

Supplementary

Comparative Compressibility of Smectite Group under Anhydrous and Hydrated Environments

Yongmoon Lee ¹, Pyosang Kim ², Hyeonsu Kim ² and Donghoon Seoung ^{2,*}

¹ Department of Geological Sciences, Pusan National University, Busan 46241, Korea; lym1229@pusan.ac.kr

² Department of Earth Systems and Environmental Sciences, Chonnam National University, Gwangju 61186, Korea; 197944@jnu.ac.kr (P.K.); 197942@jnu.ac.kr (H.K.)

* Correspondence: dseoung@jnu.ac.kr; Tel.: +82-62-530-3452

Received: 19 July 2020; Accepted: 24 August 2020; Published: date

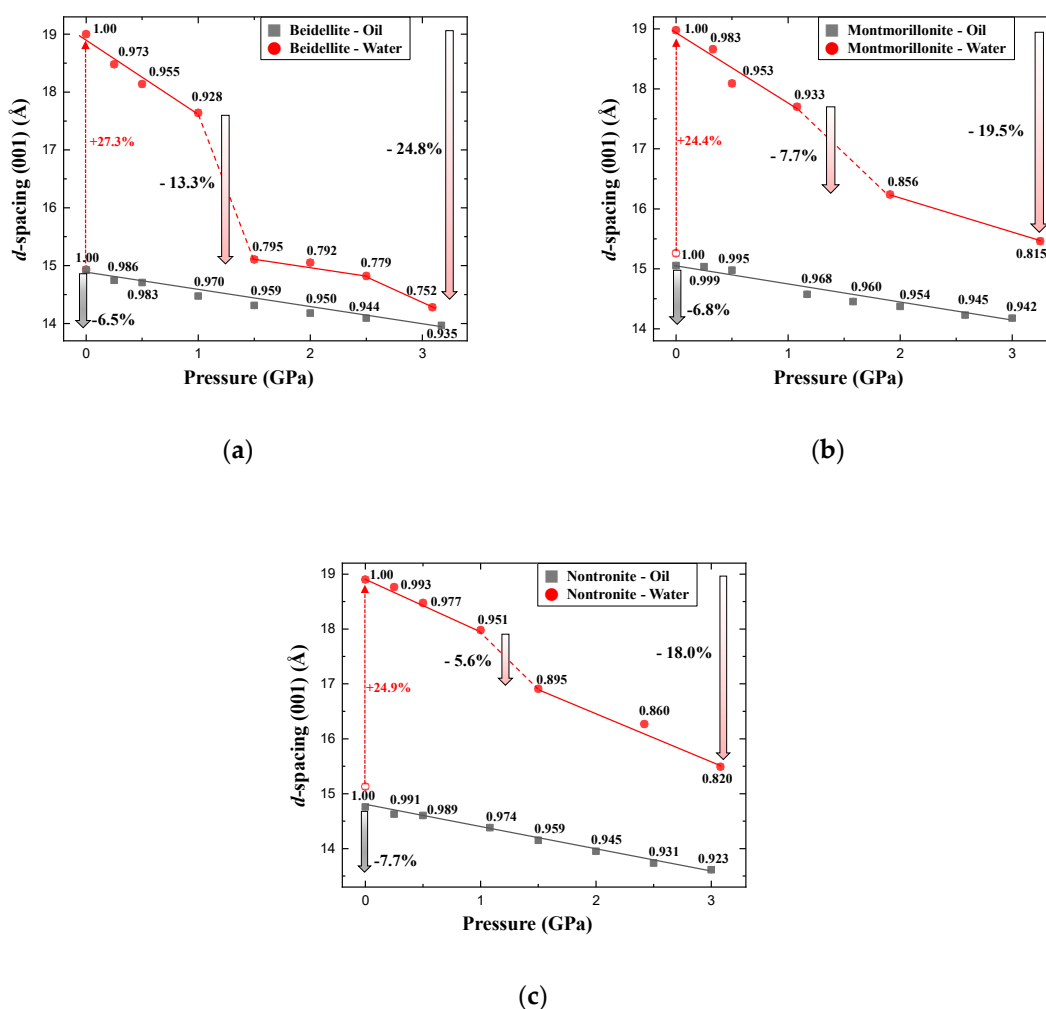


Figure S1. Pressure-dependent changes of the interplane (001) distances of (a) beidellite, (b) montmorillonite, and (c) nontronite in present of silicone-oil and distilled water PTMs for anhydrous and hydrated environments, respectively. Normalized *d-spacing* changes are shown on data points.

Table S1. Final refined unit-cell parameters, volumes, d -spacing of (001) plane, and FWHM of (001) reflections of beidellite under pressure conditions.^{a,b,c}

PTM		Silicone-Oil					
Pressure (GPa)	a (Å)	b (Å)	c (Å)	β (degrees)	Volume (Å ³)	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	5.25(1)	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)	9.00(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)
PTM		Distilled Water					
Pressure (GPa)	a (Å)	b (Å)	c (Å)	β (degrees)	Volume (Å ³)	d —Spacing (001) (Å)	FWHM (001) Reflection (°)
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	5.178(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		Silicone-Oil					
Pressure (GPa)	a (Å)	b (Å)	c (Å)	β (degrees)	Volume (Å ³)	<i>d</i> —Spacing (001) (Å)	FWHM (001) Reflection (°)
0.00	5.27(2)	9.13(4)	15.16(2)	96.7(4)	725(4)	15.05(3)	0.214(2)
0.25	5.23(7)	9.1(2)	15.13(5)	96(1)	718(9)	15.04(3)	0.208(2)
0.50	5.28(2)	9.02(3)	15.08(2)	96.8(4)	713(3)	14.98(3)	0.205(2)
1.17	5.25(2)	9.01(2)	14.71(2)	97.8(4)	689(2)	14.58(3)	0.225(3)
1.58	5.25(2)	9.00(4)	14.57(2)	97.3(4)	682(3)	14.45(3)	0.231(3)
2.00	5.25(3)	8.99(4)	14.49(3)	97.2(7)	679(4)	14.37(3)	0.234(3)
2.58	5.26(2)	8.98(2)	14.32(3)	96.6(5)	672(3)	14.23(3)	0.246(4)
3.00	5.27(1)	8.98(2)	14.26(2)	96.3(4)	670(2)	14.18(3)	0.246(4)
PTM		Distilled Water					
Pressure (GPa)	a (Å)	b (Å)	c (Å)	β (degrees)	Volume (Å ³)	<i>d</i> —Spacing (001) (Å)	FWHM (001) Reflection (°)
0.00-Dry	5.25(1)	9.16(4)	15.36(2)	96.7(3)	734(3)	15.26(5)	206(2)
0.00-Wet	5.22(2)	10.71(7)	19.03(3)	94.3(4)	1060(7)	18.98(5)	0.241(4)
0.33	5.22(1)	10.72(4)	18.71(3)	94.3(2)	1045(4)	18.66(5)	0.241(4)
0.50	5.23(2)	10.70(4)	18.14(3)	94.4(4)	1013(4)	18.09(5)	0.236(4)
1.08	5.24(2)	10.76(5)	17.75(3)	94.1(3)	998(4)	17.70(5)	0.222(3)
1.91	5.23(2)	10.73(4)	16.28(4)	94.1(3)	910(3)	16.24(5)	0.360(3)
3.25	5.241(8)	10.73(4)	15.50(4)	94.0(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			
Pressure (GPa)	a (Å)	b (Å)	c (Å)	β (degrees)	Volume (Å ³)	d —Spacing (001) (Å)	FWHM (001) Reflection (°)
0.00	5.25(2)	9.14(2)	14.89(4)	97.6(5)	708(3)	14.76(3)	0.471(3)
0.25	5.27(2)	9.12(6)	14.76(5)	97.7(6)	703(4)	14.63(3)	0.466(3)
0.50	5.28(2)	9.12(2)	14.74(4)	97.8(4)	702(3)	14.60(3)	0.452(3)
1.08	5.25(2)	9.10(4)	14.46(4)	96.0(4)	687(3)	14.38(3)	0.467(4)
1.50	5.21(2)	9.14(4)	14.24(5)	96.4(5)	675(3)	14.15(3)	0.469(4)
2.00	5.21(1)	9.15(2)	14.04(5)	96.3(4)	664(3)	13.95(3)	0.512(6)
2.50	5.20(2)	9.14(7)	13.83(5)	96.5(6)	653(5)	13.74(3)	0.606(10)
3.00	5.20(2)	9.12(7)	13.71(7)	97.0(9)	645(5)	13.62(3)	0.586(8)
PTM				Distilled Water			
Pressure (GPa)	a (Å)	b (Å)	c (Å)	β (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 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.



© 2020 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).