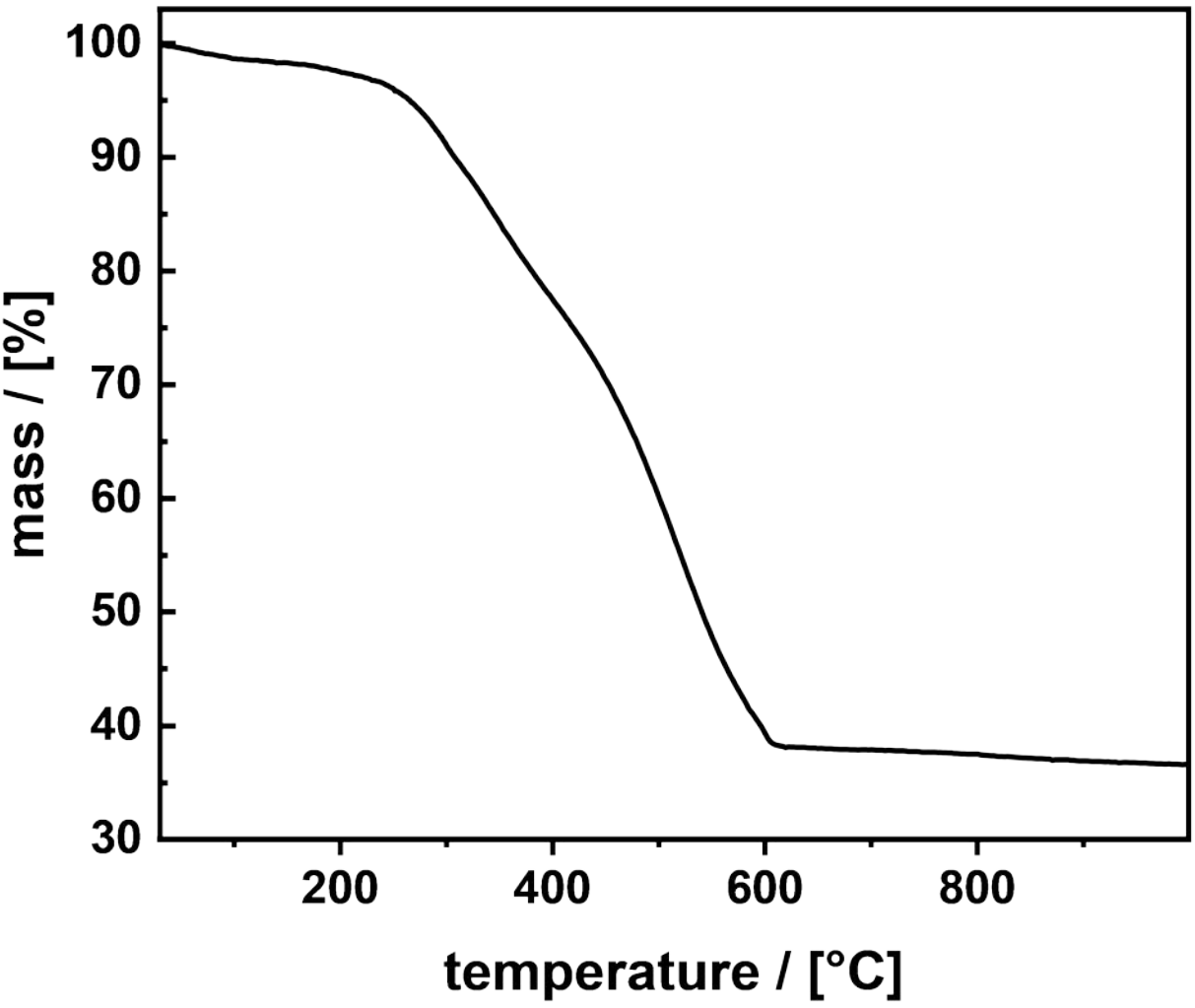
(b) N_2 physisorption isotherm; A_{BET} = 460 m^2/g.



(c) FT-IR spectrum.

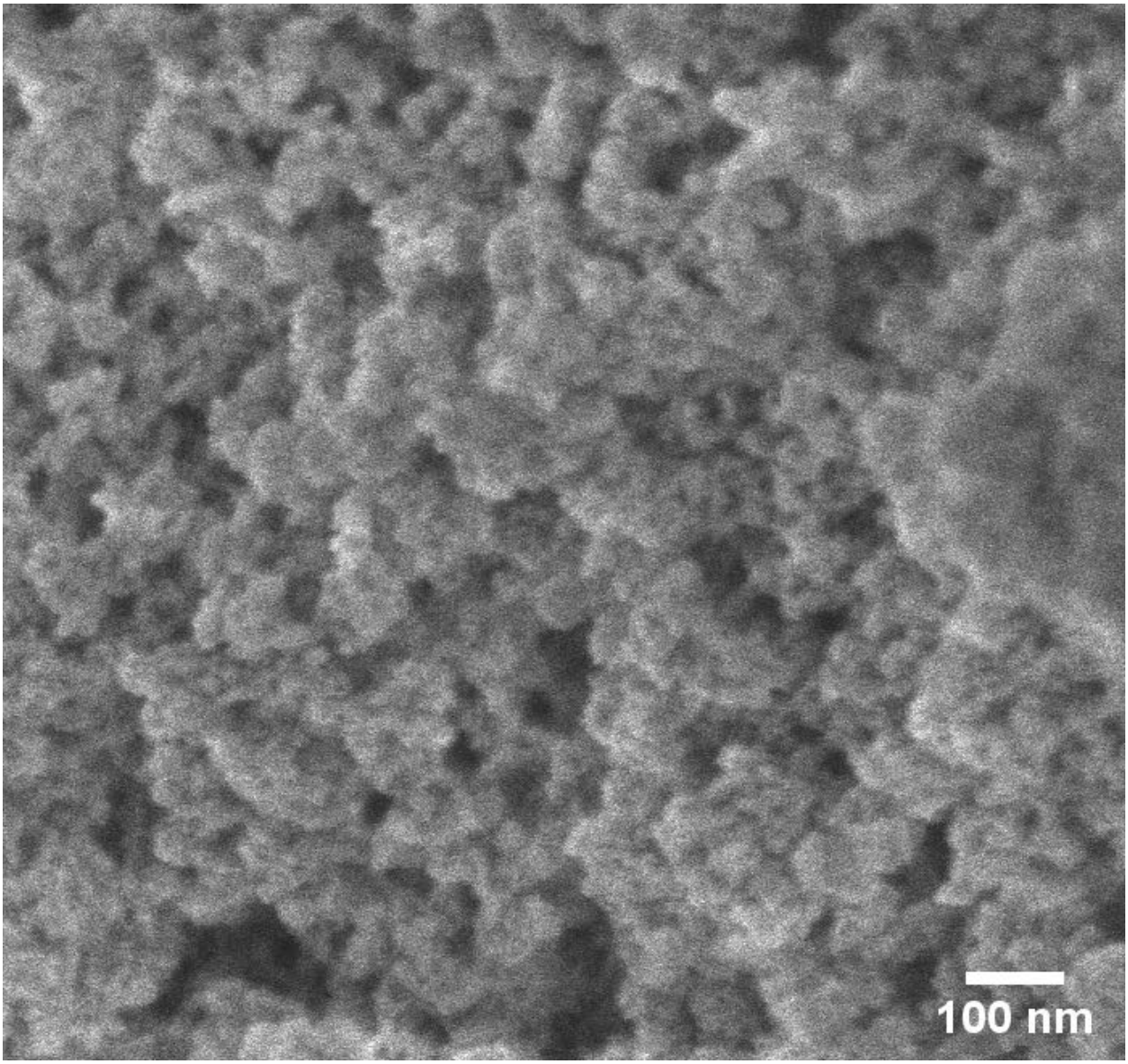


(d) ^{13}C-MAS NMR. Asterisk (*) in (C) denotes a spinning side band.

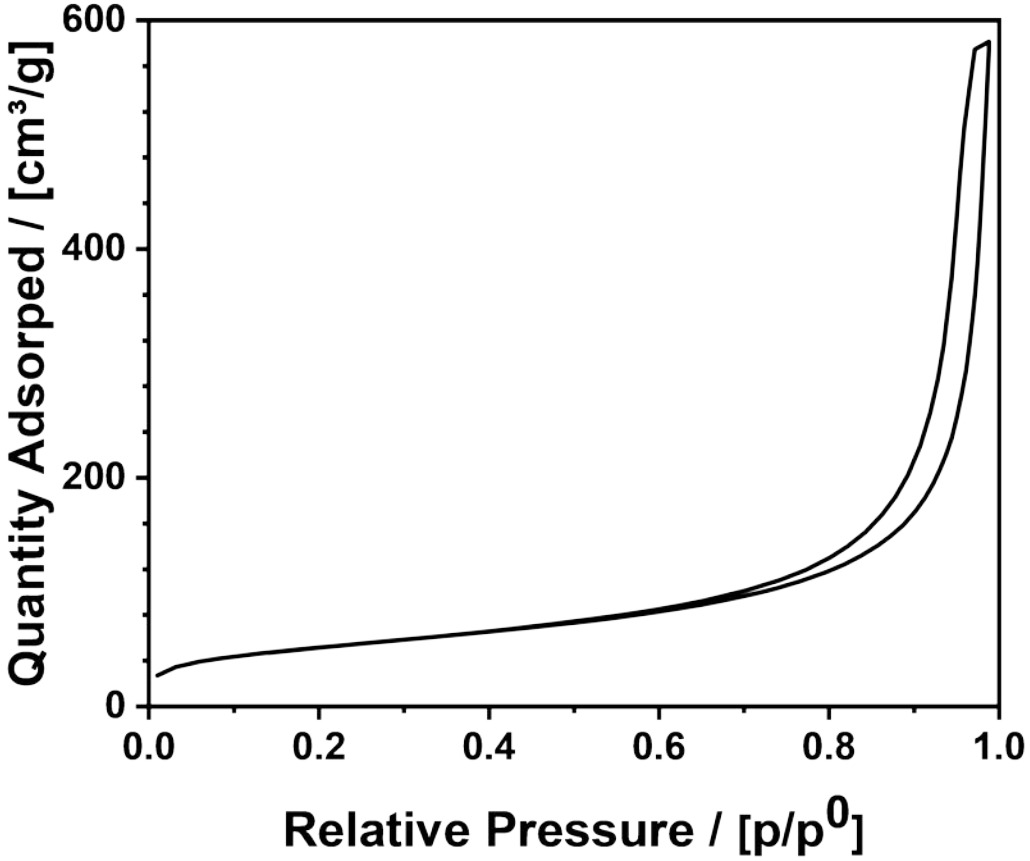


(e) TGA in air.

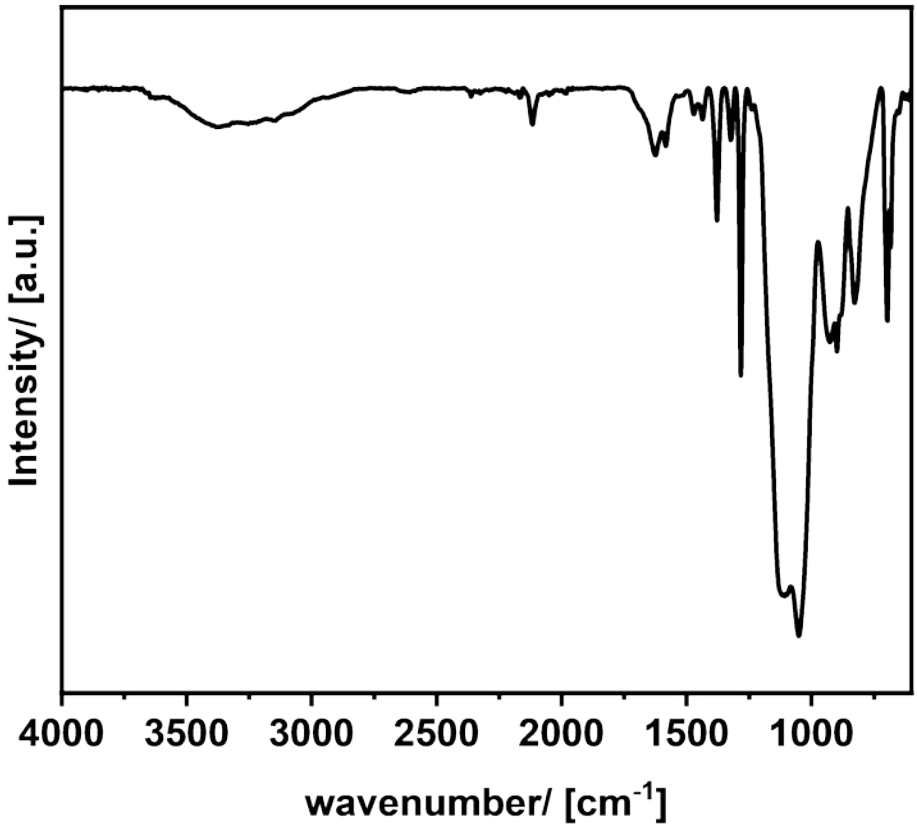
Fig. S5. Analytical Data for AmSP(c)Sil.



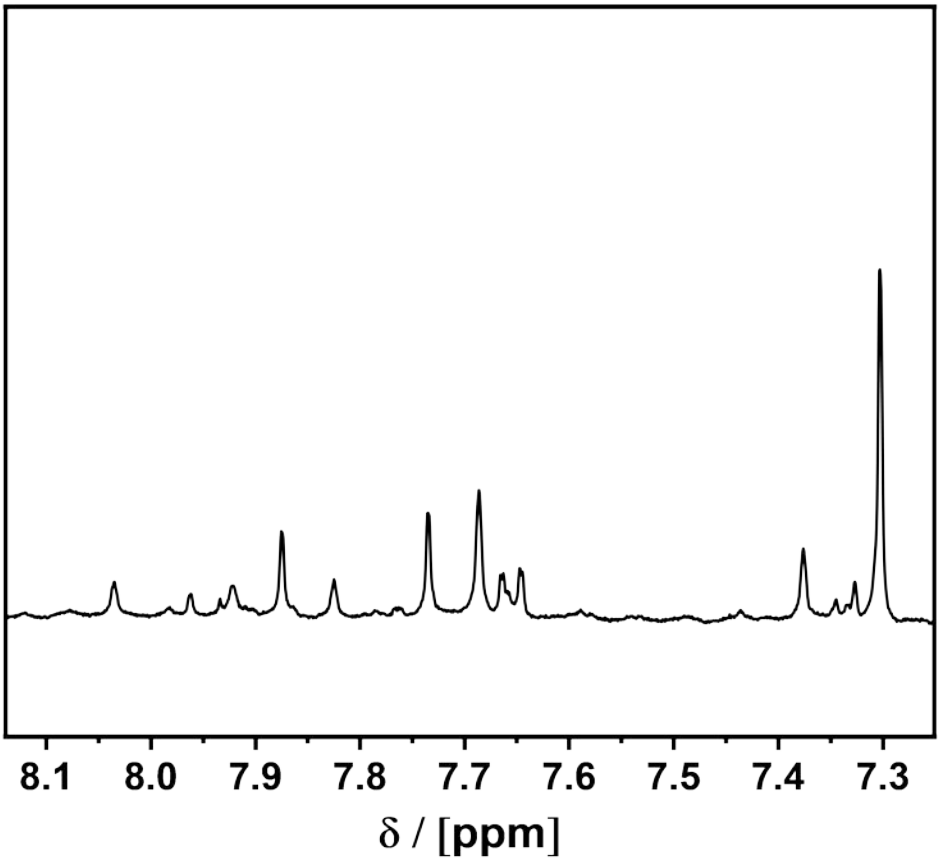
(a) SEM micrograph; scalebar = 1μm.



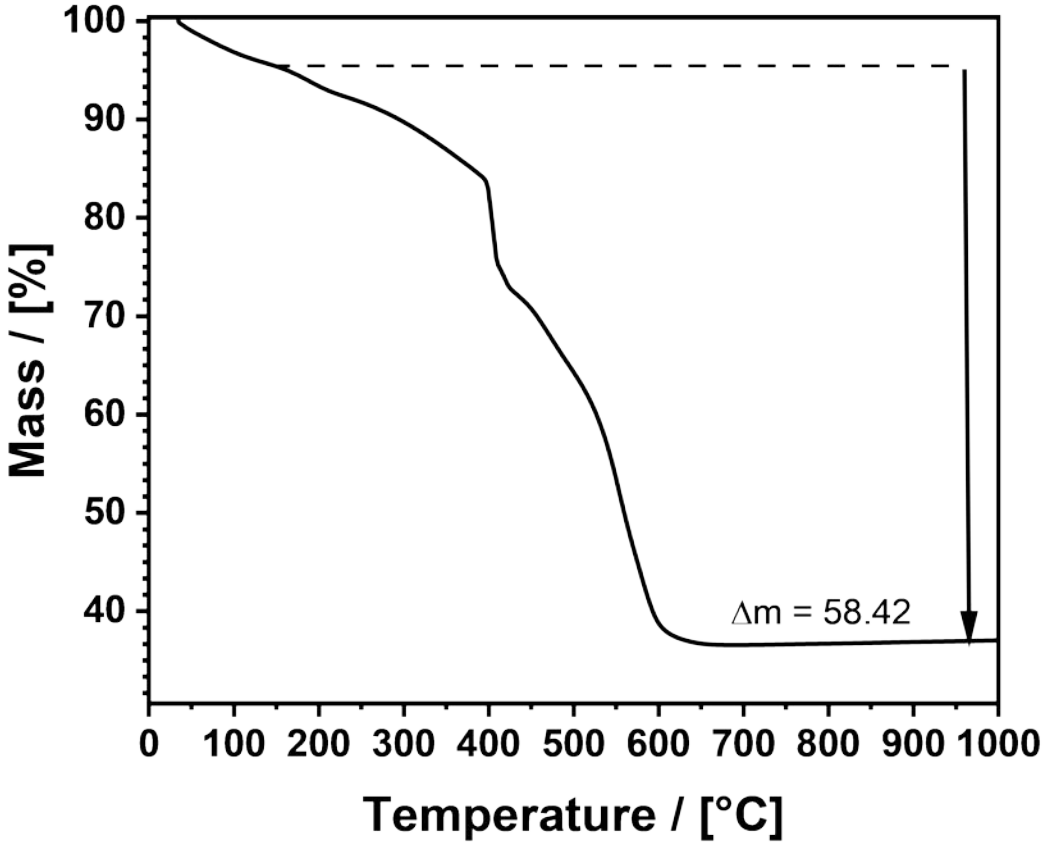
(b) N_2 physisorption isotherm; A_{BET} = 491 m^2/g.



(c) FT-IR spectrum. **ATR-IR**: ν (cm^{-1}) = 1044 (Si-O), 1114(CF3), 1288 (CF3), 1316 (C(sp3)-C(sp3)), 1466 (C(sp3)C(sp3)) , 1578 (NH3), 2115 (N_3) 2851, 2920 (C-H), 3300 (OH)

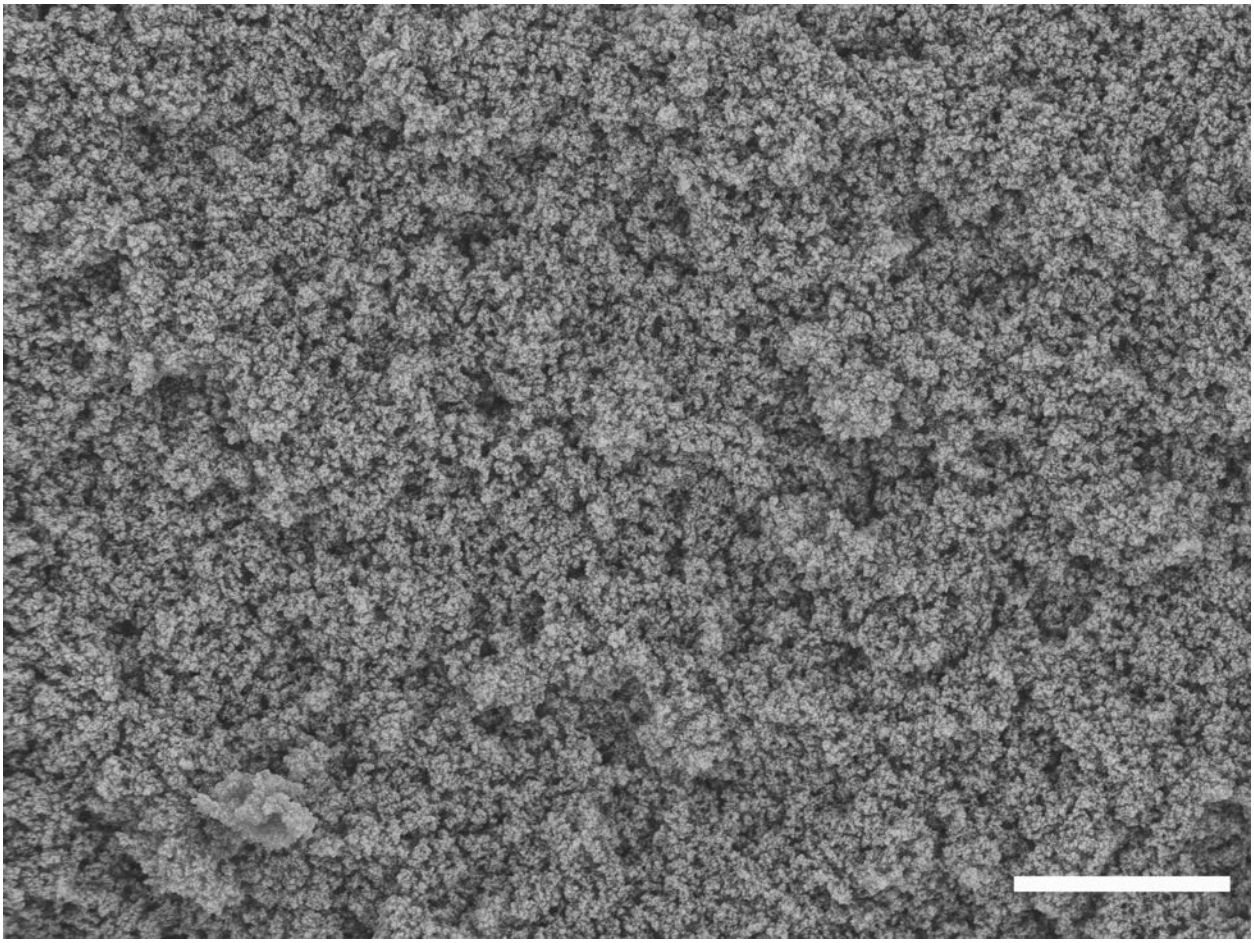


(d) ^{1}H-NMR of dissolved material.

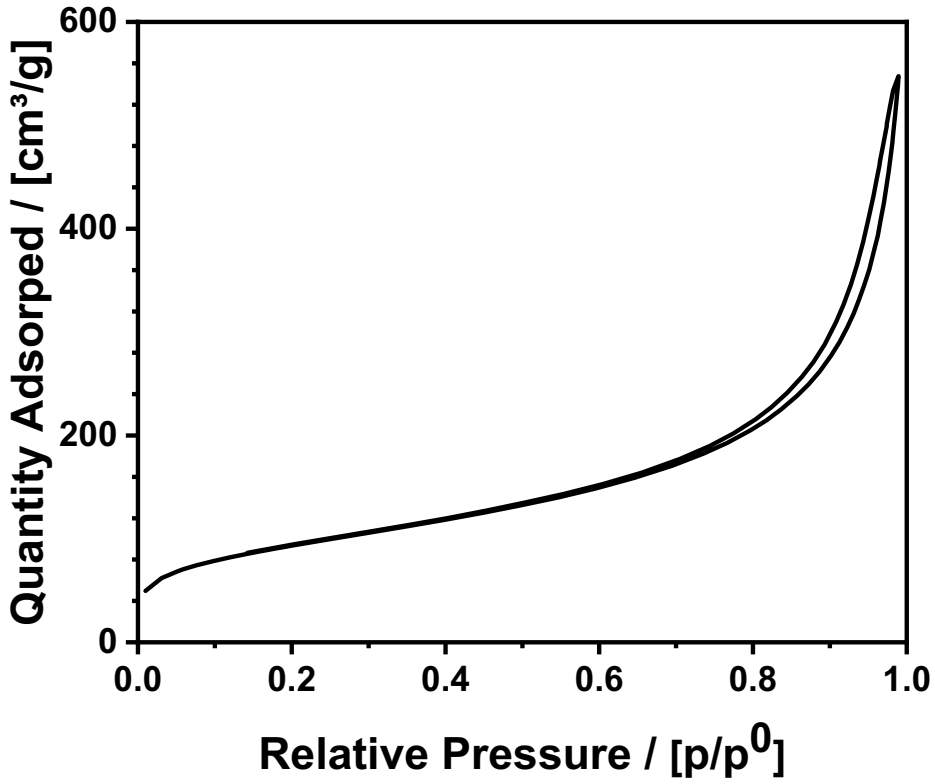

100
90
80
70
60
50
40
Mass / [%]
Δm = 58.42
0
100
200
300
400
500
600
700
800
900
1000
Temperature / [°C]

(e) TGA in air.

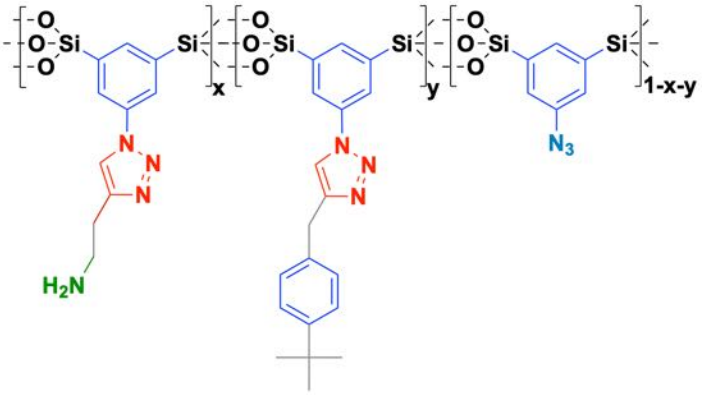
Fig. S6. Analytical Data for AmSP(d)Sil.

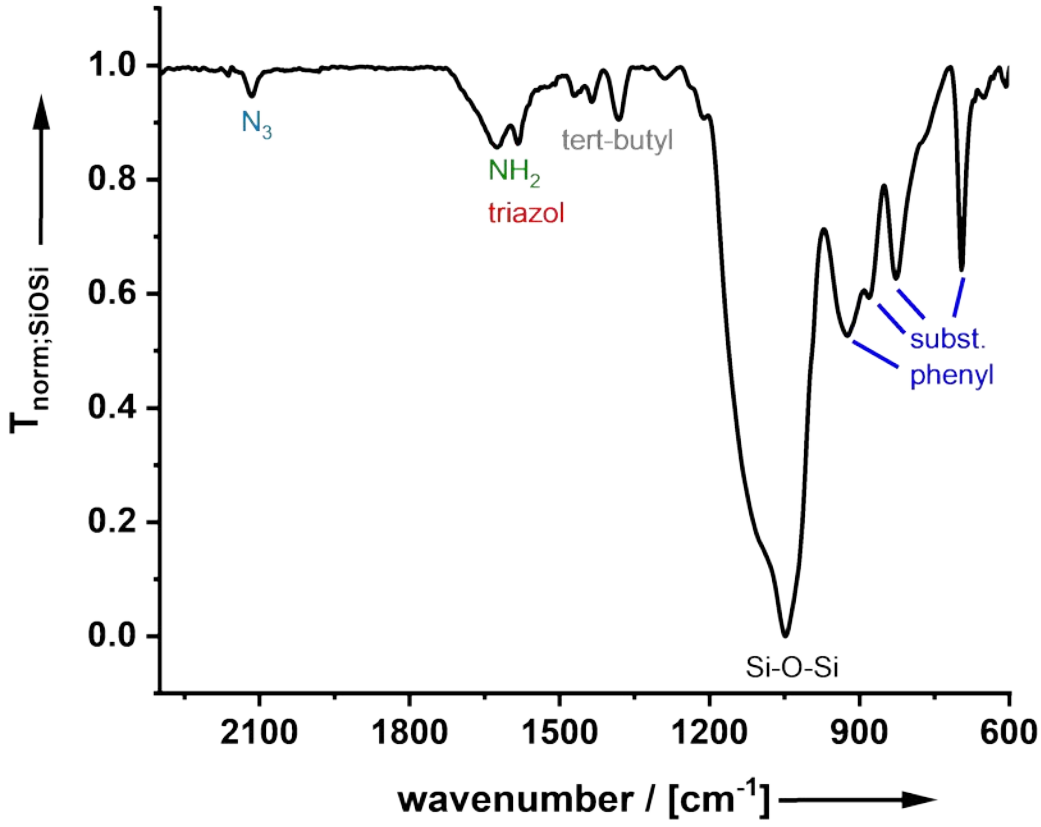


(a) SEM micrograph; scalebar = 5μm.

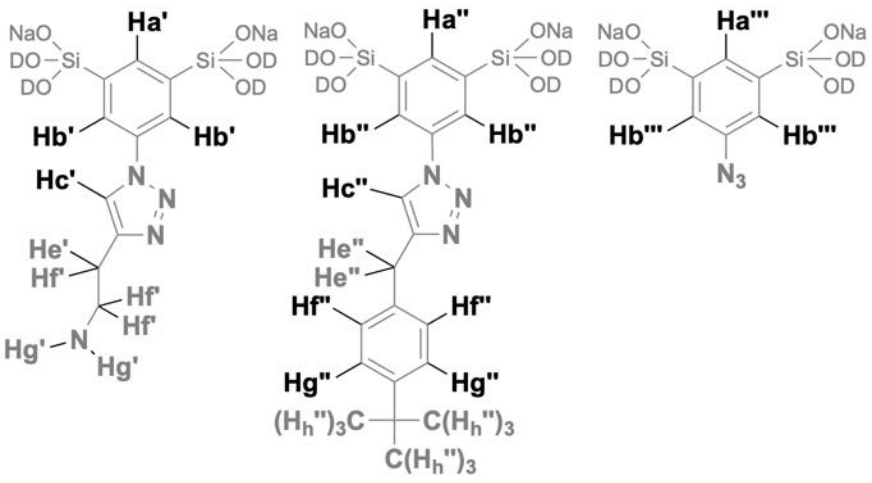


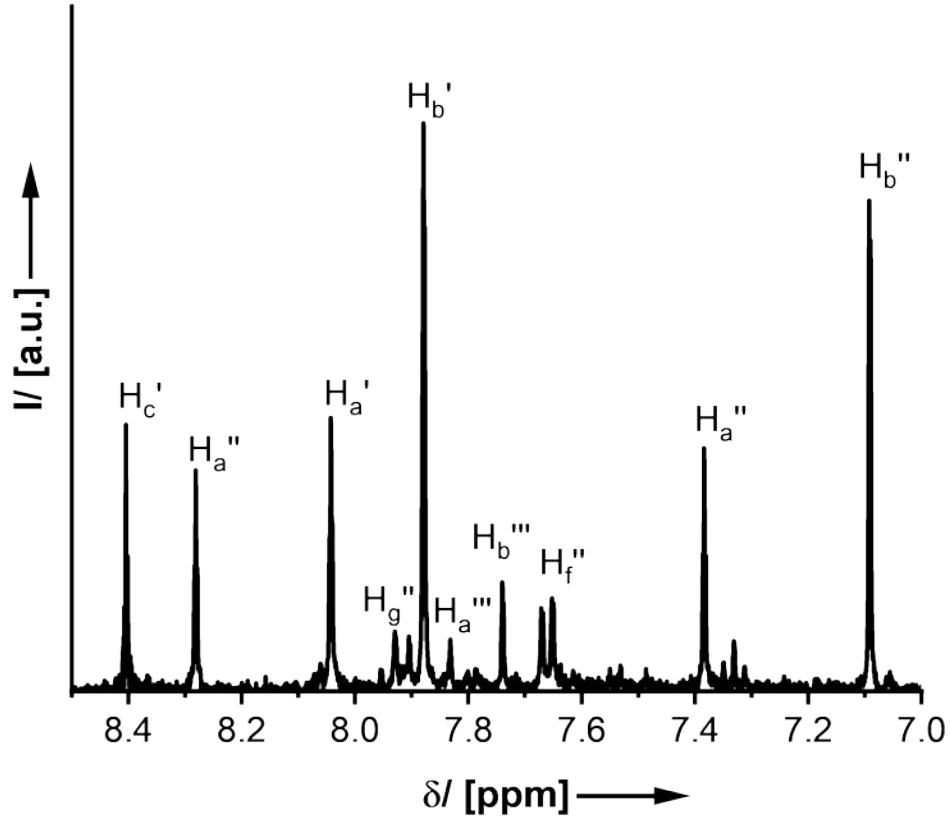
(b) N_2 physisorption isotherm; A_{BET} = 330 m^2/g.



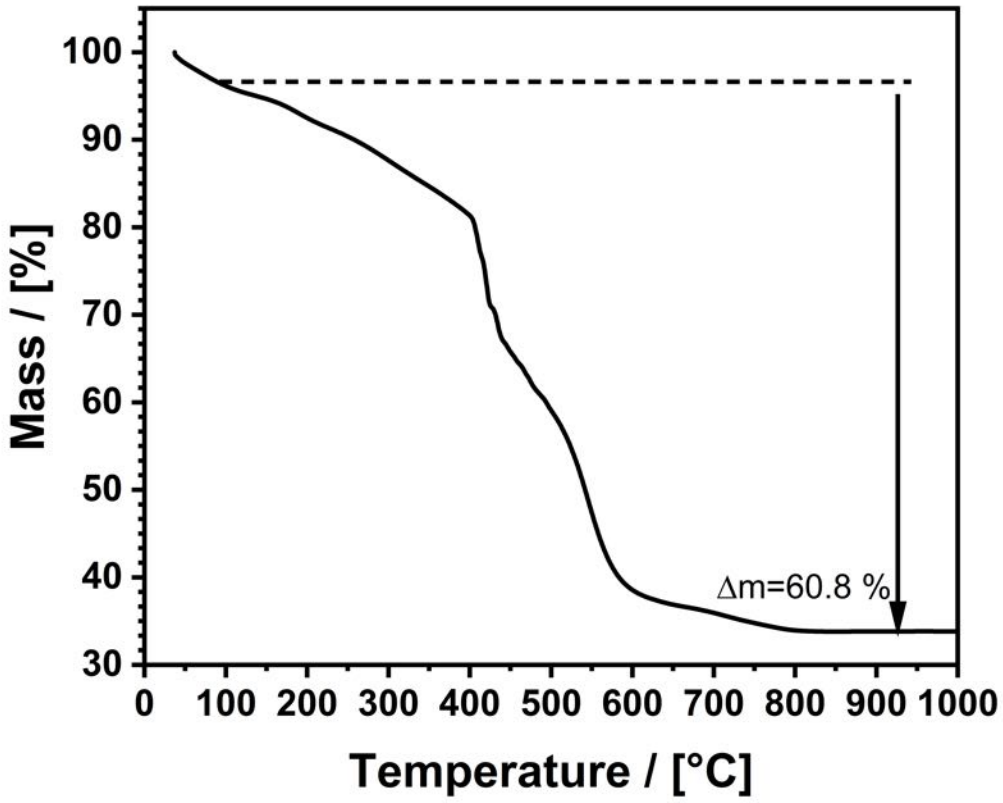


(c) FT-IR spectrum. **ATR-IR**



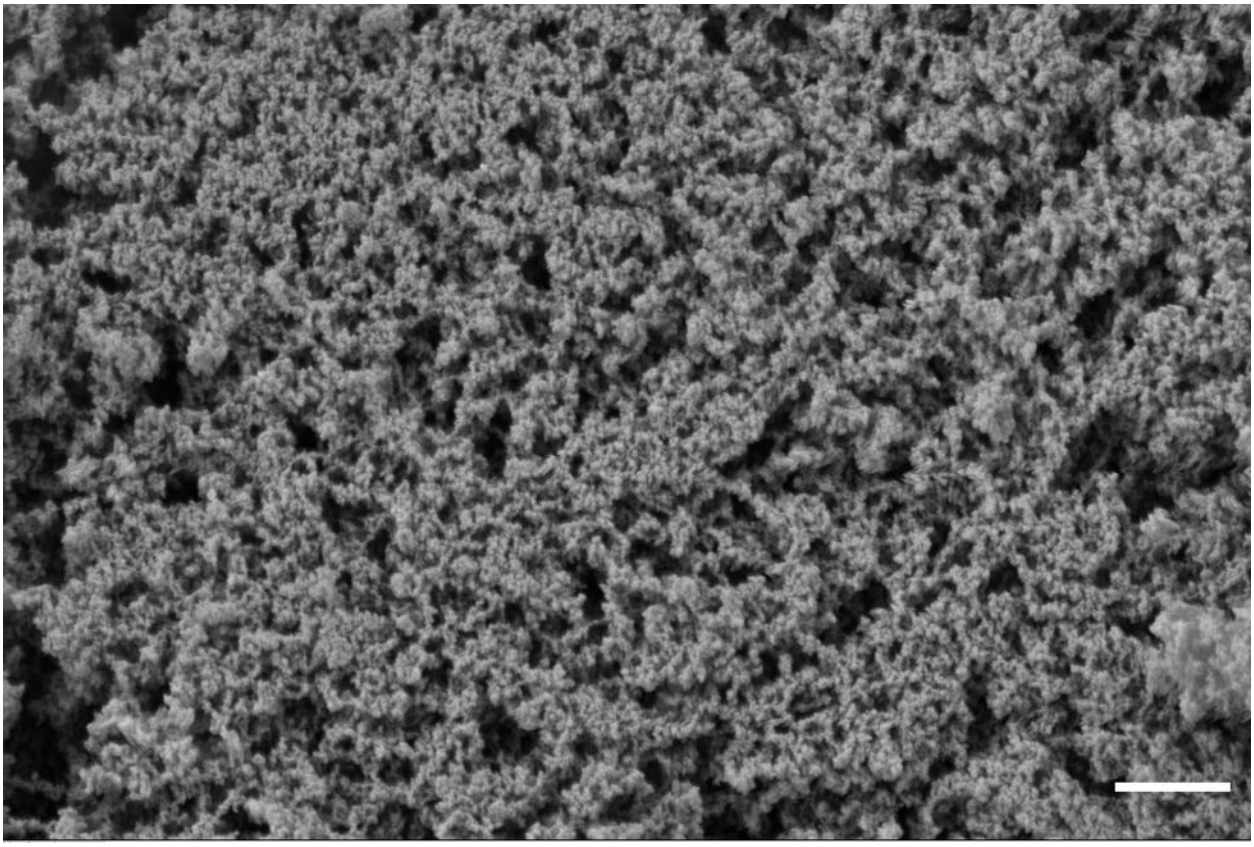


(d) ^{1}H-NMR of dissolved material (aromatic region)

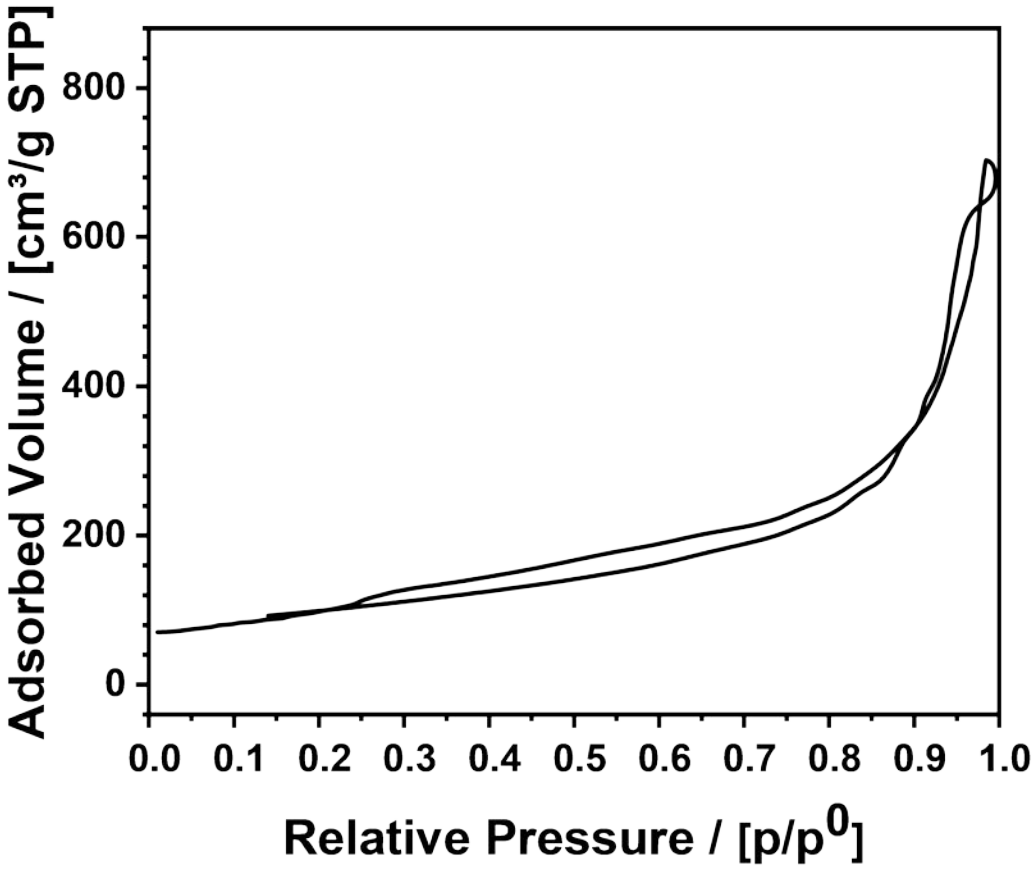

Mass / [%]
Temperature / [°C]
Δm=60.8 %
100
90
80
70
60
50
40
30
0
100
200
300
400
500
600
700
800
900
1000

(e) TGA in air.

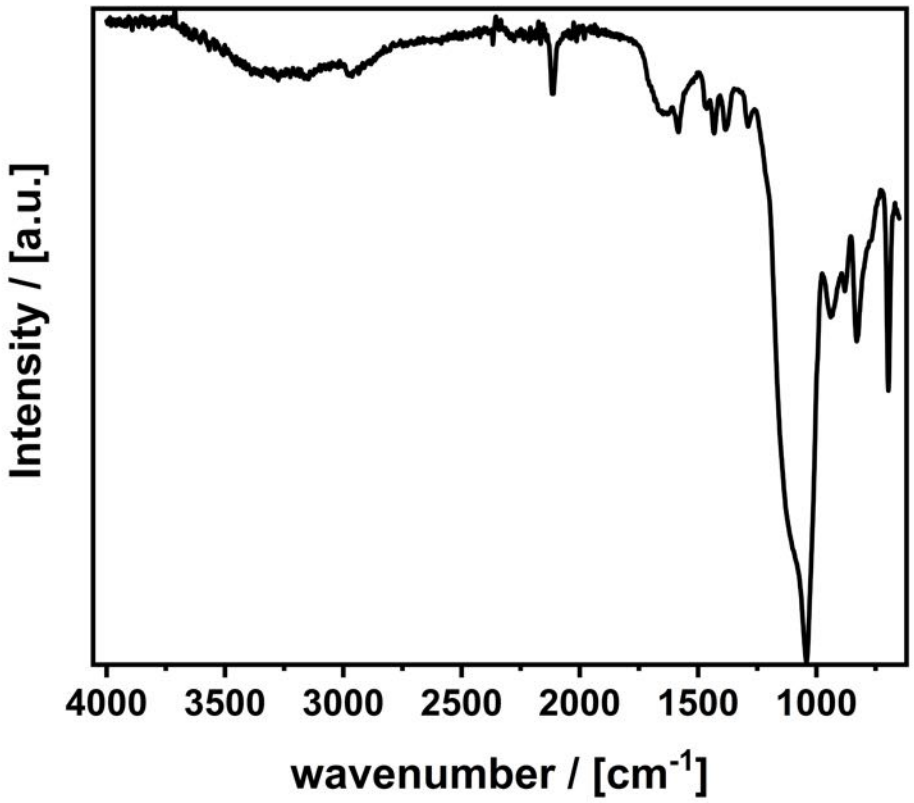
Fig. S7. Analytical Data for AmSP(e)Sil.



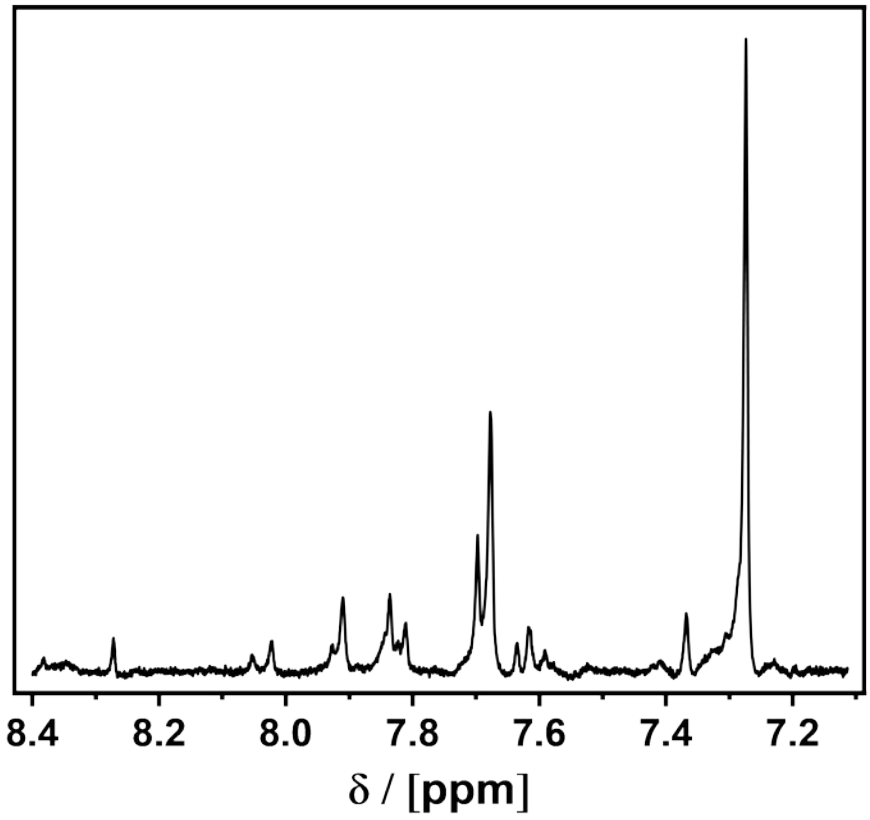
(a) SEM micrograph; scalebar = 1μm.



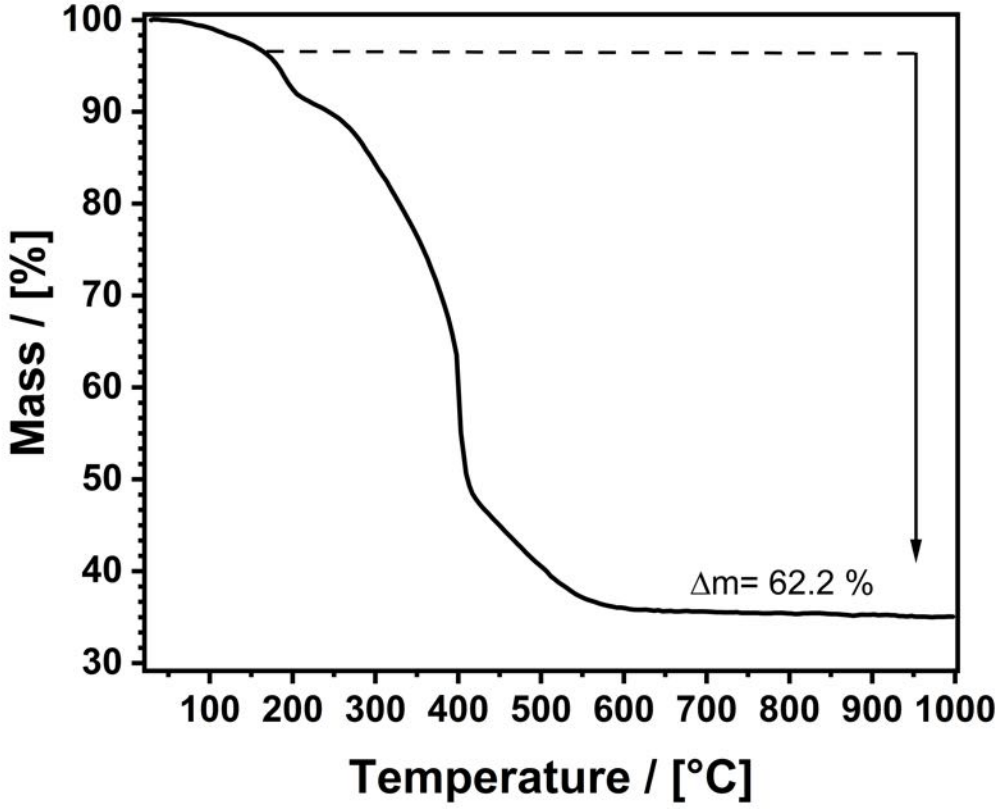
(b) N_2 physisorption isotherm; A_{BET} = 323 m^2/g.



(c) FT-IR spectrum. **ATR-IR**: ν (cm^{-1}) = 1044 (Si-O), 1316 (C(sp3)-C(sp3)), 1466 (C(sp3)C(sp3)) , 1578 (def. OH 1623 2115 (N_3), 2851, 2920 (C-H), 3300 (OH)

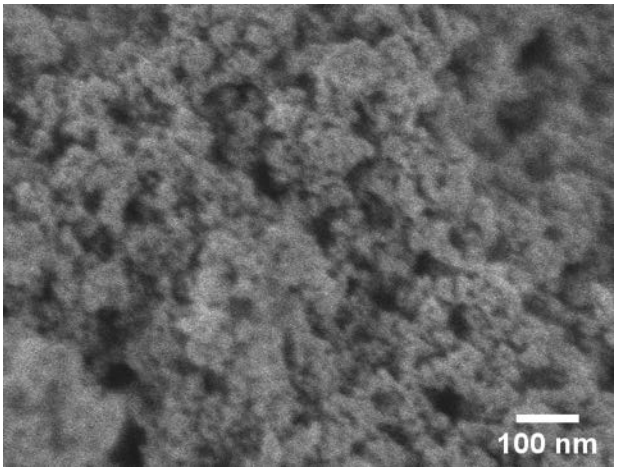


(d) ^{1}H-NMR of dissolved material.

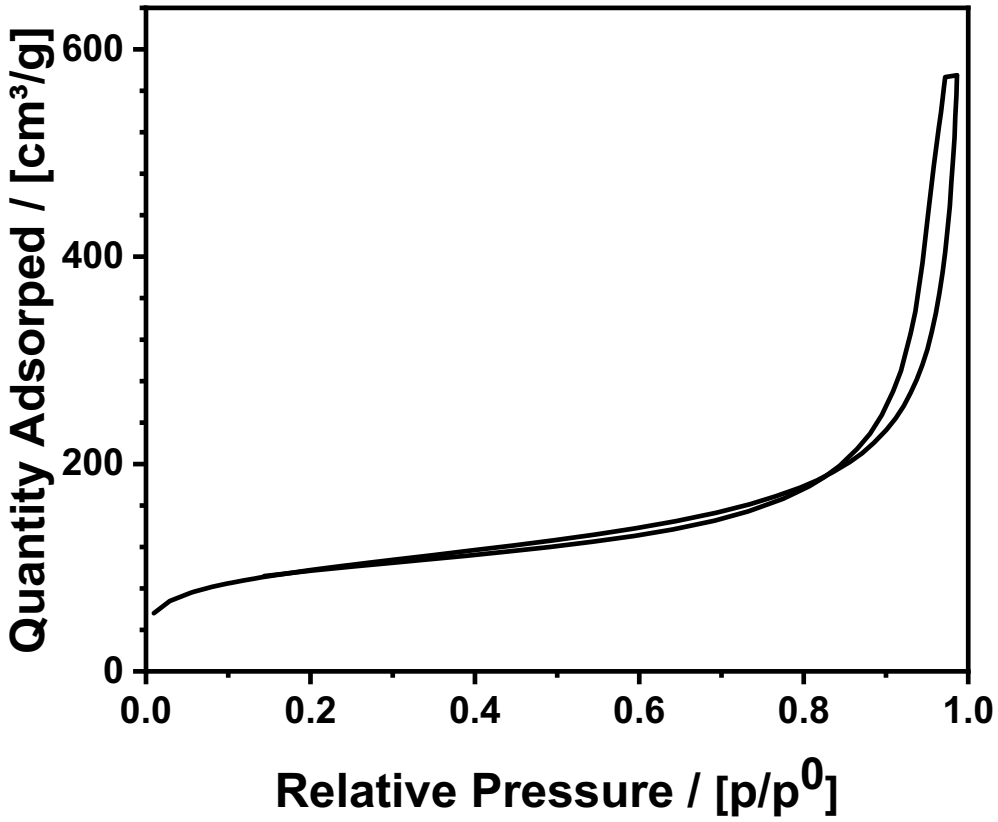

100
90
80
70
60
50
40
30
Mass / [%]
100 200 300 400 500 600 700 800 900 1000
Temperature / [°C]
Δm= 62.2 %

(e) TGA in air.

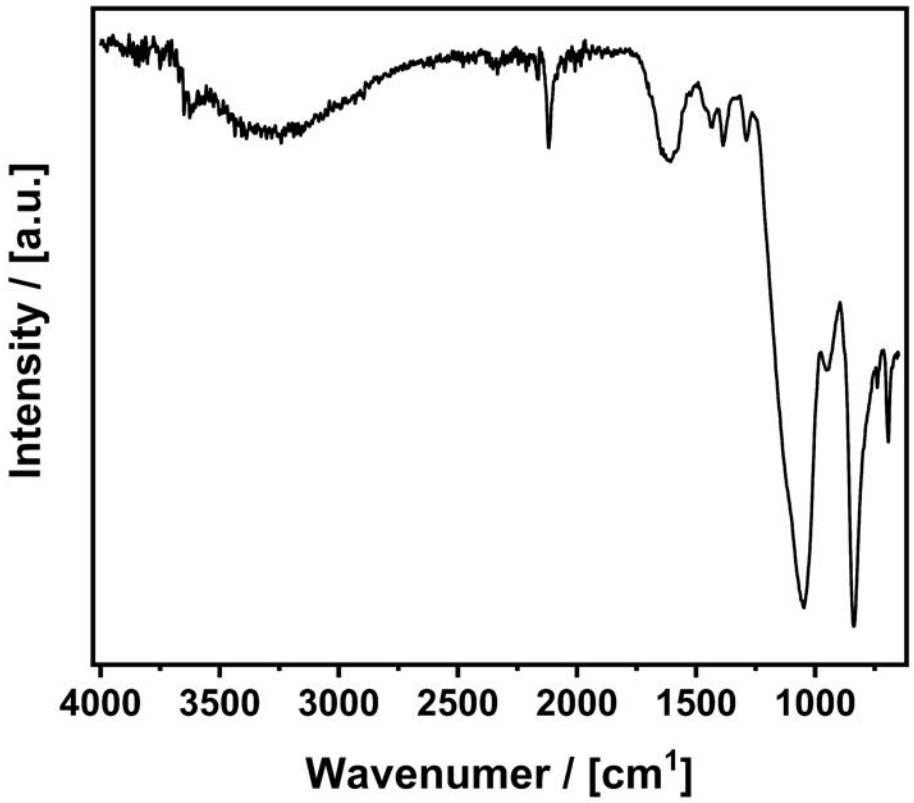
Fig. S8. Analytical Data for AmSP(f)Sil.



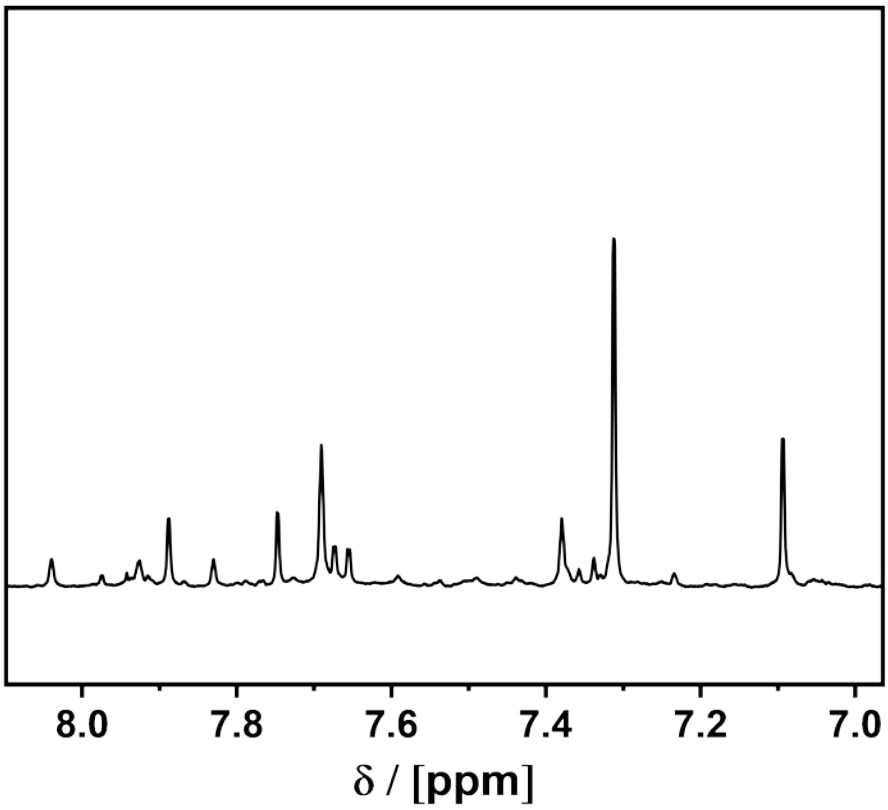
(a) SEM micrograph; scalebar = 100 nm.



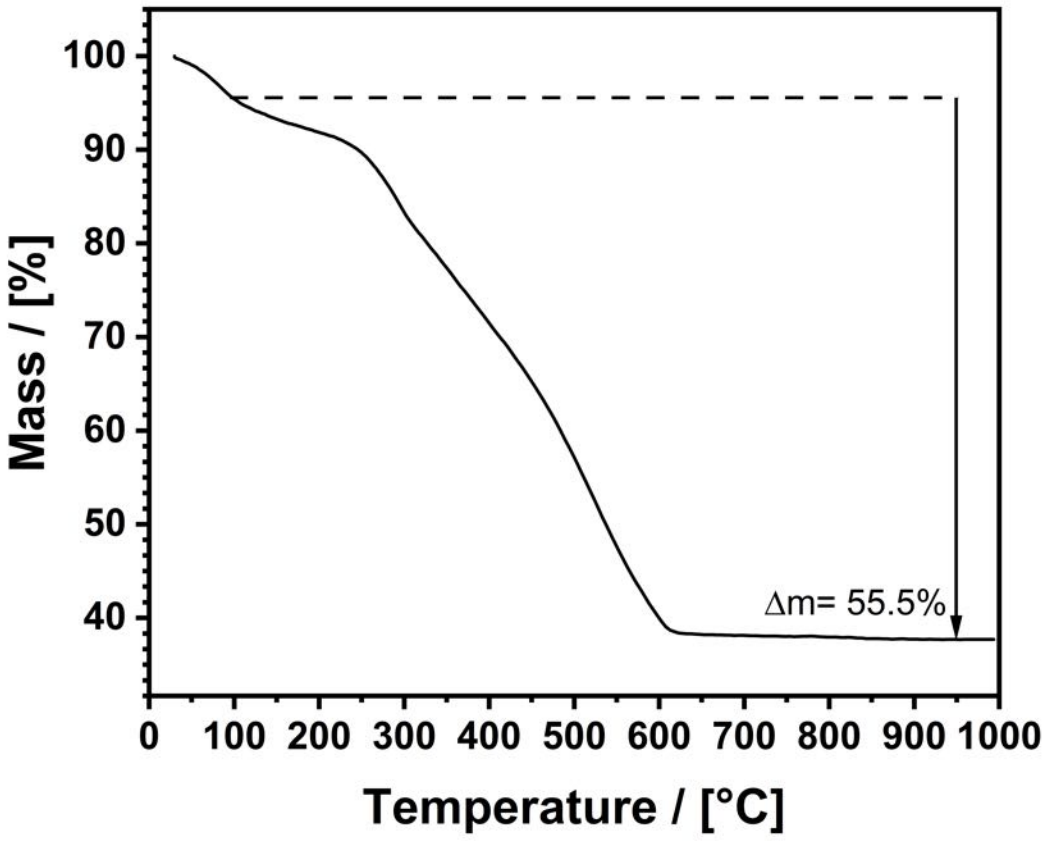
(b) N_2 physisorption isotherm; A_{BET} = 351 m^2/g.



(c) FT-IR spectrum. **ATR-IR**: ν (cm^{-1}) = 1044 (Si-O), 1316 (C(sp3)-C(sp3)), 1466 (C(sp3)C(sp3)) , 1578 (NH3) 2115 (N_3), 2851, 2920 (C-H), 3300 (OH)



(d) ^{1}H-NMR of dissolved material.


100
90
80
70
60
50
40
Mass / [%]
Δm= 55.5%
0
100
200
300
400
500
600
700
800
900
1000
Temperature / [°C]

(e) TGA in air.

Fig. S9. H_2O adsorption on organosilica materials.

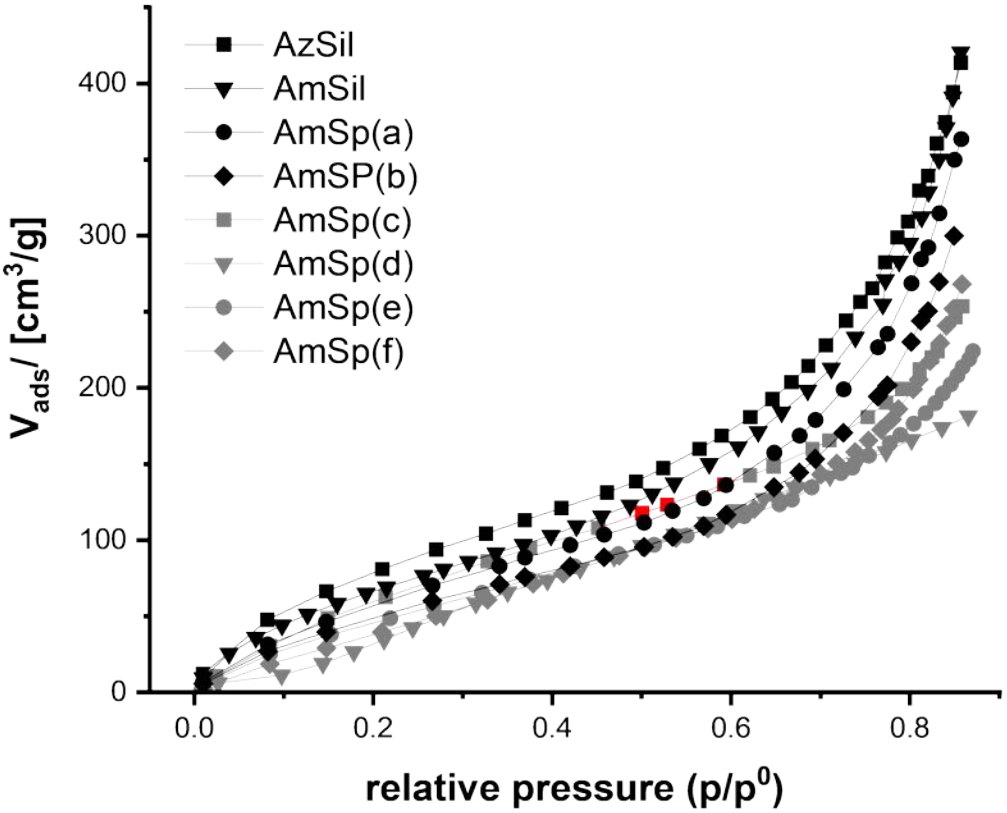
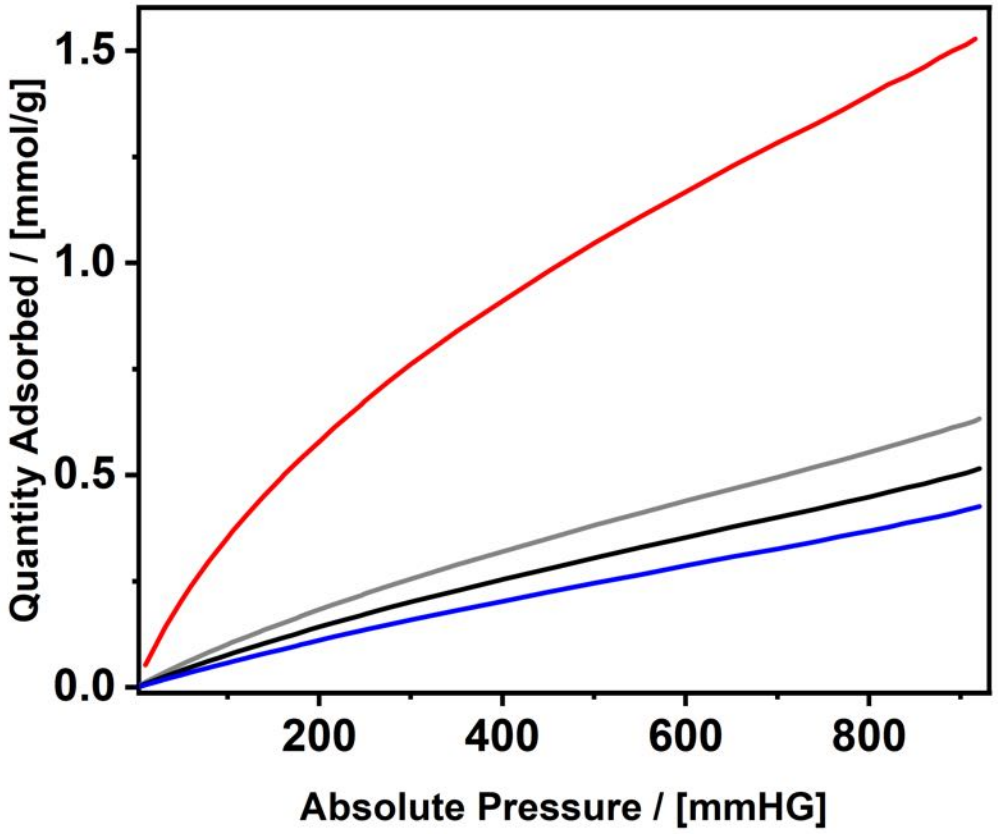
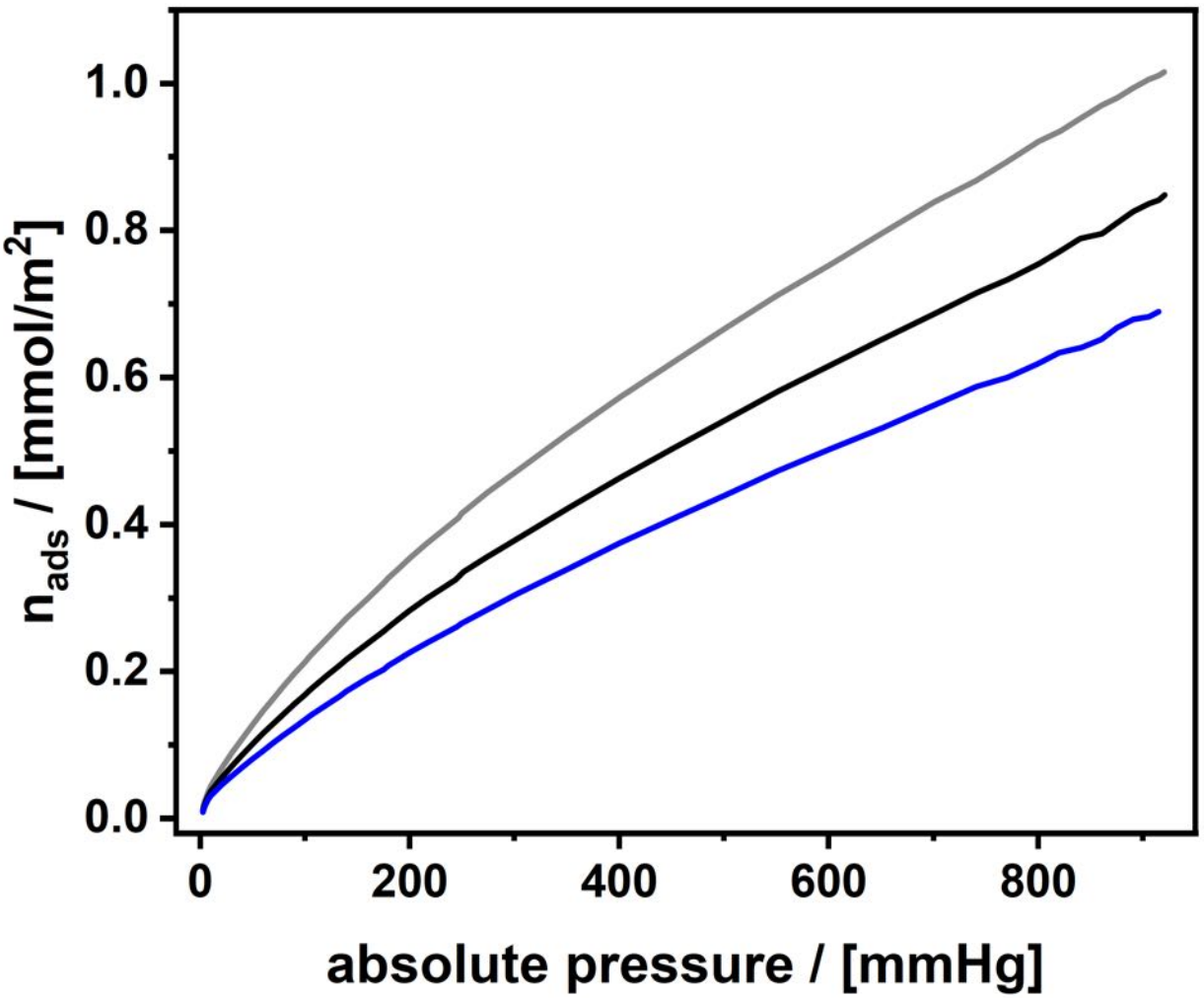


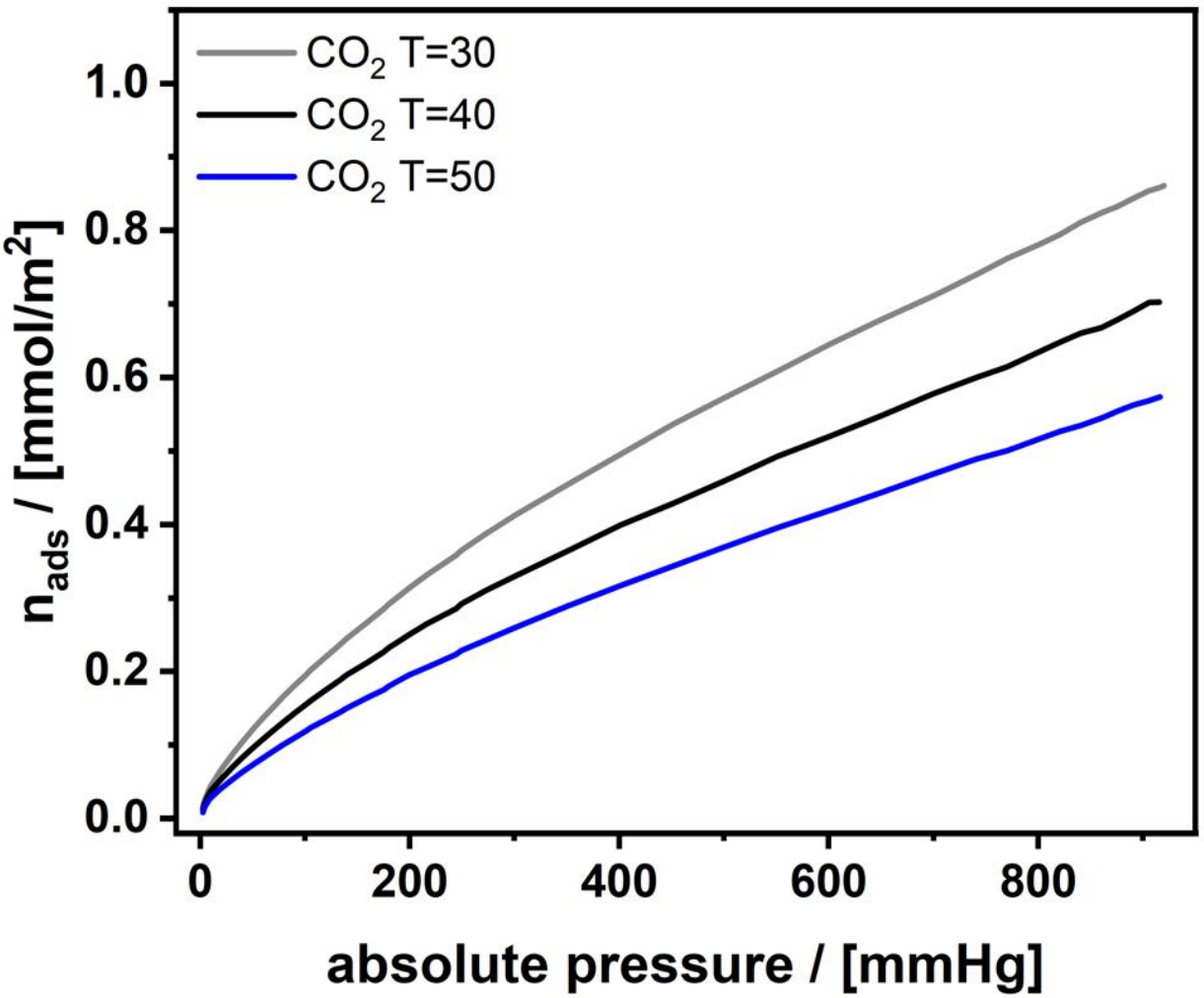
Fig. S10. Carbon Dioxide Adsorption



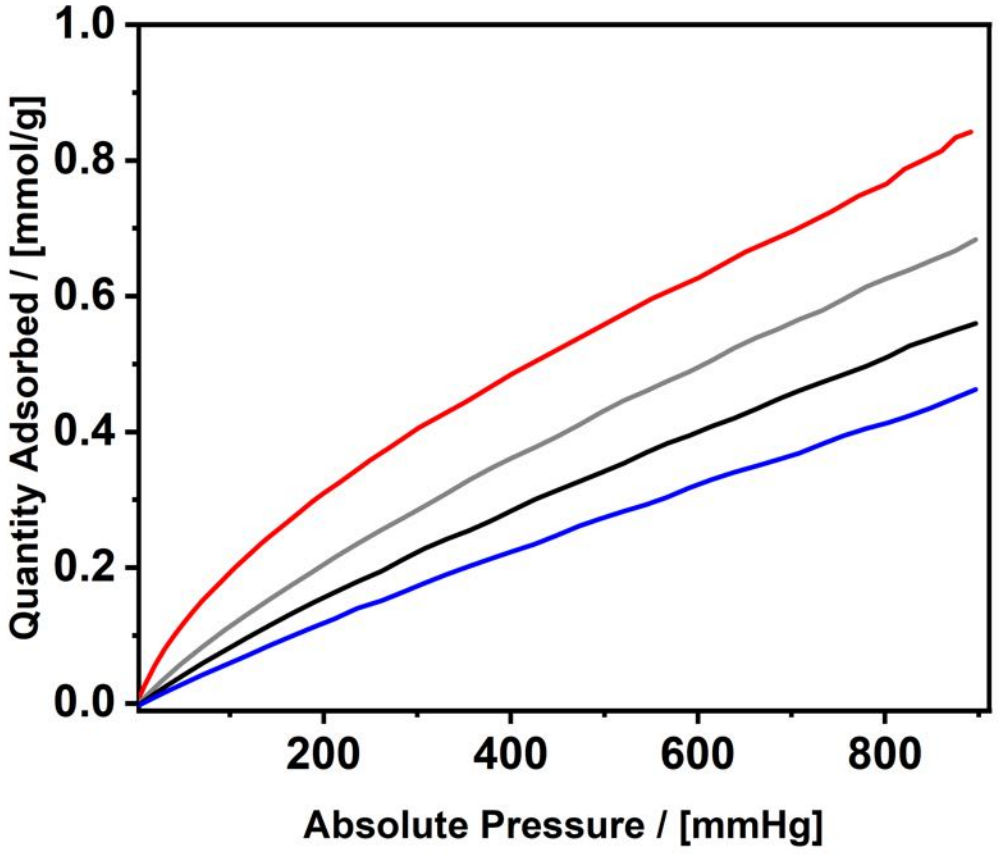
(a) CO_2(g) adsorption isotherms of AmSil measured a T = 0°C (red), 30°C (grey), 40°C (black), 50°C (blue).



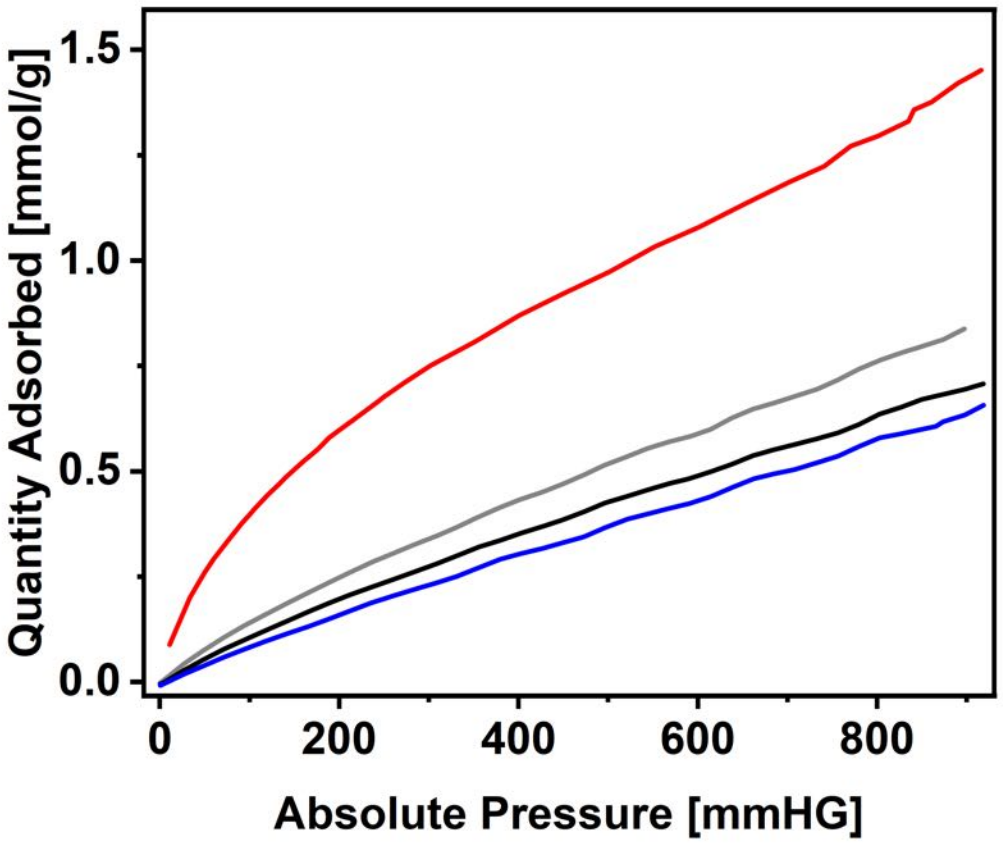
(b) CO_2(g) adsorption isotherms of AmSp(a) measured a T = 0°C (red), 30°C (grey), 40°C (black), 50°C (blue).



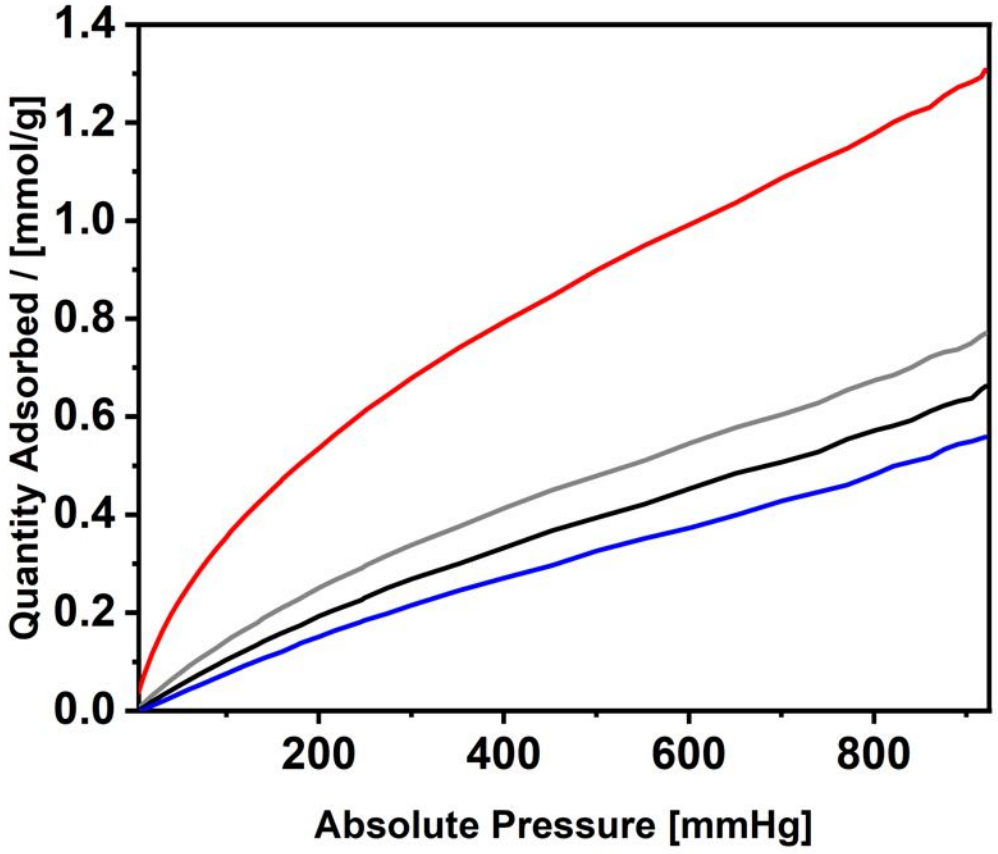
(c) CO_2(g) adsorption isotherms of AmSp(b) measured a T = 0°C (red), 30°C (grey), 40°C (black), 50°C (blue).



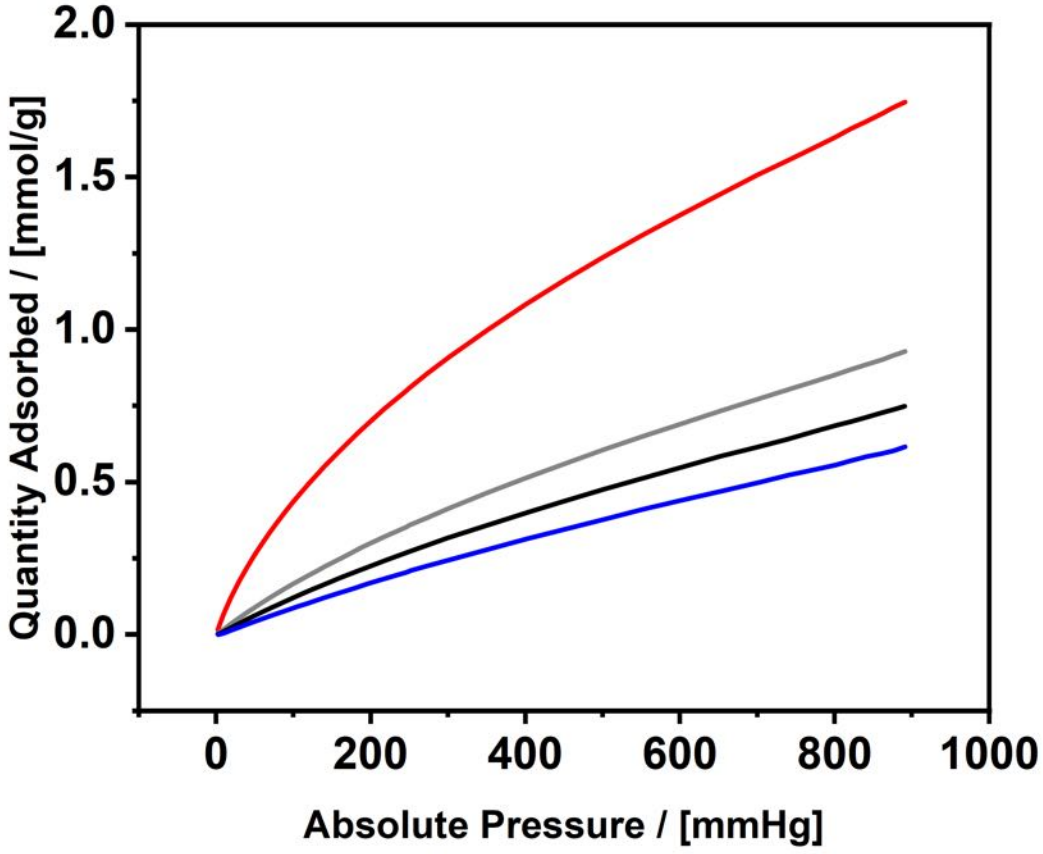
(d) CO_2(g) adsorption isotherms of AmSp(c) measured a T = 0°C (red), 30°C (grey), 40°C (black), 50°C (blue).



(e) CO_2(g) adsorption isotherms of AmSp(d) measured a T = 0°C (red), 30°C (grey), 40°C (black), 50°C (blue).

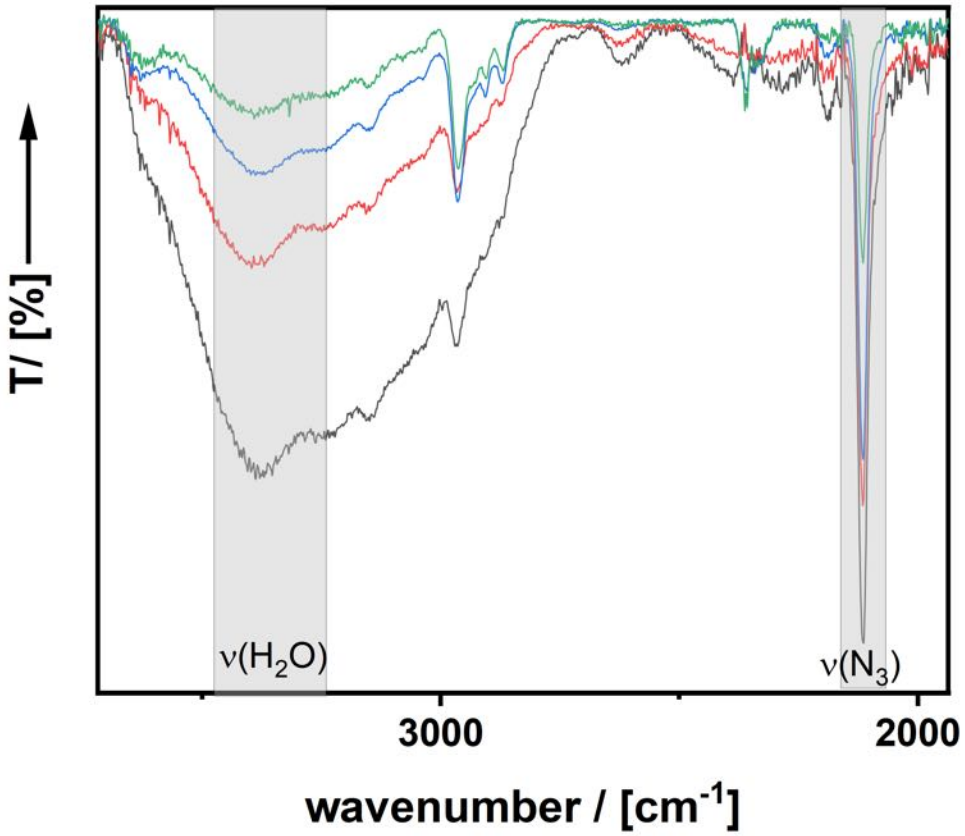


(f) CO_2(g) adsorption isotherms of AmSp(e) measured a T = 0°C (red), 30°C (grey), 40°C (black), 50°C (blue).



(g) CO_2(g) adsorption isotherms of AmSp(f) measured a T = 0°C (red), 30°C (grey), 40°C (black), 50°C (blue).

Fig. S11. Gradient Material



IR spectra recorded along the gradient.