

Supporting Information

Influence of Organic Acids Concentration on Wettability Alteration of Cap-Rock: Implications for CO₂ Trapping/Storage

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Table S1. Surface analysis of mica substrates by EDS

Concentration (Molarity)	Pure Mica					After ageing					Change due to ageing				
	wt% Si	wt% C	wt% O	wt% Al	wt% K	wt% Si	wt% C	wt% O	wt% Al	wt% K	wt% Si	wt% C	wt% O	wt% Al	wt% K
Hexanoic Acid															
10^{-2}	20.4	2.8	50.1	18.8	7.9	19.8	4.9	51.8	17.2	6.3	-0.6	+2.1	+1.7	-1.6	-1.6
10^{-3}	22.1	2.4	49.6	18.2	7.7	18.7	3.9	52.4	18.3	6.7	-3.4	+1.5	+2.8	+0.1	-1.0
10^{-5}	23.7	3.1	46.0	19.4	7.8	20.2	4.2	50.5	17.9	7.2	-3.5	+1.1	+4.5	-1.5	-0.6
10^{-7}	21.7	2.6	47.6	19.7	8.4	18.9	3.3	51.7	18.5	7.6	-2.8	+0.7	+4.1	-1.2	-0.8
10^{-9}	21.1	2.9	49.2	19.3	7.5	20.7	3.4	48.4	19.1	8.4	-0.4	+0.5	-0.8	-0.2	+0.9
0	21.5	3.7	46.8	19.8	8.2	21.5	3.7	46.8	19.8	8.2	0	0	0	0	0
Lauric Acid															
10^{-2}	22.3	3.8	44.7	20.1	9.1	19.4	7.0	46.8	19.7	7.1	-2.9	+3.2	+2.1	-0.4	-2.0
10^{-3}	22.4	2.4	46.5	20.4	8.3	21.7	4.0	48.8	18.6	6.9	-0.7	+1.6	+2.3	-1.8	-1.4
10^{-5}	21.9	2.7	47.1	19.7	8.6	22.0	3.9	48.1	17.8	8.2	+0.1	+1.2	+1.0	-1.9	-0.4
10^{-7}	21.7	2.8	48.7	19.1	7.7	21.4	3.7	48.2	19.3	7.4	-0.3	+0.9	-0.5	+0.2	-0.3
10^{-9}	23.2	3.1	46.9	18.7	8.1	19.7	3.8	50.7	17.9	7.9	-3.5	+0.7	+3.8	-0.8	-0.2
0	21.5	3.7	46.8	19.8	8.2	21.5	3.7	46.8	19.8	8.2	0	0	0	0	0
Stearic Acid															
10^{-2}	21.1	3.3	46.7	20.2	8.7	20.2	6.7	47.1	19.3	6.7	-0.9	+3.4	+0.4	-0.9	-2.0
10^{-3}	22.2	3.4	45.3	20.3	8.8	22.1	6.1	46.4	18.9	6.5	-0.1	+2.7	+1.1	-1.4	-2.3
10^{-5}	22.6	2.9	45.4	19.5	9.6	20.8	4.4	47.8	19.7	7.3	-1.8	+1.5	+2.4	+0.2	-2.3
10^{-7}	23.4	2.6	47.0	18.7	8.3	20.5	3.6	50.2	17.9	7.8	-2.9	+1.0	+3.2	-0.8	-0.5
10^{-9}	23.1	3.1	45.2	19.9	8.7	19.6	4.0	50.0	19.5	6.9	-3.5	+0.9	+4.8	-0.4	-1.8
0	21.5	3.7	46.8	19.8	8.2	21.5	3.7	46.8	19.8	8.2	0	0	0	0	0
Lignoceric Acid															
10^{-2}	22.8	3.1	47.1	17.9	9.1	19.4	6.8	48.7	17.8	7.3	-3.4	+3.7	+1.6	-0.1	-1.8
10^{-3}	21.9	2.9	47.5	18.9	8.8	20.7	5.6	45.5	19.8	8.4	-1.2	+2.7	-2.0	+0.9	-0.4
10^{-5}	23.5	2.8	45.7	19.1	8.9	19.8	4.5	48.3	19.5	7.9	-3.7	+1.7	+2.6	+0.4	-1.0
10^{-7}	23.3	3.5	44.5	19.3	9.4	20.9	5.1	49.1	18.4	6.5	-2.4	+1.6	+4.6	-0.9	-2.9
10^{-9}	21.7	3.1	47.0	20.1	8.1	21.4	4.2	48.2	18.6	7.6	-0.3	+1.1	+1.2	-1.5	-0.5
0	21.5	3.7	46.8	19.8	8.2	21.5	3.7	46.8	19.8	8.2	0	0	0	0	0

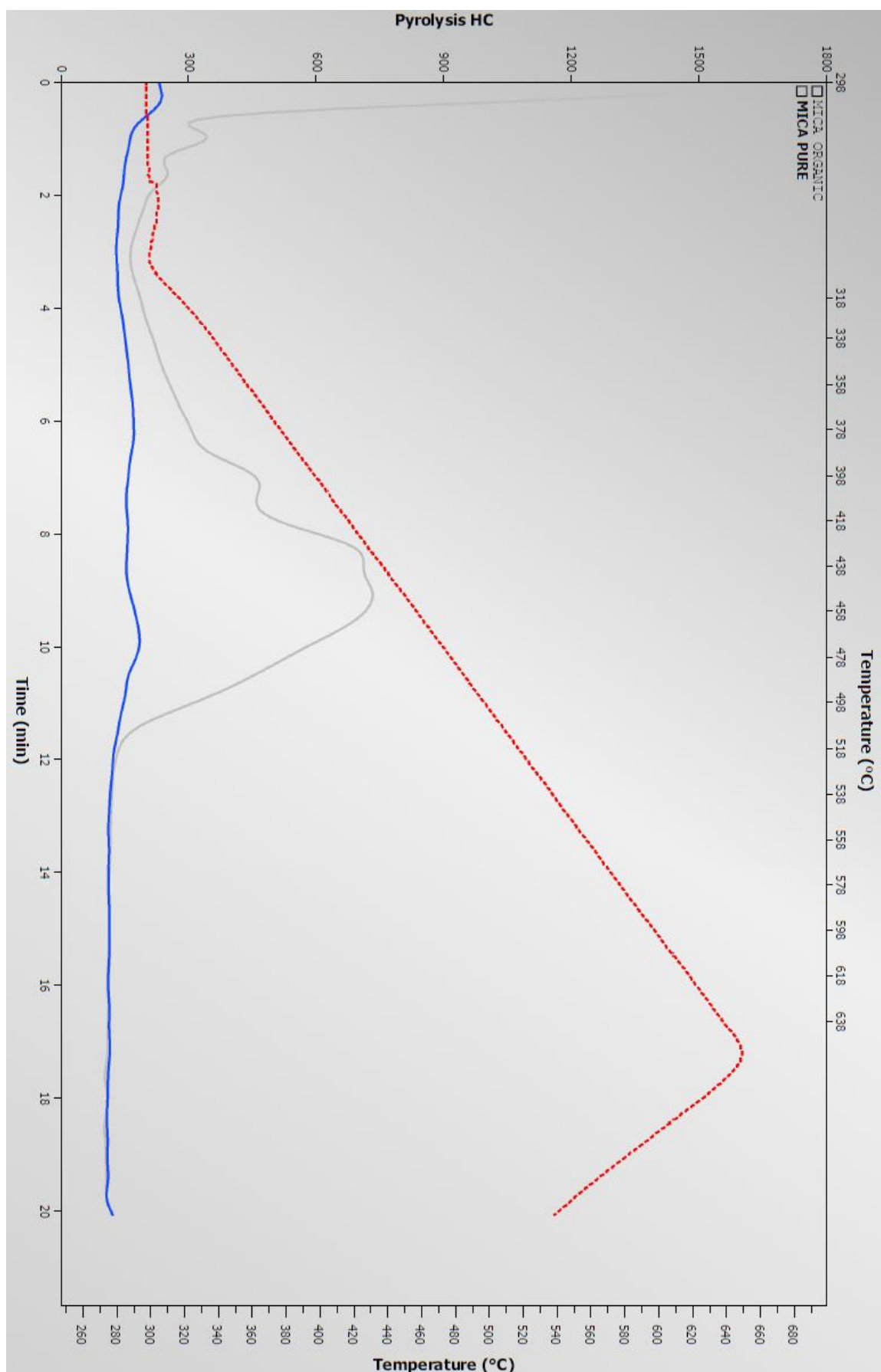


Figure S1. Total Organic Carbon (TOC) determination of pure and aged mica substrates (blue line represent the pure mica substrate and grey line represent the aged mica substrate)

X-ray Diffraction (XRD) Measurements

XRD is most commonly used to measure bulk mineralogy ¹. The XRD patterns of pure and organic aged mica samples are shown in Figure S2. The measured XRD spectra for (Mica Pure – blue line) showed oriented mica, silica and zeolite ¹; In addition to this, XRD spectra for (Mica Organic – red line) depicted oriented mica superimposed on muscovite/illite pattern with presence of silica and zeolite crystals. These minerals are also abundantly found in shale cap-rock, which makes mica a perfect proxy for cap-rock in pristine form for investigating the effects of organics on wettability.

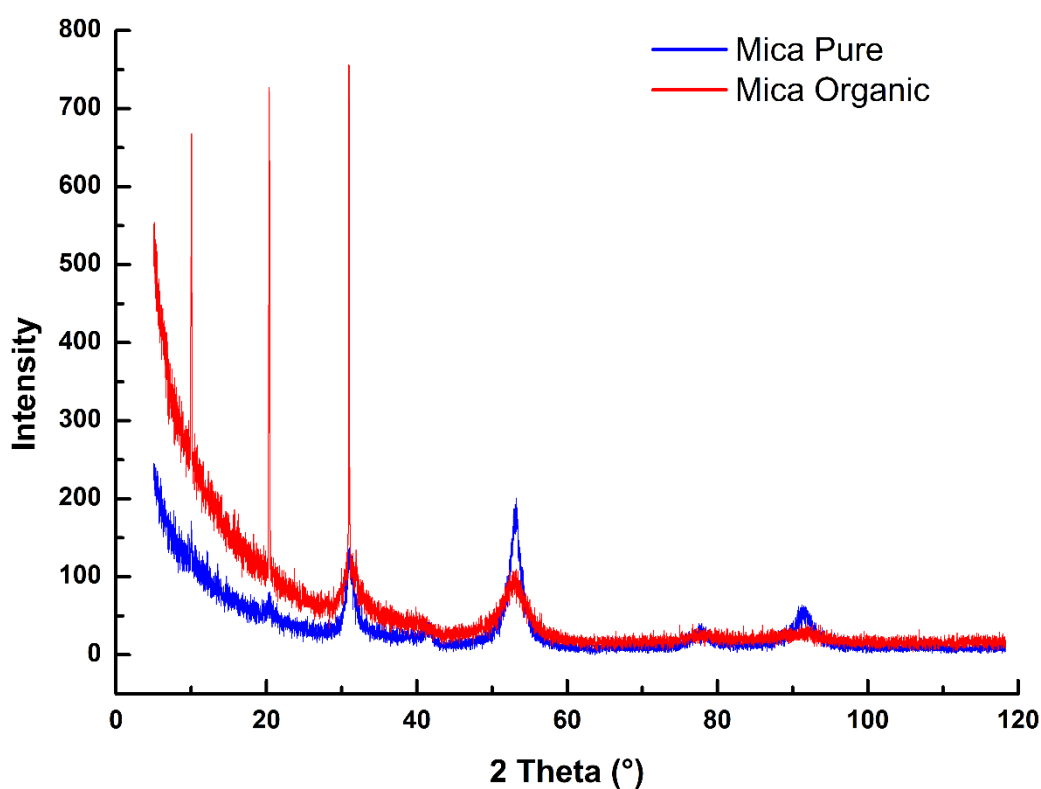


Figure S2. XRD spectra of Pure and Organic aged mica substrates.

References

1. Eskelinen, P., X-ray diffraction study of TiO₂ thin films on mica. *Journal of solid state chemistry* **1992**, *100* (2), 356-362.