Supplementary

Comparative Compressibility of Smectite Group under Anhydrous and Hydrous Environments

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**Figure S1.** Pressure-dependent changes of the interplane (001) distances of (a) beidellite, (b) montmorillonite, and (c) nontronite in present of silicone-oil and distilled water PTMs for anhydrous and hydrous environments, respectively. Normalized d-spacing changes are shown on data points.
| PTM      | Silicone-Oil | Distilled Water |
|----------|--------------|-----------------|
| Pressure (GPa) | a (Å) | b (Å) | c (Å) | β (degrees) | Volume (Å³) | d—Spacing (001) (Å) | FWHM (001) Reflection (°) |
| 0.00 | 5.236(6) | 9.01(2) | 15.07(3) | 98.0(2) | 704(1) | 14.92(3) | 0.243(2) |
| 0.25 | 5.251(8) | 9.02(2) | 14.87(3) | 97.5(3) | 698(2) | 14.75(3) | 0.247(3) |
| 0.50 | 5.251(8) | 9.03(3) | 14.84(4) | 97.6(3) | 696(3) | 14.71(3) | 0.253(4) |
| 1.00 | 5.237(7) | 9.03(2) | 14.61(3) | 97.7(2) | 684(2) | 14.47(3) | 0.259(5) |
| 1.50 | 5.23(1)  | 9.03(2) | 14.44(3) | 97.7(2) | 676(2) | 14.31(3) | 0.257(5) |
| 2.00 | 5.238(8) | 9.10(2) | 14.30(3) | 97.3(2) | 669(2) | 14.18(3) | 0.284(7) |
| 2.50 | 5.235(7) | 8.99(2) | 14.20(4) | 97.2(2) | 663(2) | 14.03(3) | 0.293(7) |
| 3.17 | 5.229(7) | 9.00(2) | 14.08(4) | 97.2(2) | 657(2) | 13.97(3) | 0.277(7) |
| 0.00-Dry | 5.235(6) | 9.01(2) | 15.08(2) | 98.0(3) | 704(2) | 14.93(5) | 0.242(5) |
| 0.00-Wet | 5.185(10) | 8.94(1) | 19.30(3) | 100.1(3) | 881(2) | 19.00(5) | 0.162(3) |
| 0.25 | 5.227(7) | 9.01(2) | 18.78(3) | 100.2(2) | 870(2) | 18.48(5) | 0.169(3) |
| 0.50 | 5.225(7) | 8.998(7) | 18.43(3) | 100.2(3) | 853(2) | 18.14(5) | 0.165(2) |
| 1.00 | 5.215(6) | 8.977(7) | 17.92(3) | 100.2(2) | 826(2) | 17.64(5) | 0.167(2) |
| 1.50 | 5.178(5) | 8.923(9) | 15.35(4) | 100.3(4) | 698(2) | 15.11(5) | 0.413(6) |
| 2.00 | 5.182(5) | 8.917(9) | 15.29(4) | 100.1(3) | 696(2) | 15.05(5) | 0.416(6) |
| 2.50 | 5.179(7) | 8.94(2) | 14.99(6) | 98.6(3) | 686(2) | 14.82(5) | 0.425(7) |
| 3.09 | 5.171(5) | 8.96(2) | 14.47(4) | 99.4(2) | 662(2) | 14.28(5) | 0.275(6) |

(a) The unit-cell parameters and volumes are derived from a series of whole profile fitting procedures using the LeBail method implemented EXPGUI program suite; (b) The interplane (001) distances and FWHM of (001) reflections were calculated using pseudo-Voigt function fitting; (c) ESD’s are in parentheses.
Table S2. Final refined unit-cell parameters, volumes, \(d\)-spacing of (001) plane, and FWHM of (001) reflections of montmorillonite under pressure conditions\(^{a,b,c}\).

| PTM       | Pressure (GPa) | \(a\) (Å) | \(b\) (Å) | \(c\) (Å) | \(\beta\) (degrees) | Volume (Å\(^3\)) | \(d\)-Spacing (001) (Å) | FWHM (001) Reflection (°) |
|-----------|----------------|-----------|-----------|-----------|----------------------|------------------|------------------------|--------------------------|
| PTM       | 0.00-Dry | 5.25(1) | 9.16(4) | 15.36(2) | 96.7(3) | 734(3) | 15.26(5) | 206(2) |
| PTM       | 0.00-Wet | 5.22(2) | 10.71(7) | 19.03(3) | 94.3(4) | 1060(7) | 18.98(5) | 0.241(4) |
| PTM       | 0.33     | 5.22(1) | 10.72(4) | 18.71(3) | 94.3(2) | 1045(4) | 18.66(5) | 0.241(4) |
| PTM       | 0.50     | 5.23(2) | 10.70(4) | 18.14(3) | 94.4(4) | 1013(4) | 18.09(5) | 0.236(4) |
| PTM       | 1.08     | 5.24(2) | 10.76(5) | 17.75(3) | 94.1(3) | 998(4)  | 17.70(5) | 0.222(3) |
| PTM       | 1.91     | 5.23(2) | 10.73(4) | 16.28(4) | 94.1(3) | 910(3)  | 16.24(5) | 0.360(3) |
| PTM       | 3.25     | 5.24(1) | 10.73(4) | 15.50(4) | 94.2(2) | 870(3)  | 15.46(5) | 0.414(4) |

(a) The unit-cell parameters and volumes are derived from a series of whole profile fitting procedures using the LeBail method implemented EXPGUI program suite; (b) The interplane (001) distances and FWHM of (001) reflections were calculated using pseudo-Voigt function fitting; (c) ESD’s are in parentheses.
### Table S3. Final refined unit-cell parameters, volumes, \(d\)-spacing of (001) plane, and FWHM of (001) reflections of nontronite under pressure conditions.\(^{a,b,c}\)

| PTM          | Silicone-Oil | Distilled Water |
|--------------|--------------|-----------------|
| **Pressure (GPa)** | **a (Å)** | **b (Å)** | **c (Å)** | **\(\beta\) (degrees)** | **Volume (Å\(^3\))** | **d—Spacing (001) (Å)** | **FWHM (001) Reflection (°)** |
| 0.00-Dry     | 5.25(1)      | 9.14(2)       | 15.22(2)   | 96.1(4)              | 727(2)             | 15.13(5)             | 0.359(1)               |
| 0.00-Wet     | 5.28(2)      | 9.08(5)       | 19.01(4)   | 96.2(4)              | 906(4)             | 18.90(5)             | 0.330(5)               |
| 0.25         | 5.30(1)      | 9.17(2)       | 18.88(4)   | 96.3(3)              | 911(2)             | 18.76(5)             | 0.346(6)               |
| 0.50         | 5.29(2)      | 9.12(3)       | 18.59(5)   | 96.2(5)              | 891(3)             | 18.48(5)             | 0.341(6)               |
| 1.00         | 5.27(2)      | 9.13(3)       | 18.08(4)   | 96.0(3)              | 865(2)             | 17.98(5)             | 0.343(5)               |
| 1.50         | 5.28(2)      | 9.11(2)       | 17.03(4)   | 96.7(3)              | 813(3)             | 16.91(5)             | 0.451(3)               |
| 2.42         | 5.30(1)      | 9.12(2)       | 16.39(6)   | 96.7(5)              | 786(3)             | 16.27(5)             | 0.472(3)               |
| 3.09         | 5.26(2)      | 9.12(4)       | 15.59(2)   | 96.3(3)              | 744(2)             | 15.49(5)             | 0.582(3)               |

(a) The unit-cell parameters and volumes are derived from a series of whole profile fitting procedures using the Le Bail method implemented EXPGUI program suite; (b) The interplane (001) distances and FWHM of (001) reflections were calculated using pseudo-Voigt function fitting; (c) ESD's are in parentheses.