

Table A2.1 - FT-IR Parameters for VES79 samples

| Sample | $X_{\text{H}_2\text{O}}^{\text{fl}}$ | Density [g/cm ³] | Thickness ^{*1} [μm] | A ₄₅₀₀ | A ₅₂₀₀ | OH [wt%] | H ₂ O _m [wt%] | H ₂ O _{tot.} [wt%] | Thickness ^{*2} [μm] | A ₁₄₃₀ | CO ₂ [wt%] |
|-------------|--------------------------------------|---------------------------------|---------------------------------|-------------------|-------------------|-------------|----------------------------------------|-------------------------------------------|---------------------------------|-------------------|--------------------------|
| VES79_0.5_1 | 0.02 | 2.435 (8) | 471 (6) | 0.0061 (96) | 0.000 (0) | 0.09 (14) | 0.00 (0) | 0.09 (14) | 112 (12) | 0.042 (7) | 280 (60) |
| VES79_0.5_6 | 0.99 | 2.435 (6) | 489 (6) | 0.0624 (0) | 0.0879 (0) | 0.94 (6) | 1.13 (4) | 2.07 (7) | 115 (5) | 0.000 (0) | |
| VES79_1_1 | 0.03 | 2.416 (20) | 417 (4) | 0.0175 (10) | 0.0000 (0) | 0.31 (3) | 0.00 (0) | 0.31 (3) | 159 (2) | 0.111 (0) | 520 (30) |
| VES79_1_2 | 0.20 | 2.434 (9) | 413 (8) | 0.0445 (10) | 0.0111 (27) | 0.80 (5) | 0.17 (4) | 0.97 (7) | 162 (4) | 0.099 (5) | 450 (30) |
| VES79_1_3 | 0.41 | 2.428 (10) | 411 (12) | 0.0659 (20) | 0.0354 (18) | 1.19 (9) | 0.55 (4) | 1.74 (10) | 161 (6) | 0.090 (7) | 410 (40) |
| VES79_1_4 | 0.62 | 2.426 (9) | 437 (1) | 0.0806 (10) | 0.0618 (0) | 1.37 (8) | 0.89 (3) | 2.26 (9) | 160 (19) | 0.075 (11) | 350 (70) |
| VES79_1_5 | 0.91 | 2.415 (28) | 444 (6) | 0.0917 (18) | 0.1148 (10) | 1.54 (10) | 1.64 (7) | 3.18 (12) | 164 (5) | 0.050 (0) | 220 (10) |
| VES79_1_6 | 0.98 | 2.413 (20) | 444 (4) | 0.0958 (10) | 0.1403 (20) | 1.61 (10) | 2.01 (8) | 3.62 (13) | 153 (16) | 0.000 (0) | |
| VES79_1.5_1 | 0.02 | 2.460 (13) | 474 (6) | 0.0157 (0) | 0.0000 (0) | 0.24 (1) | 0.00 (0) | 0.24 (1) | 105 (3) | 0.111 (5) | 770 (60) |
| VES79_1.5_6 | 1.00 | 2.409 (7) | 425 (6) | 0.0994 (47) | 0.1666 (47) | 1.75 (14) | 2.50 (12) | 4.25 (18) | 112 (6) | 0.000 (0) | |
| VES79_2_1 | 0.16 | 2.463 (28) | 485 (10) | 0.0162 (0) | 0.0000 (0) | 0.24 (2) | 0.00 (0) | 0.24 (2) | 163 (2) | 0.260 (4) | 1160 (60) |
| VES79_2_2 | 0.26 | 2.456 (15) | 481 (3) | 0.0633 (10) | 0.0284 (18) | 0.96 (6) | 0.37 (3) | 1.33 (7) | 169 (7) | 0.234 (11) | 1010 (80) |
| VES79_2_3 | 0.42 | 2.434 (9) | 463 (12) | 0.0873 (0) | 0.0914 (20) | 1.40 (9) | 1.25 (6) | 2.65 (11) | 155 (20) | 0.220 (4) | 1050 (140) |
| VES79_2_4 | 0.62 | 2.424 (8) | 472 (5) | 0.0987 (18) | 0.1397 (10) | 1.55 (10) | 1.88 (7) | 3.43 (12) | 156 (4) | 0.190 (0) | 900 (50) |
| VES79_2_5 | 0.83 | 2.392 (42) | 462 (10) | 0.1043 (10) | 0.2145 (10) | 1.70 (11) | 2.98 (13) | 4.68 (17) | 156 (9) | 0.124 (13) | 600 (80) |
| VES79_2_6 | 0.96 | 2.380 (36) | 437 (3) | 0.1084 (0) | 0.2696 (10) | 1.88 (12) | 3.99 (15) | 5.87 (19) | 155 (12) | 0.000 (0) | |
| VES79_2.5_1 | 0.02 | 2.472 (8) | 462 (8) | 0.0143 (47) | 0.0000 (0) | 0.23 (8) | 0.00 (0) | 0.23 (8) | 115 (3) | 0.227 (8) | 1430 (100) |
| VES79_2.5_6 | 1.00 | 2.380 (21) | 466 (8) | 0.1104 (0) | 0.3327 (0) | 1.79 (11) | 4.61 (18) | 6.40 (21) | 107 (6) | 0.000 (0) | |
| VES79_3_1 | 0.16 | 2.462 (14) | 484 (5) | 0.0260 (10) | 0.0000 (0) | 0.39 (3) | 0.00 (0) | 0.39 (3) | 174 (2) | 0.426 (4) | 1790 (90) |
| VES79_3_2 | 0.30 | 2.441 (36) | 490 (6) | 0.0791 (10) | 0.0495 (18) | 1.19 (8) | 0.64 (3) | 1.83 (8) | 172 (5) | 0.394 (31) | 1690 (170) |
| VES79_3_3 | 0.46 | 2.424 (17) | 484 (1) | 0.1008 (10) | 0.1069 (10) | 1.55 (9) | 1.40 (5) | 2.95 (11) | 151 (2) | 0.348 (0) | 1710 (90) |
| VES79_3_4 | 0.63 | 2.404 (6) | 472 (9) | 0.1119 (18) | 0.1969 (10) | 1.78 (12) | 2.67 (11) | 4.45 (16) | 166 (12) | 0.336 (20) | 1510 (160) |
| VES79_3_5 | 0.84 | 2.379 (9) | 482 (3) | 0.1175 (27) | 0.2895 (18) | 1.84 (12) | 3.88 (14) | 5.72 (18) | 150 (20) | 0.153 (9) | 770 (120) |
| VES79_3_6 | 0.98 | 2.357 (7) | 481 (3) | 0.1140 (20) | 0.4105 (27) | 1.81 (11) | 5.56 (20) | 7.37 (23) | 153 (9) | 0.000 (0) | |
| VES79_3_1* | 0.01 | 2.462 (14) | 469 (9) | 0.0194 (0) | 0.0000 (0) | 0.30 (2) | 0.00 (0) | 0.30 (2) | 136 (2) | 0.328 (10) | 1780 (110) |
| VES79_3_2* | 0.12 | 2.441 (36) | 450 (8) | 0.0662 (0) | 0.0369 (0) | 1.08 (6) | 0.52 (2) | 1.60 (6) | 132 (10) | 0.323 (4) | 1810 (170) |
| VES79_3_3* | 0.31 | 2.424 (17) | 436 (9) | 0.0838 (0) | 0.1072 (0) | 1.43 (8) | 1.56 (6) | 2.99 (10) | 123 (12) | 0.287 (6) | 1740 (200) |
| VES79_3_4* | 0.53 | 2.404 (6) | 402 (8) | 0.0838 (0) | 0.1774 (0) | 1.56 (8) | 2.83 (11) | 4.39 (14) | 140 (6) | 0.304 (8) | 1620 (120) |
| VES79_3_5* | 0.77 | 2.379 (9) | 173 (7) | 0.0362 (23) | 0.1091 (67) | 1.59 (14) | 4.09 (33) | 5.68 (36) | 143 (6) | 0.211 (0) | 1110 (70) |
| VES79_3_6* | 1.00 | 2.357 (7) | 396 (8) | 0.0838 (0) | 0.3492 (68) | 1.62 (8) | 5.75 (26) | 7.36 (27) | 120 (12) | 0.000 (0) | |
| VES79_80 | 0.765 | 2.387 (12) | 322 (12) | 0.0712 (0) | 0.1947 (0) | 1.67 (10) | 3.89 (20) | 5.56 (22) | 156 (5) | 0.156 (6) | 1210 (330) |

Notes: Calculated errors are shown in brackets near values.
Concentration of H₂O and CO₂ are determined by MIR. Errors of volatile contents were calculated by error propagation of density, thickness and absorbance errors.
 $X_{\text{H}_2\text{O}}^{\text{fl}}$ refers to the mole fractions of H₂O in the fluid phase present in the capsules after experiments.
Thickness^{*1} section was used for H₂O determination, thickness^{*2} was used for CO₂ determination