

Supplementary Material

Complexity of clay minerals and its effects on silicon dynamics in hypersaline coastal wetland soils, Brazil

Lucas Resmini Sartor^{A,}, Gabriel Ramatis Pugliese Andrade^B, Samantha C. Ying^C, Robert C. Graham^C, Rodrigo Santana Macedo^D, and Tiago Osório Ferreira^E*

^ADepartment of Agronomy, Federal University of Sergipe, Campus do Sertão, Nossa Senhora da Glória, Sergipe, Brazil.

^BSoil Laboratory, State University of North Fluminense Darcy Ribeiro, Campos dos Goytacazes, Rio de Janeiro, Brazil.

^CEnvironmental Sciences Department, University of California, Riverside, CA, USA.

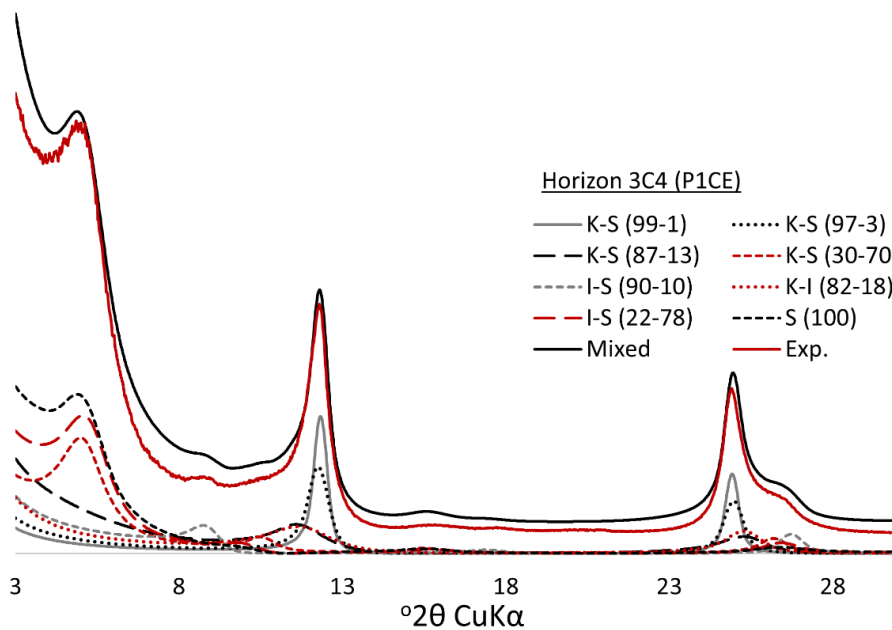
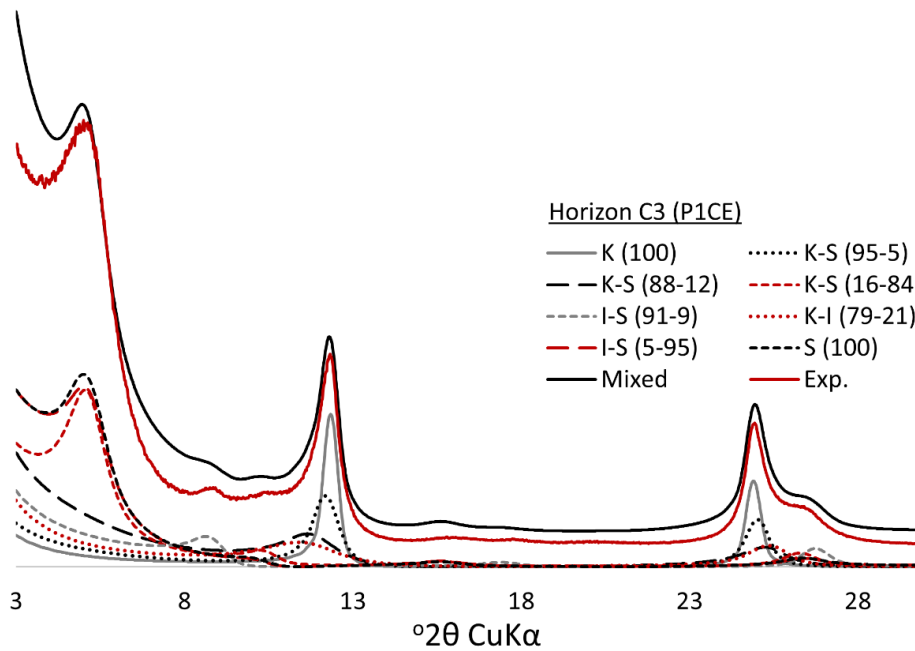
^DState University of Paraíba, Technology and Science Center, Campina Grande, Brazil.

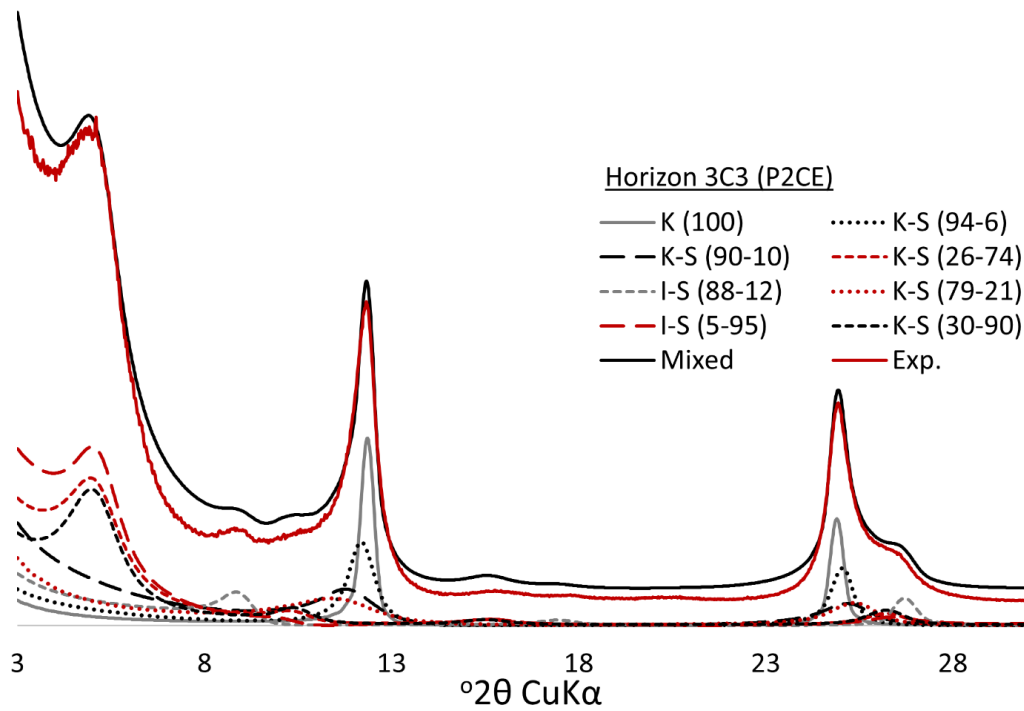
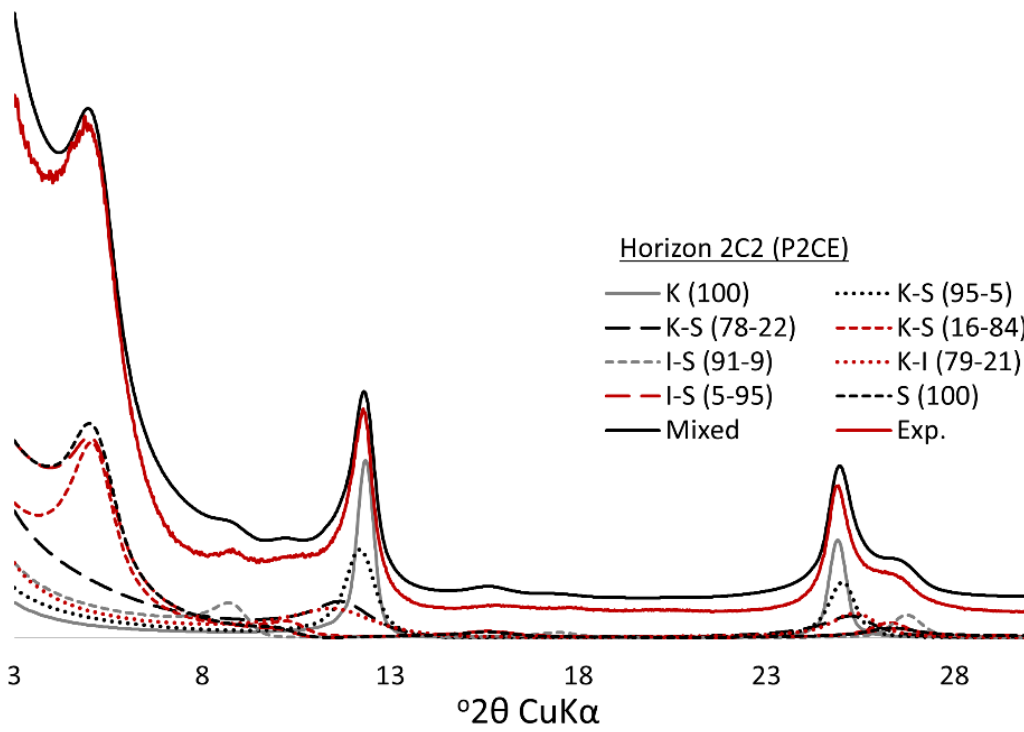
^EDepartment of Soil Science, Luiz de Queiroz College of Agriculture, University of São Paulo, Piracicaba, São Paulo, Brazil.

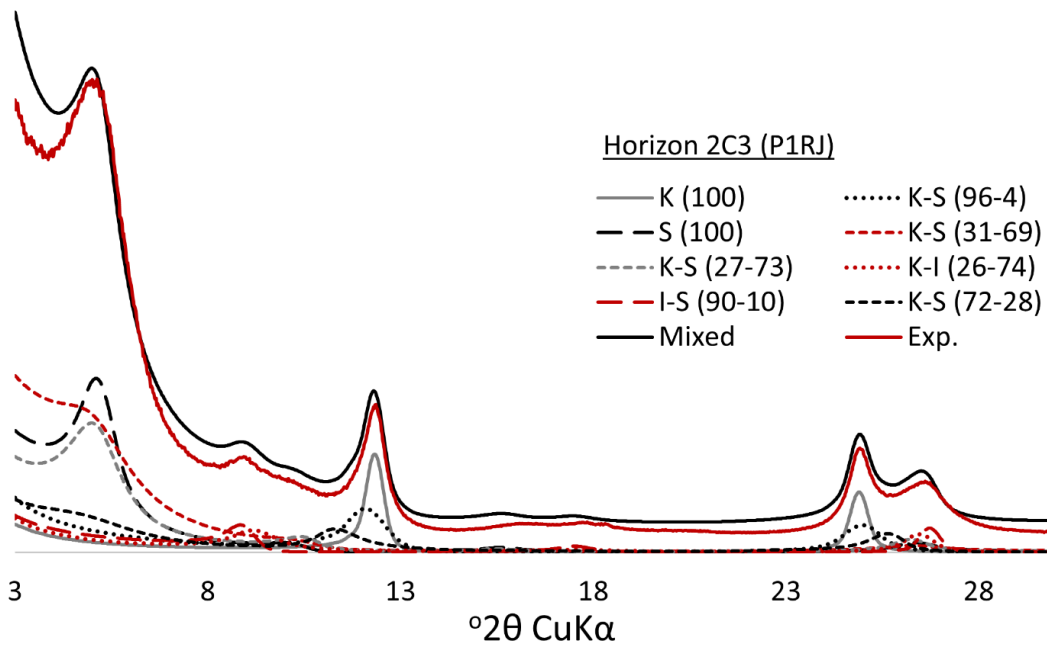
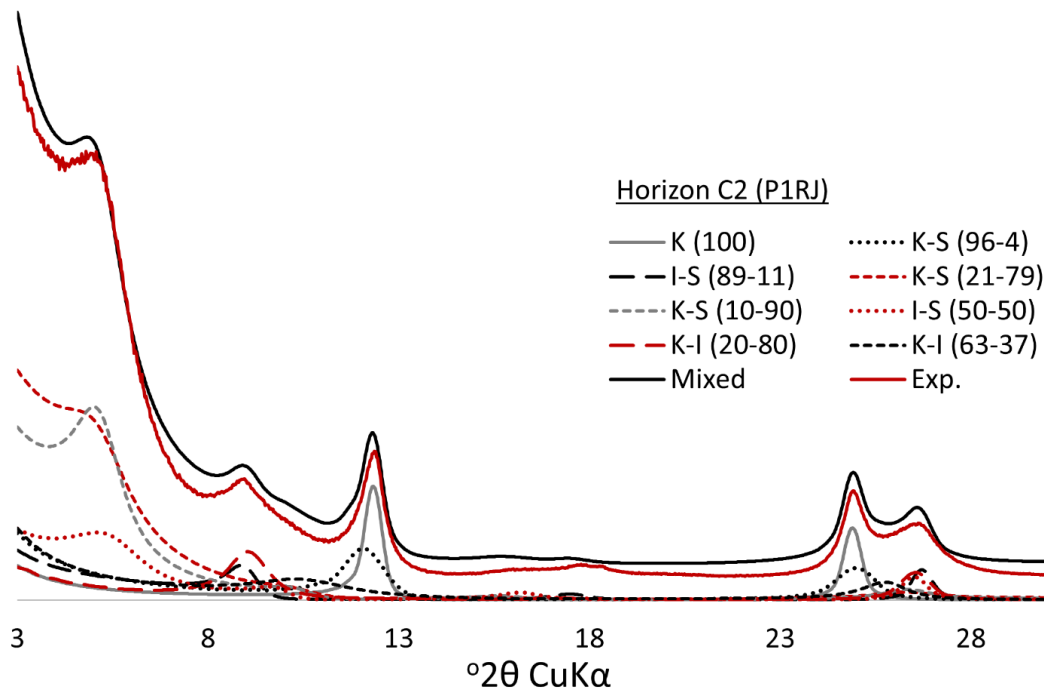
*Correspondence to: Lucas Resmini Sartor Department of Agronomy, Federal University of Sergipe, Campus do Sertão, Nossa Senhora da Glória, Sergipe, Brazil Email: lrsartor@academico.ufs.br

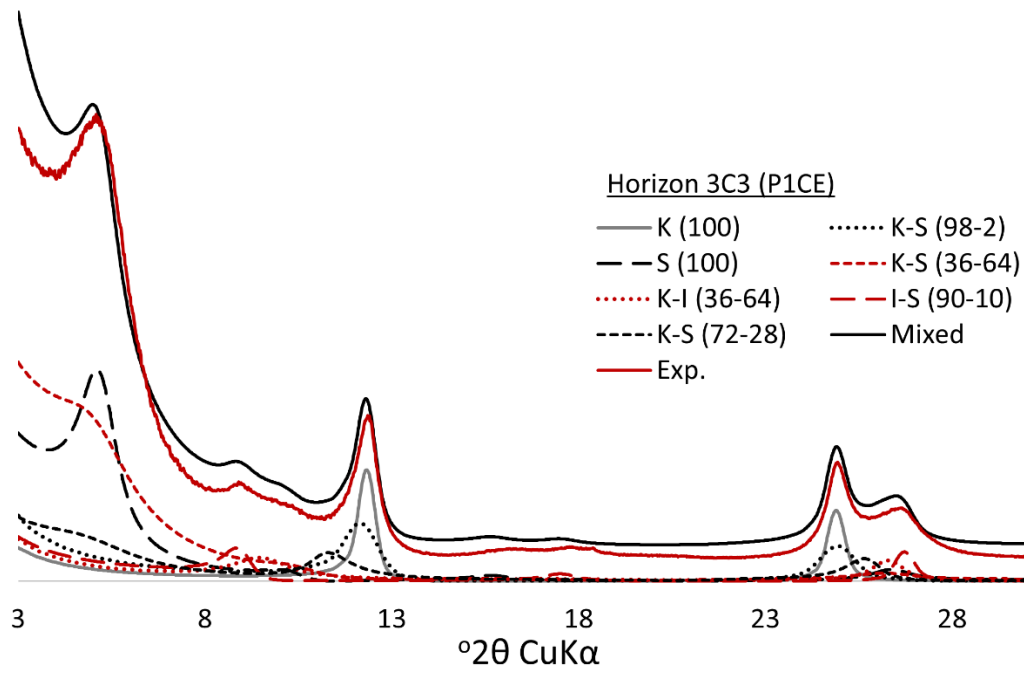
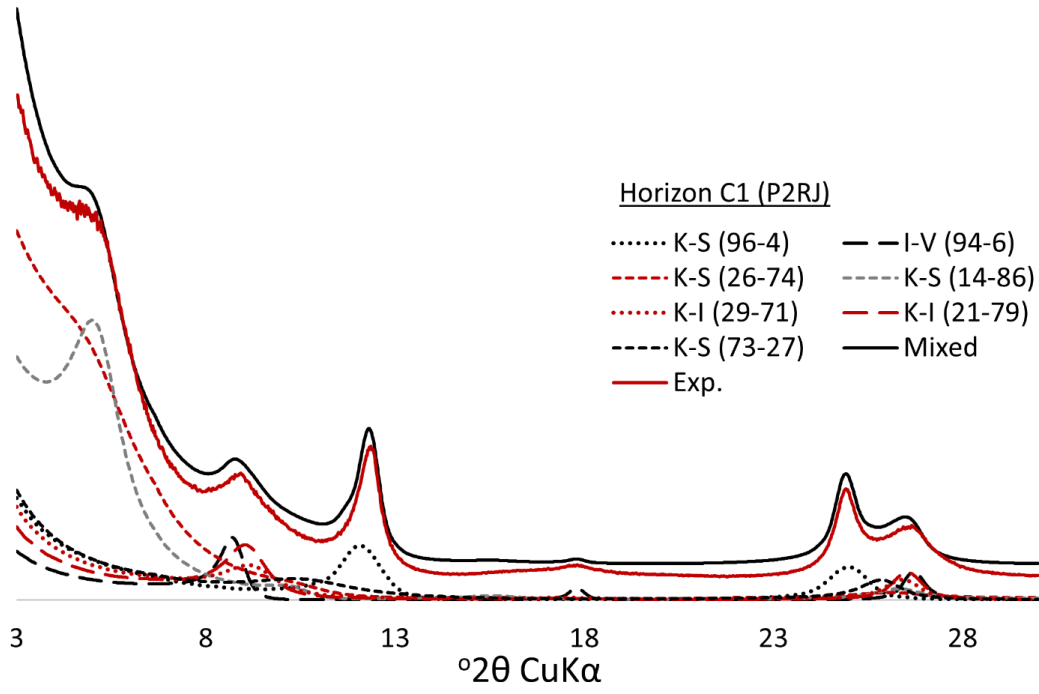
Supplementary material (Fig. 4)

XRD patterns calculated using NEWMOD 3.2.1. based on the experimental glycolated samples (Exp., solid red lines). Solid black lines (Mixed) are the result of the XRD full modeling of the sample, which is overlapped to the experimental patterns. The calculated patterns of each mineral phase are presented individually, together with the proportion in the sample.









Supplementary material (Table 2)

Table S1. Parameters from the XDR modelling of glycolated samples.

Mineral	% layers	Fe				K illite	Nmax	Nave	% phase
		K	S	V	I				
A horizon (P1CE)									
K-S	99-1	<0.01	0.50	-	-	-	30	15.0	16.9
K-S	95-5	<0.01	0.50	-	-	-	15	7.0	24.2
K-S	80-20	<0.01	0.35	-	-	-	8	3.1	20.6
K-S	60-40	<0.01	0.35	-	-	-	8	3.0	17.1
I-S	96-4	<0.01	<0.01	-	0.50	0.75	16	10.9	6.4
K-I	44-56	<0.01	-	-	0.40	0.80	15	10.0	7.3
I-S	70-30	-	0.21	-	0.10	0.80	15	7.0	3.9
K-S	37-63	<0.01	0.32	-	-	-	7	3.0	3.6
C3 horizon (P1CE)									
K	100	<0.01	-	-	-	-	30	19.0	12.9
K-S	95-5	<0.01	0.64	-	-	-	23	14.8	16.4
K-S	88-12	<0.01	0.76	-	-	-	18	3.1	17.1
K-S	16-84	0.04	0.69	-	-	-	9	1.8	13.8
I-S	91-9	-	0.50	-	0.46	0.80	11	4.9	10.4
K-I	79-21	<0.01	-	-	0.40	0.80	14	7.0	9.9
I-S	5-95	-	0.70	-	0.53	0.75	7	1.2	14.1
S	100	-	0.87	-	-	-	6	1.2	5.4
3C4 horizon (P1CE)									
K-S	99-1	<0.01	0.50	-	-	-	35	20.2	12.6
K-S	97-3	<0.01	0.64	-	-	-	26	14.8	15.2
K-S	87-13	<0.01	0.76	-	-	-	13	3.5	15.1
K-S	30-70	<0.01	0.35	-	-	-	11	2.7	12.3
I-S	90-10	-	0.45	-	0.56	0.80	13	5.9	8.6
K-I	82-18	<0.01	-	-	0.40	0.75	16	6.8	13.4
I-S	22-78	-	0.91	-	0.58	0.75	7	1.7	9.0
S	100	-	0.71	-	-	-	5	1.1	13.9
A horizon (P2CE)									
K-S	99-1	<0.01	0.35	-	-	-	30	16.0	18.6
K-S	93-7	<0.01	0.50	-	-	-	18	9.9	21.2
K-S	86-14	<0.01	0.35	-	-	-	8	3.1	15.9
K-S	55-45	<0.01	0.35	-	-	-	8	3.0	17.0
I-S	94-6	-	0.45	-	0.56	0.77	16	9.6	9.3
K-I	48-52	<0.01	-	-	0.40	0.80	17	12.9	9.6
I-S	50-50	-	0.24	-	0.19	0.80	11	7.0	4.4
K-S	50-50	<0.01	0.20	-	-	-	7	2.1	4.1
2C2 horizon (P2CE)									
K	100	<0.01	-	-	-	-	30	19.0	10.9
K-S	95-5	<0.01	0.50	-	-	-	23	14.8	15.7
K-S	78-22	<0.01	0.50	-	-	-	18	3.1	17.3
K-S	16-84	<0.01	0.69	-	-	-	9	1.8	14.0
I-S	91-9	-	0.50	-	0.46	0.80	12	5.9	10.5
K-I	79-21	<0.01	-	-	0.40	0.80	14	7.0	10.0
I-S	5-95	-	0.70	-	0.53	0.75	7	1.2	14.3

S	100	-	0.87	-	-	-	6	1.2	7.3
3C3 horizon (P2CE)									
K	100	<0.01	-	-	-	-	36	28.2	14.5
K-S	94-6	<0.01	0.93	-	-	-	31	18.8	14.5
K-S	90-10	<0.01	0.76	-	-	-	15	3.7	14.5
K-S	26-74	<0.01	0.35	-	-	-	9	1.8	11.2
I-S	88-12	-	0.45	-	0.46	0.70	14	10.9	8.1
K-I	79-21	<0.01	-	-	0.40	0.60	14	7.0	14.5
I-S	5-95	-	0.60	-	0.53	0.70	7	1.2	13.2
K-S	30-70	<0.01	0.43	-	-	-	7	3.2	9.4
A horizon (P1RJ)									
K	100	<0.01	-	-	-	-	26	14.9	18.4
K-S	93-7	<0.01	<0.01	-	-	-	13	7.2	13.4
I	100	-	-	-	1.31	0.70	11	7.1	6.4
K-S	7-93	<0.01	0.55	-	-	-	8	1.1	19.8
K-I	45-55	<0.01	-	-	0.93	0.74	10	3.4	15.9
K-I	37-63	<0.01	-	-	1.08	0.79	12	6.0	16.0
I-S	91-9	<0.01	-	-	1.08	0.70	16	9.7	10.1
C2 horizon (P1RJ)									
K	100	<0.01	-	-	-	-	29	14.9	14.4
K-S	96-4	<0.01	0.86	-	-	-	14	9.2	13.1
I-S	89-11	-	0.90	-	0.41	0.71	23	12.8	12.0
K-S	21-79	<0.01	1.34	-	-	-	8	1.0	14.1
K-S	10-90	<0.01	1.12	-	-	-	8	1.4	18.2
I-S	50-50	-	<0.01	-	0.62	0.70	15	6.0	4.9
K-I	20-80	<0.01	-	-	1.01	0.70	13	6.0	7.8
K-I	63-37	<0.01	-	-	0.37	0.77	19	4.7	15.6
2C3 horizon (P1RJ)									
K	100	<0.01	-	-	-	-	29	14.9	13.6
K-S	96-4	<0.01	0.97	-	-	-	15	8.2	15.5
S	100	-	0.94	-	-	-	9	1.4	15.5
K-S	31-69	<0.01	1.26	-	-	-	8	1.1	15.5
K-S	27-73	<0.01	0.95	-	-	-	11	2.0	10.0
K-I	26-74	<0.01	-	-	0.28	0.74	17	11.9	15.2
I-S	90-10	-	<0.01	-	0.29	0.70	17	10.9	9.3
K-S	72-28	0	<0.01	-	-	-	15	8.9	5.6
A horizon (P2RJ)									
K	100	<0.01	-	-	-	-	29	14.9	17.1
K-S	92-8	<0.01	<0.01	-	-	-	14	9.2	17.6
I	100	-	-	-	0.15	0.71	16	13.8	5.6
K-S	33-67	<0.01	0.55	-	-	-	8	1.3	19.5
K-I	30-70	<0.01	-	-	1.40	0.70	9	2.4	16.8
K-I	35-65	<0.01	-	-	1.23	0.70	12	6.0	10.5
I-S	93-7	-	0.21	-	0.72	0.70	18	11.0	12.9
C1 horizon (P2RJ)									
K	100	<0.01	-	-	-	-	29	14.9	15.7
K-S	96-4	<0.01	0.86	-	-	-	14	9.2	13.9
I-V	94-6	-	-	0	0.55	0.71	23	13.8	6.1
K-S	26-74	<0.01	1.34	-	-	-	8	1.1	18.9

K-S	14-86	<0.01	1.05	-	-	-	8	1.4	11.6
K-I	29-71	<0.01	-	-	0.62	0.70	15	6.0	11.0
K-I	21-79	<0.01	-	-	1.20	0.70	15	11.0	13.0
K-S	73-27	<0.01	<0.01	-	-	0.77	19	4.7	9.8
3C3 horizon (P2RJ)									
K	100	<0.01		-	-	-	29	14.9	15.7
K-S	98-2	<0.01	0.97	-	-	-	15	8.2	13.9
S	100	-	0.94	-	-	-	9	1.4	18.1
K-S	36-64	<0.01	1.26	-	-	-	8	1.1	18.1
K-I	36-64	<0.01		-	0.28	0.74	17	11.9	17.0
I-S	90-10	-	<0.01	-	0.29	0.70	17	10.9	10.8
K-S	72-28	<0.01	<0.01	-	-	-	15	8.9	6.5

% layers: proportion of layers of each mineral phase; Fe – K, S, V, and I: octahedral Fe for kaolinite, smectite, vermiculite, or illite; K illite: interlayered K in illite layers; Nave and Nmax: medium and maximum number of layers per coherent scattering domain; % phase: final proportion of each mineral phase in the sample.