

## **SUPPLEMENTARY MATERIAL**

related to

### **Interaction of corroding iron with seven bentonites in the alternative buffer materials field experiment (ABM2)**

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## **S3 XRD and XRF data**

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Counts

Position [°2Theta] (Copper (Cu))

Ibicoseal raw (4x 1 h, averaged)  
Ibicoseal raw (10 h, re-crushed, disoriented)

cal: calcite (96-901-6707)  
cbl: cristobalite (96-901-1579)  
dol: dolomite (96-900-4929)  
gyp: gypsum (96-9013165)  
hem: hematite (96-900-9783)  
ill: illite (96-901-3724)  
mmt: monmorillonite  
qtz: quartz (96-101-1098)  
pyr: pyrite (00-041-1340)

fel: feldspar including  
-albite (96-900-5080)  
-anorthite (96-900-6347)  
-microcline (96-900-5038)  
-orthoclase (96-900-6347)  
-sanidine (96-900-5266)

Counts

different mica ?

Na-Ca exchange

anh

fel

cbl

cal

qtz

cal

cal

anh: anhydrite (96-500-0041)

Position [°2Theta] (Copper (Cu))

Legend:

- Ibecoseal raw (dome)
- ABM2#11bulk (dome)
- ABM2#11contact (dome)
- ABM2#11crust (dome)

S2-1

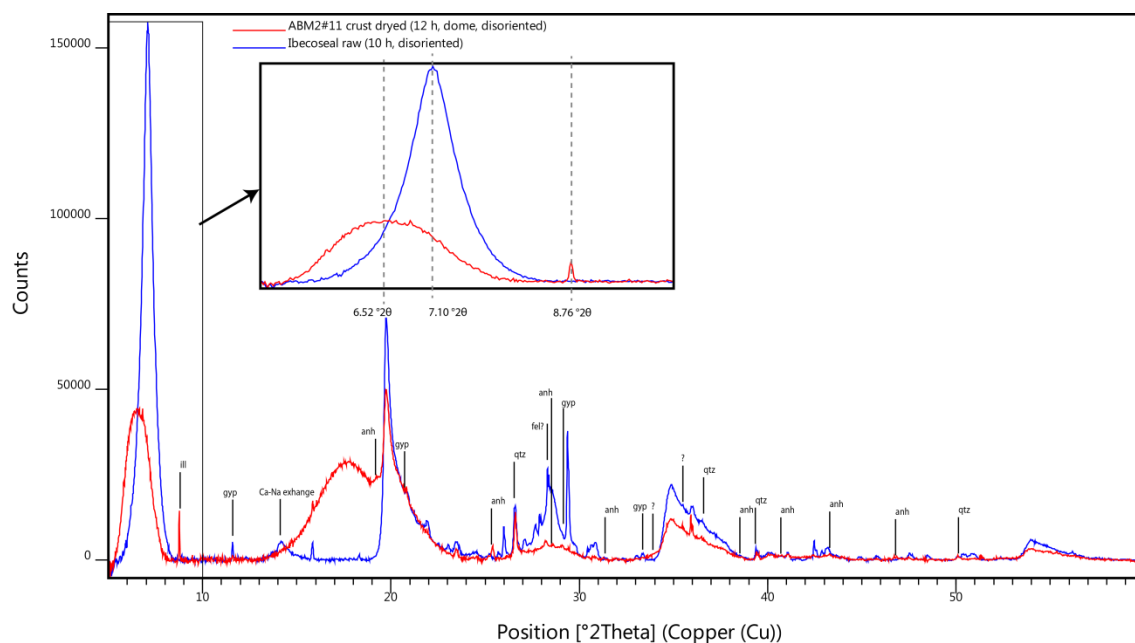


Fig. S3-3 Diffractograms (slow scan rate) of (red) the domed crust sample from block ABM2#11 and (blue) the undomed raw Ibeseal.

### S3-2 XRD data of Ikosorb (Block #12)

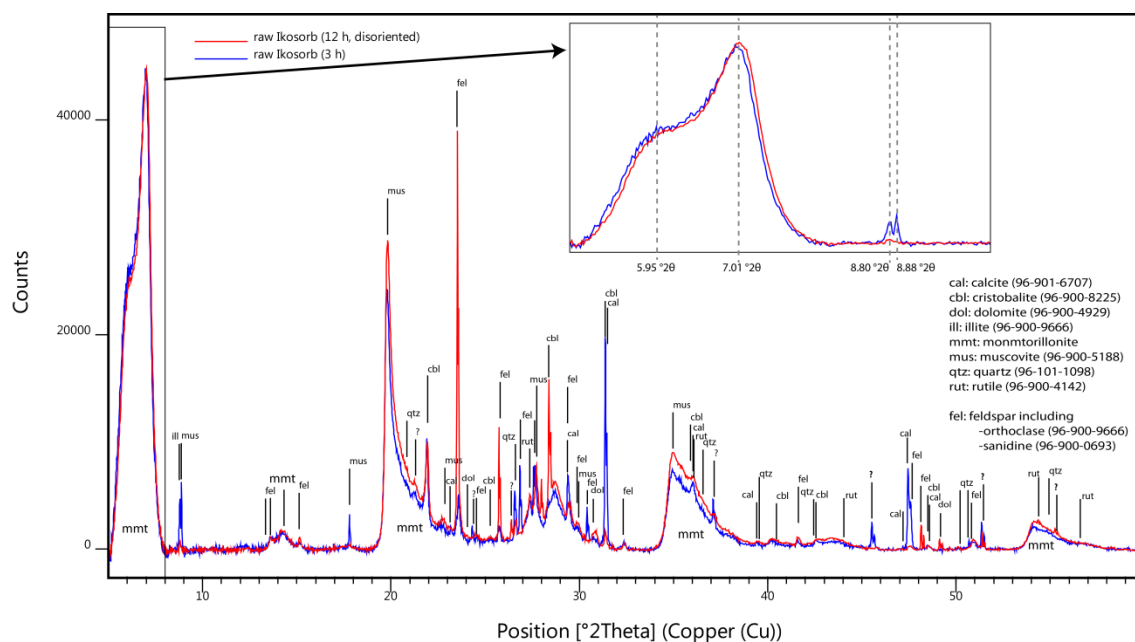


Fig. S3-4 Diffractograms of the raw Ikosorb bentonites (two different aliquots with scan rates).

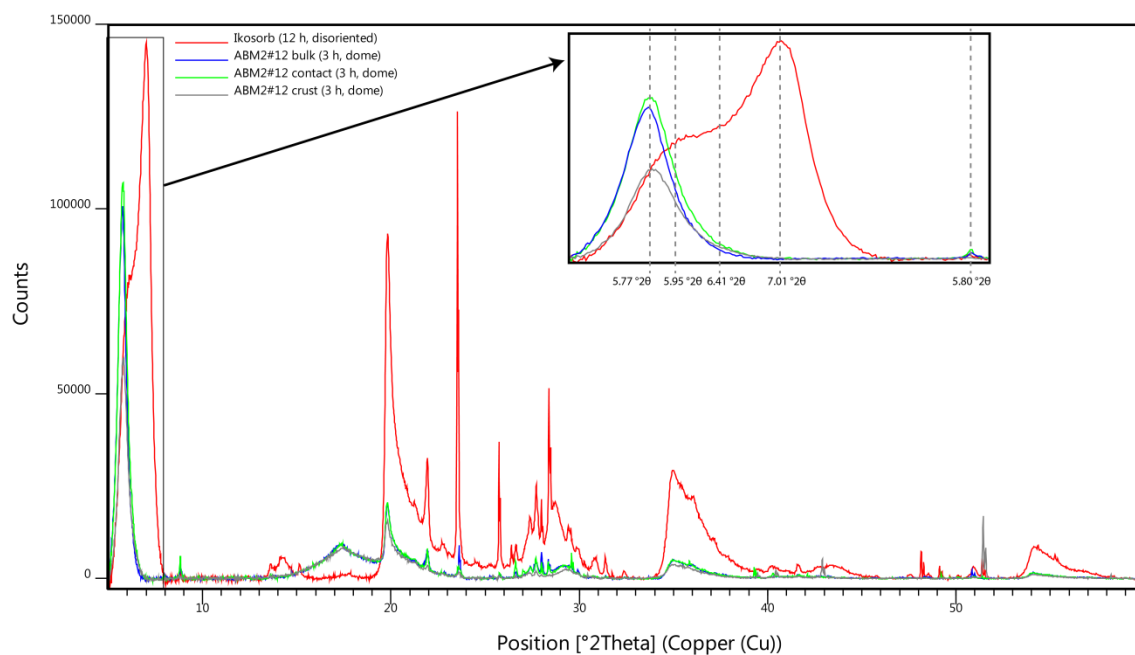


Fig. S3-5 Diffractograms of the profile samples (bulk/contact/crust) from block ABM2#12 and of the undomed raw material.

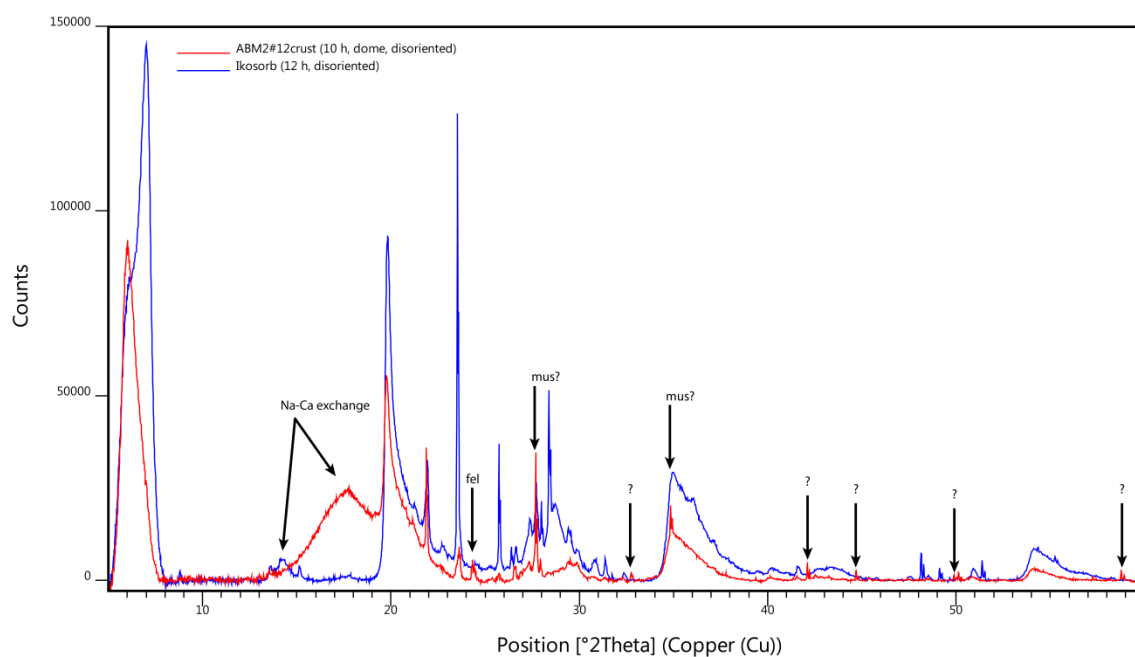


Fig. S3-6 Diffractograms of the crust (disorientated, slow scan rate) and of the undomed raw material.

### S3-3 XRD data of MX-80/qz (Block #25)

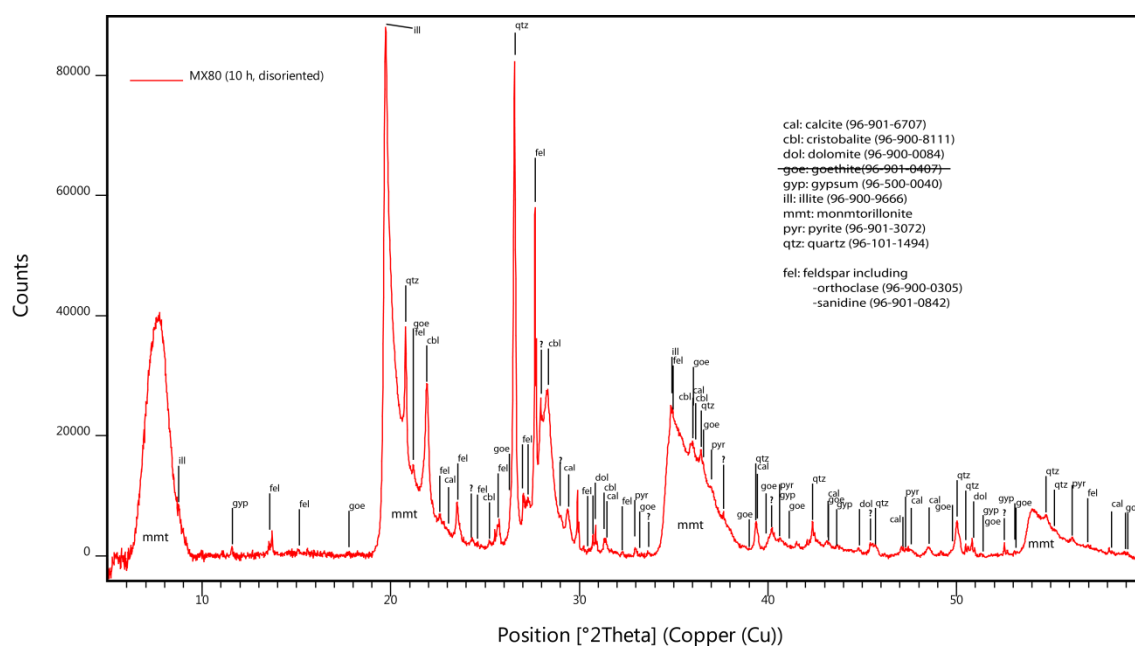


Fig. S3-7 Diffractograms of the raw MX80 bentonites.

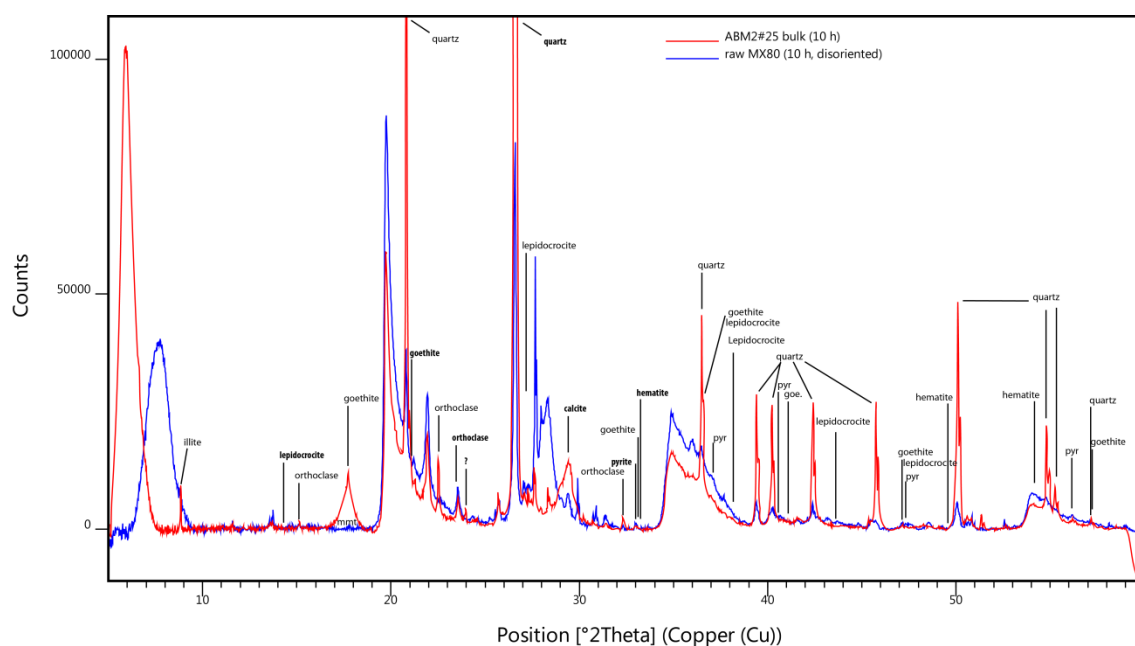


Fig. S3-8 Diffractograms of bulk sample from block ABM2#25 (MX80+quartz) and of the raw MX80 material (both undomed). The positions of some accessory phase of original material (quartz, orthoclase and calcite), as well as common Fe bearing oxides expected to be found in the raw material or in the corrosion product are indicated (the main reflections indicated in bold)

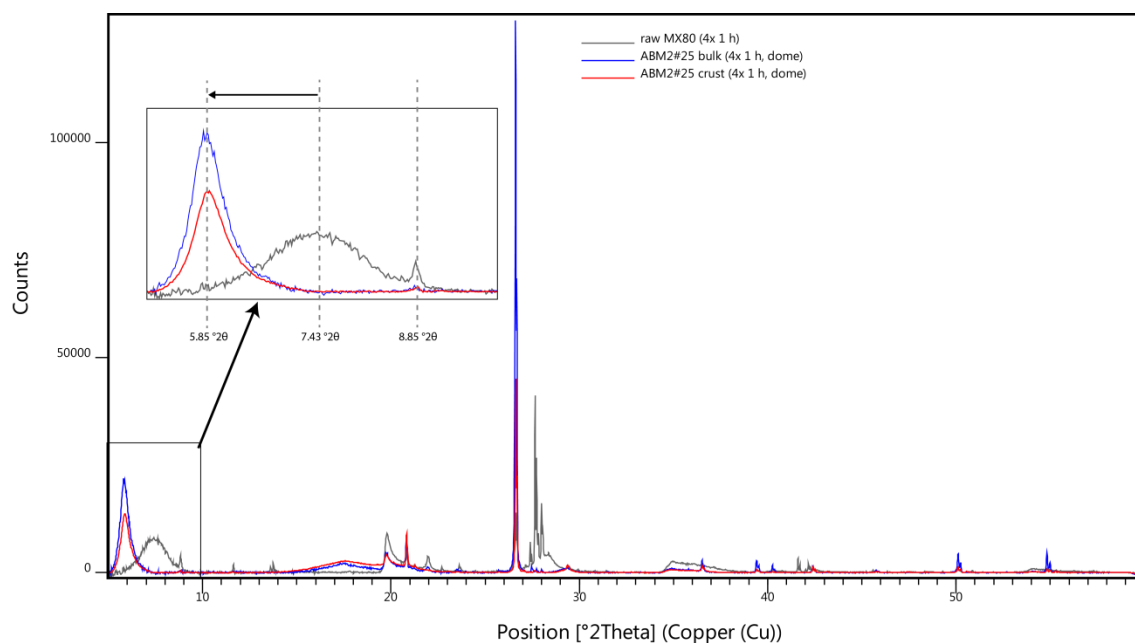


Fig. S3-9 Diffractograms of profile samples (bulk/crust) from block ABM2#25 and of the undomed raw material.

### S3-4 XRD data of Deponit (Block #26)

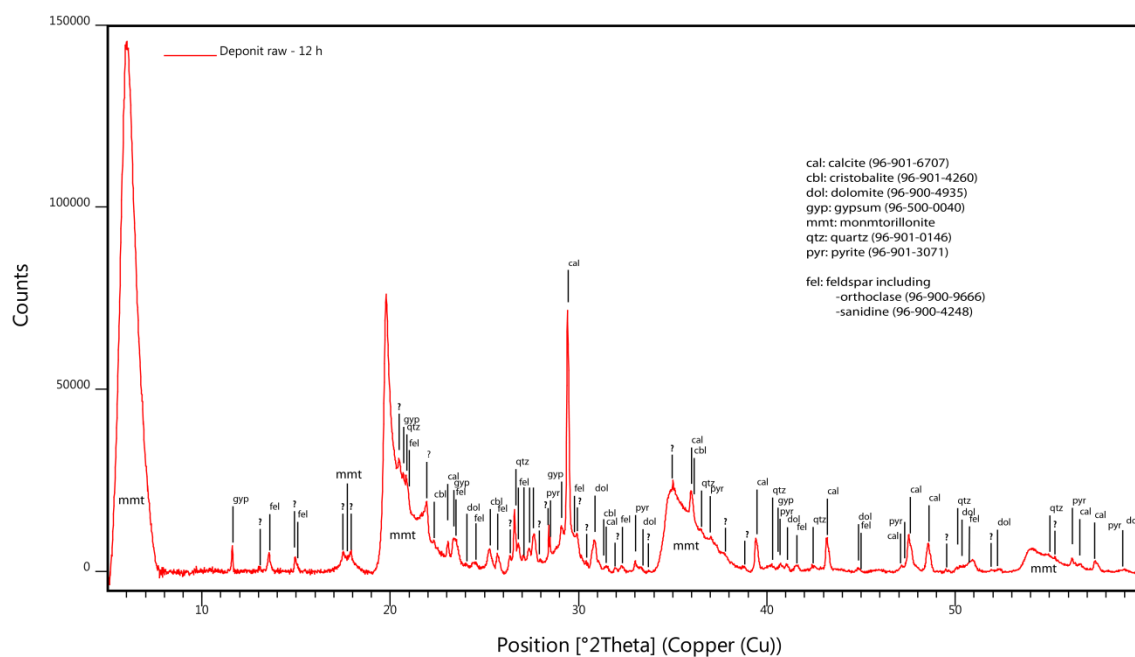


Fig. S3-10 Diffractograms of the raw Deponit bentonites (the fit is an arbitrary sum of pseudo Voigtian curves).

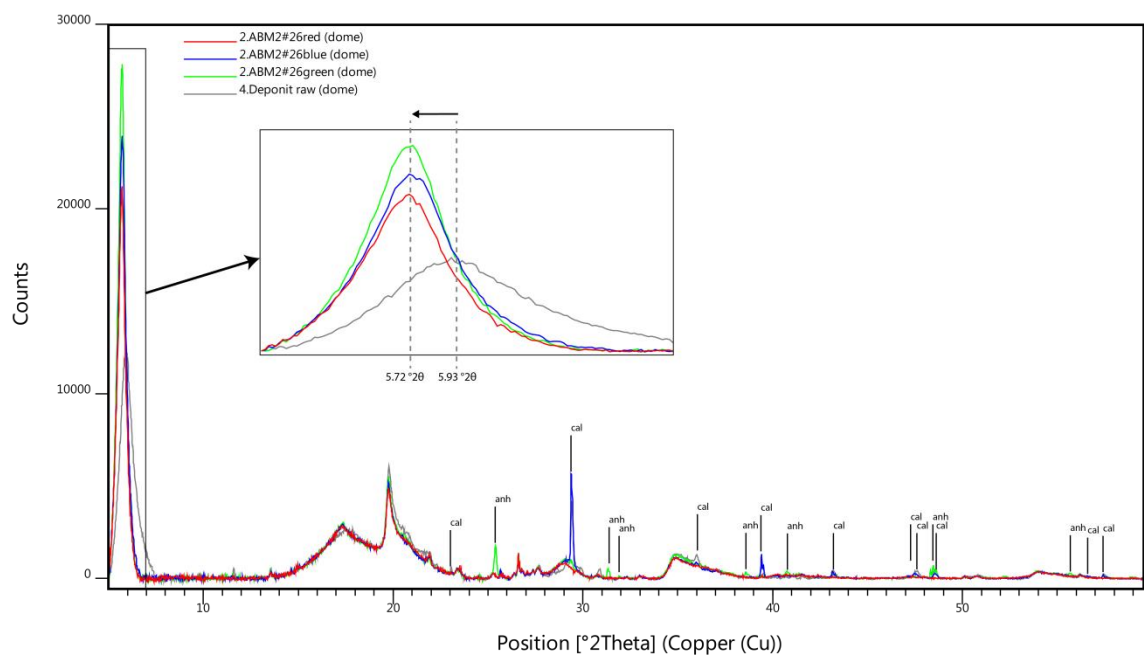


Fig. S3-11 Diffractograms of the red/green/blue samples from block ABM2#26 and of the raw Deponit bentonites (all domed).

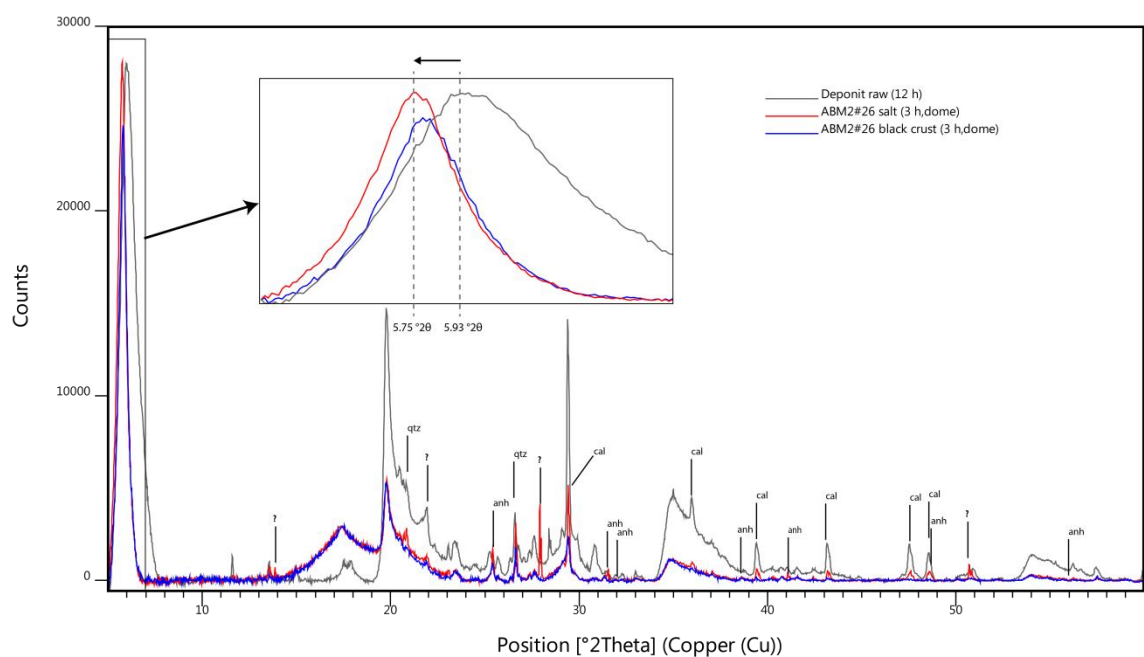


Fig. S3-12 Diffractograms two domed profile samples (black crust and salt) from block ABM2#36 and of the undomed raw Deponit bentonites.

## S3-5 XRF data

Table S3-1 XRF data

Material	MX80	Ibecoseal	Ibecoseal	Ikosorb	Ikosorb	Ikosorb	Kunigel	MX80/qz	MX80/qz	MX80/qz	MX80/qz	Deponit	Deponit	Deponit	Deponit	Deponit	MX80	MX80
Sample ID	08B	11B	11Co	12B	12Co	12H	13C	25B	25Cr	25Co2	25Co3	26Blue	26Green	26Red	26RC	26S	27Co	27H
Type	bulk	bulk	contact	bulk	contact	heart	contact	bulk	crust	contact	contact	blue	green	red	crust	salt	contact	heart
%H <sub>2</sub> O	10.25	15.32	16.36	14.4	12.47	12.81	9.3	9.22	7.93	9.37	9.19	13.98	14.22	14.62	13.29	13.95	14.05	14.28
LOI	7.54	10.62	8.96	8.74	8.34	8.26	6.58	5.78	8.54	5.78	5.77	10.53	9.81	9.56	9.33	11.01	8.25	7.89
S	101.02	100.26	100.01	100.02	99.41	99.87	100.02	100.71	100.19	100.06	100.07	99.21	99.03	100.14	101.02	100.26	100.01	100.02
majors elements (in oxide wt.%)																		
SiO <sub>2</sub>	67.65	62.32	61.68	62.72	62.18	62.69	75.85	77.09	64.45	73.91	73.94	60.8	60.82	60.53	60.67	60.41	65.63	66.64
TiO <sub>2</sub>	0.17	0.47	0.47	0.26	0.25	0.27	0.16	0.17	0.14	0.15	0.16	0.85	0.86	0.85	0.85	0.84	0.16	0.17
Al <sub>2</sub> O <sub>3</sub>	21.39	19.92	19.77	25.16	24.97	25.25	14.48	14.77	11.82	14.21	14.6	19.46	19.33	19.31	19.37	19.4	20.44	20.88
Fe <sub>2</sub> O <sub>3</sub>	4.38	4.59	7.61	2.77	4.14	3.39	2.44	3.37	11.83	5.18	4.86	6.81	6.25	11.07	7.2	5.63	5.57	4.7
MnO	0.01	0.13	0.06	0.02	0.02	0.01	0.06	0.02	0.09	0.05	0.04	0.08	0.14	0.04	0.14	0.08	0.03	0.01
MgO	2.4	4.09	4.72	1.98	2.05	2.02	2.42	1.59	5.45	2.57	2.2	2.83	4.39	2.71	4.7	2.9	2.56	2.27
CaO	3.16	6.22	3.5	4.02	3.16	3.52	3.33	2.09	5.16	2.51	2.53	6.32	5.25	3.64	4.52	7.73	3.7	2.92
Na <sub>2</sub> O	1.14	0.86	0.83	1.5	1.2	1.31	0.84	0.75	0.62	0.7	0.89	0.75	0.7	0.72	0.75	0.78	0.86	0.9
TiO <sub>2</sub>	0.54	1.31	1.14	1.21	1.11	1.09	0.22	0.74	0.49	0.65	0.7	0.95	0.93	0.91	0.96	0.95	0.5	0.52
P <sub>2</sub> O <sub>5</sub>	0.05	0.12	0.12	0.05	0.05	0.05	0.04	0.04	0.03	0.04	0.04	0.16	0.16	0.16	0.16	0.16	0.05	0.05
MnO	67.65	62.32	61.68	62.72	62.18	62.69	75.85	77.09	64.45	73.91	73.94	60.8	60.82	60.53	60.67	60.41	65.63	66.64
Trace elements (in ppm)																		
Ba	423	423	1402	277	2487	1920	1937	1054	239	189	231	325	1013	917	993	532	1074	353
Cr	7	7	17	20	7	4<	10	8	4<	29	12	11	30	36	34	34	35	10
Cu	9	9	13	12	-0<	-1<	-1<	1<	2<	25	1<	3	27	29	27	27	28	1<
Nb	30	30	14	12	23	24	23	10	23	18	21	21	11	11	11	9	11	29
Ni	11	11	9	11	5	4	7	7	9	25	9	9	15	17	16	14	15	7
Pb	39	39	31	23	7<	7<	7<	22	25	14	4<	4<	30	49	23	15	25	5<
Rb	5	5	44	39	31	31	26	7	17	12	15	17	63	64	64	69	64	5
Sr	397	397	552	411	430	402	411	427	282	494	316	324	443	471	422	426	466	434
V	7	7	81	77	26	29	25	10	6	5	2<	12	165	171	170	172	170	0<
Y	48	48	31	29	30	31	32	49	34	31	34	34	24	23	24	23	24	45
Zn	111	111	90	106	44	67	44	92	77	38	28	30	127	180	142	101	114	68
Zr	209	209	186	188	238	255	250	141	169	135	174	164	171	169	173	169	173	206

%H<sub>2</sub>O: water content measured from water loss at 105 °C

LOI: loss on ignition

Σ: sum of elements (excluding %H<sub>2</sub>O and LOI)