

Table A2.2 - FT-IR Parameters for SULm samples

Sample	X _{H₂O} ^{fl}	Density [g/cm ³]	Thickness [μm]	A ₄₅₀₀	A ₅₂₀₀	OH [wt%]	H ₂ O _m [wt%]	H ₂ O _{tot.} [wt%]	Int ₉₇₀	A ₁₄₃₀ norm.	CO ₂ [ppm]
SULm_0.5_1	0.05	2.703 (24)	479 (6)	0.0105 (0)	0.0000 (0)	0.35 (2)	0.00 (0)	0.35 (2)	100.9 (1)	0.384 (9)	1610 (60)
SULm_0.5_6	1.00	2.731 (10)	475 (6)	0.0523 (0)	0.0591 (58)	1.77 (9)	0.84 (11)	2.61 (14)			
SULm_1_1	0.05	2.704 (12)	501 (8)	0.0150 (14)	0.0000 (0)	0.47 (5)	0.00 (0)	0.47 (5)	98.1 (23)	0.700 (17)	2940 (100)
SULm_1_2	0.14	2.700 (12)	501 (14)	0.0345 (0)	0.0202 (39)	1.09 (6)	0.27 (6)	1.36 (8)	100.5 (1)	0.634 (16)	2660 (90)
SULm_1_3	0.29	2.658 (31)	482 (5)	0.0477 (0)	0.0301 (38)	1.60 (8)	0.42 (7)	2.02 (10)	97.0 (17)	0.523 (13)	2200 (80)
SULm_1_4	0.52	2.675 (5)	485 (18)	0.0588 (38)	0.0577 (0)	1.94 (17)	0.80 (8)	2.74 (19)	100.8 (2)	0.423 (10)	1780 (60)
SULm_1_5	0.76	2.647 (10)	501 (1)	0.0709 (0)	0.0501 (0)	2.29 (11)	1.19 (11)	3.48 (15)	99.4 (2)	0.317 (8)	1330 (50)
SULm_1_6	1.00	2.644 (5)	486 (3)	0.0676 (0)	0.1062 (38)	2.26 (11)	1.49 (14)	3.75 (18)			
SULm_1.5_1	0.03	2.706 (14)	464 (6)	0.0105 (0)	0.0000 (0)	0.36 (2)	0.00 (0)	0.36 (2)	94.5 (46)	0.915 (22)	3850 (140)
SULm_1.5_6	0.97	2.666 (14)	482 (11)	0.0622 (73)	0.1826 (74)	2.08 (27)	2.56 (26)	4.65 (37)			
SULm_2_1	0.02	2.712 (15)	428 (7)	0.0136 (0)	0.0000 (0)	0.50 (3)	0.00 (0)	0.50 (3)	99.1 (1)	1.351 (33)	5680 (200)
SULm_2_2	0.18	2.709 (30)	463 (4)	0.0389 (38)	0.0224 (38)	1.33 (15)	0.32 (6)	1.65 (16)	98.1 (1)	1.297 (32)	5450 (190)
SULm_2_3	0.31	2.674 (9)	465 (6)	0.0577 (0)	0.0610 (0)	1.99 (10)	0.88 (8)	2.87 (13)	100.5 (2)	1.107 (27)	4650 (160)
SULm_2_4	0.52	2.650 (17)	438 (2)	0.0643 (0)	0.0941 (0)	2.38 (11)	1.46 (13)	3.84 (17)	99.0 (1)	0.888 (22)	3730 (130)
SULm_2_5	0.77	2.661 (11)	458 (6)	0.0651 (90)	0.1658 (60)	2.29 (34)	2.45 (24)	4.74 (41)	101.2 (1)	0.585 (14)	2460 (90)
SULm_2_6	1.00	2.623 (13)	462 (5)	0.073 (0)	0.2183 (60)	2.58 (13)	3.24 (31)	5.82 (33)			
SULm_2.5_1	0.02	2.718 (11)	488 (4)	0.0115 (36)	0.0000 (0)	0.37 (12)	0.00 (0)	0.37 (12)	98.5 (1)	1.503 (37)	6320 (220)
SULm_2.5_6	0.99	2.640 (11)	465 (13)	0.0675 (63)	0.1909 (0)	2.36 (26)	2.80 (27)	5.16 (37)			
SULm_3_1	0.03	2.713 (4)	459 (3)	0.019 (0)	0.0000 (0)	0.65 (3)	0.00 (0)	0.65 (3)	99.3 (4)	2.012 (49)	8460 (300)
SULm_3_2	0.13	2.689 (14)	459 (5)	0.0490 (61)	0.0331 (61)	1.71 (23)	0.48 (10)	2.19 (25)	98.0 (2)	1.832 (45)	7700 (270)
SULm_3_3	0.32	2.667 (11)	464 (3)	0.0666 (3)	0.0872 (24)	2.31 (11)	1.27 (12)	3.58 (16)	98.4 (1)	1.568 (38)	6590 (230)
SULm_3_4	0.55	2.671 (12)	434 (8)	0.0648 (57)	0.1516 (146)	2.40 (24)	2.36 (31)	4.76 (40)	100.3 (3)	1.365 (33)	5740 (200)
SULm_3_5	0.79	2.644 (7)	440 (2)	0.0680 (57)	0.2440 (111)	2.51 (24)	3.78 (38)	6.29 (45)	98.3 (2)	0.879 (22)	3700 (130)
SULm_3_6	0.96	2.568 (27)	438 (5)	0.0729 (55)	0.2811 (55)	2.78 (25)	4.51 (42)	7.29 (49)			
SULm_0.5		2.716 (11)	338 (2)	0.0156 (0)	0.0000 (0)	0.71 (3)	0.00 (0)	0.71 (3)			
SULm_1.0		2.705 (17)	332 (4)	0.0215 (68)	0.0036 (42)	1.03 (33)	0.07 (8)	1.10 (34)			

Notes:

Calculated errors are shown in brackets near values.

Concentration of H₂O determined by NIR, Concentration of CO₂ determined by ATR.

Errors of H₂O species were calculated by error propagation of density, thickness and absorbance errors.

CO₂ content errors were calculated by error propagation of peak height, Int970 and baseline error.

X_{H₂O}^{fl} refers to the mole fractions of H₂O in the fluid phase present in the capsules after experiments.

$$A_{1430\text{norm.}} = (A_{1430} * 10000) / \text{Int}_{970}$$