P-06-12

Oskarshamn site investigation

Borehole KLX03: Characterisation of pore water

Part 1: Methodology and analytical data

H N Waber, Rock Water Interaction, University of Bern

J A T Smellie, Conterra AB

January 2006

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel 08-459 84 00
+46 8 459 84 00
Fax 08-661 57 19
+46 8 661 57 19

ISSN 1651-4416
SKB P-06-12

Oskarshamn site investigation

Borehole KLX03: Characterisation of pore water

Part 1: Methodology and analytical data

H N Waber, Rock Water Interaction, University of Bern

J A T Smellie, Conterra AB

January 2006

Keywords: Site investigations, Matrix pore water, Diffusion experiments, Mineral chemistry, Analytical data, AP PS400-04-043.

Abstract

Drillcore material has been successfully sampled from borehole KLX03 for studies relating to characterisation of the connected pore-water chemistry. The methodology to extract and analyse the pore-water is outlined and the raw analytical data are tabulated.

Summary

Pore-water that resides in the pore space between minerals and along grain boundaries in crystalline rocks of low permeability cannot be sampled by conventional groundwater sampling techniques and therefore has to be characterised by applying indirect methods based on drillcore material. Accessible, interconnected pore-water has been extracted successfully by laboratory out-diffusion methods using some 16 drillcore samples from borehole KLX03 as part of the Oskarshamn hydrogeochemical site investigation programme. The objective was to characterise these pore-waters chemically and isotopically and relate these data to the present and past groundwater evolution of the site. This report outlines the methodology to extract and analyse the pore-water and tabulates the raw analytical data.

Sammanfattning

Porvatten som uppehåller sig i porutrymmen mellan mineral och längs mineralkorns-gränser i kristallint berg med låg permeabilitet kan inte provtas med konventionella provtagningstekniker för grundvatten och måste därför karakteriseras genom att använda indirekta metoder baserade på borrkärnematerial. Tillgängligt, sammanbundet porvatten har framgångsrikt extraherats på laboratorium med hjälp av diffusionsmetoder på 16 stycken borrkärneprover från borrhål KLX03 som en del i det hydrogeokemiska platsundersökningsprogrammet i Oskarshamn. Syftet var att karakterisera dessa porvatten kemiskt och isotopiskt och att relatera dessa data till platsens nutida och dåtida grundvattenutveckling. Denna rapport sammanfattar metodiken för att extrahera och analysera porvattnet och tabellerar analysrådatan.

Contents

1	**Introduction**	9
2	**Materials and methods**	11
2.1	Samples and sample preparation	11
2.2	Analytical methods	13
2.3	Data handling	15
2.4	Noncomformities	15
3	**Tabulation of analytical data**	17
4	**Acknowledgements**	39
5	**References**	41

1 Introduction

This document reports performance and results of the activity *characterisation of pore-water* in drillcore samples within the site investigation programme at Oskarshamn. The drillcore samples were selected during drilling of the telescopic borehole KLX03 and the work was carried out according to activity plan "Pore space groundwaters in low permeable crystalline rock in KLX03", SKB AP PS 400-04-043, version 1.0 (internal controlling document). The data from this activity are reported to the database SICADA.

Crystalline rocks are characterised in general by two hydraulic regimes. The first regime includes the water-conducting zones related to regional or local fracture networks. The second regime includes the bedrock mass of low permeability between the water-conducting zones. Depending on the residence time of formation groundwater in the water-conducting zones, interaction with water present in the pore space of the low permeable bedrock might become significant. In addition, since repository construction will be restricted largely to bedrock of low permeability, this pore-water over time will interact with the repository barrier materials (e.g. bentonite; canister) potentially leading to a deterioration in their physical properties. For safety assessment considerations it is therefore important to know the composition of such pore-water and its evolution over recent geological time, certainly during the last thousands to hundreds of thousands of years in accordance with the expected lifespan of a repository. Pore-water compositions can be assessed by combining the information gained from pore-water profiles within bedrock of low permeability and the chemical and isotopic data of formation groundwaters circulating in the adjacent fracture zones.

Pore-water that resides in the pore space between minerals and along grain boundaries in crystalline rocks of low permeability cannot be sampled by conventional groundwater sampling techniques and therefore has to be characterised by applying indirect methods based on drillcore material. Such techniques have been tested during the Matrix Fluid Chemistry Experiment in the Äspö HRL /Smellie et al. 2003/ and borehole KSH02 from the Oskarshamn site investigation /Waber and Smellie 2004/. One of these techniques, the laboratory out-diffusion method, hs been applied successfully to borehole KFM06A at Forsmark to trace the pore-water chemistry in low permeable bedrock to depths of around 1,000 m /Waber and Smellie 2005/.

A similar approach has been carried out for borehole KLX03. The methodology employed and the resulting analytical data are reported in this present report; preliminary interpretation of the data has been reported in /Laaksoharju 2006/.

2 Materials and methods

From borehole KLX03 16 drillcore sections were sampled between June 1st and September 6th 2004 for pore-water characterisation. The sections of about 20–50 cm in length were taken at regular depth intervals of approximately 100 m. This protocol required the samples to be taken from homogeneous, non-fractured bedrock volumes at least 5 m away from any water-conducting fractures or fracture zones. To safeguard against the selection of unsuitable samples, which might not be obvious at the time, extra core lengths were taken along the borehole length when good rock properties occurred.

An important requirement for pore-water characterisation using rock samples is the preservation of the fully water-saturated state of the rock material immediately following drilling and sampling and during transportation from the site to the laboratory. This precaution is to inhibit possible water-rock interactions induced by exposure of the rock sample to air. To minimise these potential perturbing effects the samples were immediately wiped clean with a dry towel following drilling and selection, wrapped into a heavy-duty PVC bag which was repeatedly flushed with nitrogen, evacuated and heat sealed. This procedure was repeated with a second PVC bag and finally sealed in a plastic coated Al-foil. The samples were then air freighted to the laboratory at the University of Bern, Switzerland, where they were immediately stored at 4°C in a cooling room and prepared for the various measurements and experiments within about 20 hours after arrival.

Once exposed to the air and/or stored over too long a time period, the drillcore samples lose their value for pore-water characterisation. Therefore, all samples received had to be rapidly conditioned so that the different laboratory experimental procedures could be initiated. For the out-diffusion experiments this involved all the drillcore samples collected (some 16).

In February 2005 a final decision was made as to which samples involved in the on-going out-diffusion experiments were considered unsuitable (e.g. areas of high fracture frequency) or at least potentially problematic for future interpretation. This selection initially was based on a personal on-site drillcore inspection, use of available drillcore mapping information, BIPS logs and also hydraulic data from downhole differential flow measurements. Guidance of the field personnel was invaluable. Ten samples were selected for the full analytical programme.

2.1 Samples and sample preparation

For legibility reasons the sample labelling adopted in this report is a subsequent numbering of the samples with depth using the borehole name as prefix; similar labelling was used for the laboratory studies. The conversion of this sample description to the SKB sample number and the vertical depth along borehole is given in Table 2-1. The analytical programme performed on the rock samples and experiment solutions is given in Table 2-2.

Following arrival at the laboratory the core sections were cut by dry sawing into full-diameter samples of about 19 cm length to be used specifically for the out-diffusion experiments. The remaining material from the top and bottom of the core section was used for the isotope diffusive-exchange method and the determination of the water content. For these methods the outer rim of the core (~ 0.5 cm) was first removed by chisel and hammer to minimise any small-scale sample effects resulting from de-saturation during initial perturbations by

Table 21. KLX03 borehole: list of samples used for pore-water studies.

Sample No	SKB sample No	Average depth (m)	Lithology	Alteration/ tectonisation[1)]	Fracture intensity
KLX03-1	SKB 007250	159.22	Avrö granite	± 5 m	moderate
KLX03-2	SKB 007251	202.66	Avrö granite	± 5 m	moderate
KLX03-3	SKB 007252	253.72	Avrö granite	± 5 m	moderate
KLX03-4	SKB 007423	303.10	Avrö granite	± 10 m	moderate
KLX03-5	SKB 007424	355.66	Avrö granite	± 10 m	moderate
KLX03-6	SKB 007425	411.70	Avrö granite	± 10 m	moderate
KLX03-7	SKB 007426	462.76	Avrö granite	± 5 m	moderate
KLX03-8	SKB 007427	524.63	Avrö granite	± 20 m	weak
KLX03-9	SKB 007428	590.12	Avrö granite	± 20 m	weak
KLX03-10	SKB 007429	643.14	Qtz-monzodiorite	± 10 m	moderate
KLX03-11	SKB 007430	695.95	Qtz-monzodiorite	± 1 m	high
KLX03-12	SKB 007431	803.21	Qtz-monzodiorite	± 1 m	very high
KLX03-13	SKB 007432	841.15	Qtz-monzodiorite	± 15 m	weak
KLX03-14	SKB 005349	894.53	Qtz-monzodiorite	± 5 m	weak
KLX03-15	SKB 005351	942.47	Qtz-monzodiorite	± 20 m	weak
KLX03-16	SKB 005352	979.78	Qtz-monzodiorite	± 15 m	weak

[1)] approximate distance to next major alteration zone above and below sample.

Table 2–2. KLX03 borehole: experiments and measurements performed on drillcore samples.

Sample	Mineralogy, geochemistry, fluid inclusions	Aqueous leaching	Water-content porosity	Physical porosity	Isotope diffusive exchange	Out-diffusion experiment
KLX03-1			X		X	X
KLX03-2			X		X	X
KLX03-3			X		X	X
KLX03-4			X		O	X
KLX03-5			X		X	X
KLX03-6			X		X	X
KLX03-7			X		X	X
KLX03-8			X		X	X
KLX03-9			X		–	X
KLX03-10			X		–	X
KLX03-11	X	X	X	X	X	X
KLX03-12			X		X	X
KLX03-13			X		O	X
KLX03-14			X		X	X
KLX03-15			X		O	X
KLX03-16			X		X	X

X = experiment performed, analyses available.

– = inadequate material to perform the experiment.

O = experiment performed, analytical data not produced based on final sample selection.

drilling activities and subsequent sample preparation. The wet weight of such material was determined immediately after preparation. The remaining rim material was further prepared for mineralogical and geochemical investigations.

2.2 Analytical methods

Most of the analytical work of this study has been conducted at the Institute of Geological Sciences, University of Bern, Switzerland. Thus, if not otherwise stated the analytics have been performed at this institution.

Mineralogical investigations were performed by optical microscopy of thin sections and X-ray diffractometry on pulped rock material of sample KLX03-11. Bulk chemical analyses were performed by X-ray fluorescence at University of Fribourg on homogenised rock material of less than 60 µ of grain size.

Mineral chemical analyses were performed with a Joel JXA-8200 electron microprobe The beam conditions used were 15 kV and 20 nA with peak and background analysis times of 20–30 seconds each. Standards used are natural or synthetic silicates. Estimated detection limits in µg/g are: Si 140; Ti 75; Cr 400; Al 120; Fe 450; Mn 400; Mg 75; Ca 120; Na 120; K 55; F 300; Cl 40.

Bulk density (ρ_{bulk}) was determined on sample cubes of about 1 cm^3 from the core centre by the Hg-displacement method. The sample cubes were then ground to < 60 µm and the grain density (ρ_{grain}) was measured by He-pycnometry.

The water content was determined by the gravimetric determination of the water loss by drying subsamples at 105°C until stable weight conditions (± 0.002 g). If the material received allowed it, then the weight of these samples was chosen to be more than about 200 g to minimise possible de-saturation effects and to account for variations in the grain size of the rocks.

The water content was also determined on the material used for the isotope diffusive-exchange method using the same technique. These samples remained saturated throughout the experiment because they were placed in a vapour-tight vessel at 100% humidity during the equilibration procedure (see also below). The water-content porosity was calculated from the water loss and the volumetrically determined bulk wet density (see below) or the grain density measured by He-pycnometry if available.

A measure for the bulk wet density of the rocks investigated was obtained from the volume and saturated mass of the core samples used for out-diffusion experiments. The volume was calculated from measurements of height and diameter of the core samples using a vernier calliper with an error of ± 0.01 mm. Variations in the core diameter over the lengths of the samples was found to be less than 0.05 mm for most samples and a constant diameter was used in the calculation of the volume. For the so-derived wet bulk density this results in an error of less than 3%.

Fluid inclusion petrography and microthermometry was conducted using a Linkham THMSG-600 heating-cooling stage with a Linkham TMS 91 temperature control on a Olympus BX51 microscop equipped with a 100/0.80 LM PlanFI objective lens. Laser Raman micro-spectroscopy was performed using a Jobin Yvon LabRam HR 800 confocal-laser Raman microprobe with a frequency-doubled Nd-YAG laser. The Raman microprobe is equipped with an Olympus BX41 microscope with an Olympus 100/0.95 UM PlanFI objective lens and a Linkham MDS-600 heating-cooling stage with a Linkham TMS

94 temperature. Measurement conditions were a laser beam at 532.12 nm, a hole width of 400 µm, a slit of 100 µm, and an accumulation time of 3×40 seconds. The relative abundance of fluid inclusions was done by image analysis of individual quartz grains.

Aqueous leaching tests were performed on different grain-size fractions prepared from the centre material of core KLX03-11. Leaching was performed in double-distilled water by gently shaking the PE tubes end over end over 24 hours under ambient conditions. Measurements of pH and alkalinity (by titration) were determined immediately after termination of the experiment. Major cations and anions were determined using a Metrohm 861 Compact ion-chromatograph with a relative error of ± 5%.

The stable water isotope composition of the pore-water was determined by the isotope diffusive-exchange method as originally described by /Rogge 1997/, /Rübel 2000/ and /Rübel et al. 2002/. In this method the isotope exchange occurs through the gaseous phase without any direct contact between the rock sample and the test water. Rock pieces of about 1 cm in diameter from the centre of the core and a small petri dish filled with a test water are stored together in a vapour-tight glass container. The mass and stable water isotope composition of the test water are known. In the test water about 0.3 mol NaCl are dissolved to lower the water vapour pressure above the test-water surface. This is to minimise loss of test water from the petri dish and condensation on the rock fragments and the glass container walls. The petri dish with the test water and the whole container are weighed before and after the exchange experiment to check that no water is lost from the container and there was no transfer of test water to the sample by possible swelling of the rock material. Equilibrium in the three reservoir system – rock sample, test water, and the air inside the container as a diaphragm – is achieved in about 10 to 20 days at room temperature depending on the size and water content of the rock pieces. After complete equilibration the test water was removed and analysed by ion-ratio mass spectrometry.

The isotope diffusive-exchange method was originally designed for rocks with water contents in the order of several percent. To account for the much lower water content in the crystalline rocks of borehole KLX03, the method was modified in that an artificial test water was used, which is strongly enriched in ^2H and depleted in ^{18}O ($\delta^{18}O = -109.84‰$ and $\delta^2H = +425.5‰$ V-SMOW). This modification was necessary in order to obtain a modified test water composition after equilibration that is outside the standard analytical error of the mass-spectrometer. Obviously, solutions so much enriched in ^2H are difficult to analyse for δ^2H and certain memory effects cannot be excluded for some of the samples. In contrast, the oxygen isotope data are more reliable.

Out-diffusion experiments were performed on complete core samples of about 190 mm in height by immersion into the same artificial test water as used for the isotope diffusive-exchange method (Figure 2-1). To accelerate the out-diffusion, the vapour-tight PVC containers were placed into a water bath with a constant temperature of 45°C. The weight of the core sample, the experiment container, and the artificial test water used was measured before and after the experiment to ensure that no loss of test water has occurred during the entire experiment. Weighing of the core before and after the experiment in addition gives valuable information about the saturation state of the core at the beginning of the experiment.

At specific time intervals, initially a few days and later a few weeks, 0.5 mL of solution were sampled for the determination of the chloride concentration as a function of time. The small samples were analysed on a Metrohm 861 Compact ion-chromatograph. The analytical error of these determinations is about 5% based on multiple measurements of the standard solutions.

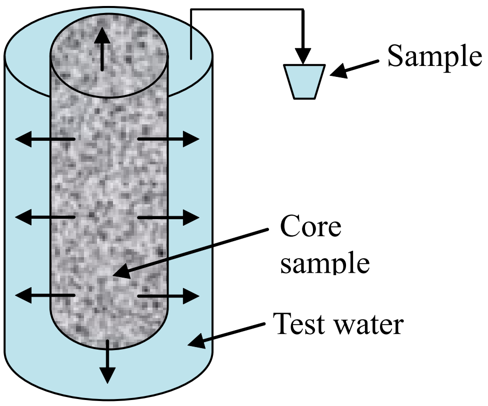

Figure 2–1. *Schematic picture of out-diffusion experiments performed.*

After steady state with respect to chloride was achieved, the core was removed from the container and the solution was immediately analysed for pH and alkalinity (by titration). The remaining solution was split into different aliquots for chemical and isotopic analyses. Major cation and anion were analysed by ion-chromatography at Hydroisotop GmbH with a relative error of 5%.

The isotopic compositions of oxygen and hydrogen in the various test solutions (diffusive-exchange method, and out-diffusion experiments) were determined by conventional ion-ratio mass spectrometry at Hydroisotop GmbH. The results are reported relative to the V-SMOW standard with a precision of ± 0.15‰ for $\delta^{18}O$ and ± 1.5‰ for $\delta^{2}H$.

The $^{87}Sr/^{86}Sr$ isotope ratio was measured at the University of Bern using a modified VG Sector® thermal ionisation mass spectrometer (TIMS) in simple collector mode, using oxidised Ta filaments. The analytical uncertainty is given with 2 σ of multiple measurements of the same sample. Total Sr concentrations are given in ppm.

The $^{37}C1/^{35}C1$ isotopic ratio, expressed as $\delta^{37}C1$ relative to SMOC, was measured at the University of Waterloo Environmental Isotope Lab (EIL) using a VG SIRA 9 Mass Spectrometer. Measurements were made with a precision of ± 0.15% (1 σ) based on repeat analyses of SMOC.

2.3 Data handling

All data from this activity are stored in SKB's database SICADA, where they are traceable by the Activity Plan number.

2.4 Noncomformities

The activity has been performed according to the activity plan without any significant nonconformities.

3 Tabulation of analytical data

Table 3-1. Mineralogical composition of sample KLX03-11 compared to samples of borehole KSH02 /Waber and Smelie 2004/.

Borehole Sample Vertical depth (m)		KLX03 KLX03-11 695.80–696.10	KSH02 785 G 785.30–785.52	KSH02 879 G 879.28–879.53	KSH02 997 G 997.01–997.26
Quartz	wt.%[1)]	18	12	16	14
K-feldspar	wt.%	16	20	19	14
Plagioclase	wt.%	34	28	34	32
Clinopyroxene	vol.%	1–5	1–5	5–10	5–10
Amphibole	vol.%	5–10	10–15	15–20	10–15
Biotite	vol.%	10–15	15–20	5–10	15–20
Opaque Phases	vol.%	1–5	5–10	1–5	1–5
Calcite	wt.%	0.5	0.6	0.9	< 0.5
Accessories	Chlorite, epidote, sericite, prehnite, vesuvianite, sphene, zircon, monazite, apatite, few clay minerals		Chlorite, sericite, clay minerals (very few), apatite, monazite, sphene, zircon		

[1)] wt.% from XRD analysis; vol.% from thin section analysis.

Table 3-2. Average chemical compositions of major mineral phases in the quartz-monzodiorite sample KLX03-11.

	Plagioclase center	Plagioclase rim	K-feldspar center	K-feldspar rim	Diopside	Amphibole	Biotite	Magnetite
SiO_2	58.80	60.05	65.06	64.91	52.51	54.67	37.01	0.02
TiO_2	0.10	0.01	0.02	0.01	0.14	0.31	3.05	0.04
Cr_2O_3	0.02	0.02	0.02	0.01	0.08	0.03	0.03	0.14
Al_2O_3	26.75	26.16	19.52	18.91	1.00	2.68	14.92	0.02
Fe_2O_3	0.00	0.00	0.00	0.02	0.54	0.00	0.00	0.00
FeO	0.10	0.16	0.05	0.00	9.75	13.31	19.89	93.08
MnO	0.02	0.01	0.05	0.03	0.68	0.46	0.21	0.02
MgO	0.00	0.00	0.00	0.00	12.38	13.76	10.96	0.01
CaO	8.19	7.23	0.89	0.00	22.72	11.98	0.01	0.04
Na_2O	6.68	7.23	1.83	0.75	0.36	0.33	0.10	0.03
K_2O	0.23	0.18	12.96	15.87	0.01	0.17	9.89	0.00
H_2O						2.06	3.86	
F							b.d.	
Cl							b.d.	
Total	100.89	101.04	100.40	100.52	99.99	99.74	99.92	93.39

b.d. = below detection.

Table 3-3. Chemical composition of sample KLX03-11 (quartz-monzodiorite) compared to samples from borehole KSH02 /Waber and Smellie 2004/.

Borehole **Sample** **Depth (m)**		**KLX03** **KLX03-11** **695.80–696.10**	**KSH02** **785 G** **785.30–785.52**	**KSH02** **879 G** **879.28–879.53**	**KSH02** **997 G** **997.01–997.26**
SiO_2	wt.%	58.09	58.90	57.46	58.06
TiO_2	wt.%	1.03	0.95	0.95	1.02
Al_2O_3	wt.%	16.77	15.53	15.73	16.24
Fe_2O_3	wt.%	7.25	7.20	6.60	7.53
MnO	wt.%	0.12	0.12	0.11	0.12
MgO	wt.%	3.05	3.38	2.45	2.70
CaO	wt.%	5.84	5.38	5.17	5.64
Na_2O	wt.%	3.33	2.91	3.22	3.02
K_2O	wt.%	3.02	3.71	3.68	3.04
P_2O_5	wt.%	0.42	0.27	0.29	0.30
LOI	wt.%	0.59	0.40	0.54	0.67
Sum	wt.%	99.70	99.05	96.49	98.64
Ba	ppm	789	915	868	782
Cr	ppm	68	81	19	8
Cu	ppm	20	< 2	26	8
Nb	ppm	14	14	13	14
Ni	ppm	14	25	11	13
Pb	ppm	15	30	20	36
Rb	ppm	84	98	102	77
Sr	ppm	666	593	597	594
V	ppm	25	< 5	< 5	< 5
Y	ppm	86	22	20	22
Zn	ppm	157	93	89	88
Zr	ppm	789	218	201	188

LOI = loss on ignition.

Table 3-4. Mineral chemistry data of sample KLX03-11: Plagioclase I (normalised to 32 charges and 8 cations).

	KLX03-11 plg3	KLX03-11 plg4	KLX03-11 plg5	KLX03-11 plg6	KLX03-11 plg7	KLX03-11 plg8	KLX03-11 plg1
Weight %							
SiO_2	60.93	60.79	59.81	60.10	59.37	59.35	59.017
TiO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.000
Cr_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.000
Al_2O_3	25.48	25.56	25.93	25.98	25.47	25.65	26.578
Fe_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.000
FeO	0.05	0.14	0.00	0.05	0.13	0.14	0.057
MnO	0.01	0.00	0.00	0.00	0.00	0.00	0.020
MgO	0.00	0.00	0.00	0.00	0.00	0.00	0.000
CaO	6.77	6.72	7.54	7.47	7.42	7.53	8.010
Na_2O	7.41	7.52	7.12	7.13	7.23	7.20	6.751
K_2O	0.24	0.19	0.22	0.20	0.12	0.20	0.078
Total	100.89	100.93	100.61	100.93	99.73	100.08	100.511
Cations (Fe^{2+}/Fe^{3+} charge balance)							
Si	2.697	2.689	2.658	2.663	2.660	2.650	2.63
Ti	0.000	0.000	0.000	0.000	0.000	0.000	0.00
Cr	0.000	0.000	0.000	0.000	0.000	0.000	0.00
Al	1.330	1.332	1.358	1.357	1.345	1.350	1.40
Fe^{3+}	0.000	0.000	0.000	0.000	0.000	0.000	0.00
Fe^{2+}	0.002	0.005	0.000	0.002	0.005	0.005	0.00
Mn	0.000	0.000	0.000	0.000	0.000	0.000	0.00
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.00
Ca	0.321	0.318	0.359	0.355	0.356	0.360	0.38
Na	0.636	0.645	0.613	0.612	0.628	0.623	0.58
K	0.013	0.011	0.012	0.011	0.007	0.011	0.00
Total	5.000	5.000	5.000	5.000	5.000	5.000	5.00
Endmembers							
$CaAl_2Si_2O_8$ (An)	0.331	0.327	0.365	0.362	0.359	0.362	0.394
$NaAlSi_3O_8$ (Alb)	0.655	0.662	0.623	0.626	0.634	0.626	0.601
$KAlSi_3O_8$	0.014	0.011	0.013	0.012	0.007	0.011	0.005
Total endmembers	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Residuals and ratios							
Al_Fe3_deficit	–0.001	0.005	–0.007	–0.006	–0.015	–0.012	0.002
Si deficit	0.028	0.016	0.022	0.026	0.019	0.012	0.025
An/An+Ab	0.335	0.331	0.369	0.367	0.362	0.366	0.396
Fe3/Fetot	0.000	0.000	–	0.000	0.000	0.000	0.000
Charge deficit	–0.075	–0.054	–0.048	–0.059	–0.030	–0.015	–0.070
Sum feldspar	0.971	0.974	0.984	0.978	0.990	0.995	0.970

Table 3-4 (cont.). Plagioclase II (normalised to 32 charges and 8 cations).

	KLX 03-11 plgc3	KLX 03-11 plgc4	KLX 03-11 plgr6	KLX 03-11 plgr7	KLX 03-11 plgr8	KLX 03-11 plgc9	KLX 03-11 plgc10	KLX 03-11 plgc11	KLX 03-11 plgr12	KLX 03-11 plgr13	KLX 03-11 plgr14
Weight %											
SiO_2	58.72	60.33	61.00	61.59	60.57	58.21	58.64	58.08	59.08	61.60	58.03
TiO_2	0.01	0.02	0.01	0.01	0.00	0.02	0.00	0.43	0.02	0.00	0.01
Cr_2O_3	0.04	0.04	0.00	0.01	0.00	0.00	0.03	0.00	0.02	0.00	0.06
Al_2O_3	27.02	25.88	25.72	25.38	26.10	27.21	27.10	26.56	26.40	23.19	27.21
Fe_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FeO	0.08	0.14	0.21	0.15	0.03	0.11	0.13	0.06	0.20	0.07	0.19
MnO	0.00	0.00	0.00	0.01	0.00	0.03	0.02	0.04	0.00	0.01	0.02
MgO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CaO	8.34	7.08	6.71	6.32	7.12	8.68	8.44	8.39	7.36	4.71	8.62
Na_2O	6.68	7.35	7.61	7.46	7.38	6.32	6.56	6.51	7.26	4.87	6.45
K_2O	0.23	0.20	0.30	0.15	0.09	0.26	0.21	0.26	0.08	5.88	0.26
Total	101.11	101.04	101.54	101.07	101.29	100.82	101.14	100.33	100.41	100.34	100.84
Cations (Fe^{2+}/Fe^{3+} charge balance)											
Si	2.602	2.667	2.680	2.723	2.670	2.592	2.600	2.599	2.627	2.775	2.581
Ti	0.000	0.001	0.000	0.000	0.000	0.001	0.000	0.015	0.001	0.000	0.000
Cr	0.001	0.001	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000	0.002
Al	1.411	1.349	1.332	1.323	1.356	1.428	1.416	1.401	1.383	1.232	1.426
Fe^{3+}	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Fe^{2+}	0.003	0.005	0.008	0.006	0.001	0.004	0.005	0.002	0.007	0.003	0.007
Mn	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.002	0.000	0.000	0.001
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ca	0.396	0.336	0.316	0.299	0.336	0.414	0.401	0.402	0.351	0.227	0.411
Na	0.574	0.630	0.648	0.640	0.631	0.545	0.564	0.565	0.626	0.425	0.557
K	0.013	0.011	0.017	0.008	0.005	0.015	0.012	0.015	0.005	0.338	0.015
Total	5.000	5.000	5.000	5.000	5.000	5.000	5.000	5.000	5.000	5.000	5.000
Endmembers											
$CaAl_2Si_2O_8$ (An)	0.403	0.344	0.322	0.316	0.346	0.425	0.411	0.410	0.357	0.230	0.418
$NaAlSi_3O_8$ (Alb)	0.584	0.645	0.661	0.675	0.649	0.560	0.577	0.575	0.638	0.429	0.567
$KAlSi_3O_8$	0.013	0.011	0.017	0.009	0.005	0.015	0.012	0.015	0.005	0.341	0.015
Total endmembers	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Residuals and ratios											
Al_Fe3_deficit	0.008	0.005	0.010	0.007	0.010	0.003	0.006	–0.009	0.026	0.002	0.008
Si deficit	0.005	0.011	0.002	0.039	0.016	0.017	0.011	0.008	–0.016	0.004	–0.001
An/An+Ab	0.408	0.347	0.328	0.319	0.348	0.431	0.416	0.416	0.359	0.349	0.425
Fe3/Fetot	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Charge deficit	–0.029	–0.045	–0.028	–0.123	–0.061	–0.053	–0.042	–0.048	–0.009	–0.018	–0.020
Sum feldspar	0.983	0.977	0.980	0.947	0.972	0.974	0.977	0.982	0.981	0.990	0.982

plgc: centre of plagioclase crystal.

plgr: rim of plagioclase crystal.

Table 3-4 (cont.). K-feldspar I (normalised to 32 charges and 8 cations).

	KLX03-11 kf1	KLX03-11 kf2	KLX03-11 kf3	KLX03-11 kf4
Weight %				
SiO_2	64.85	64.46	64.28	64.22
TiO_2	0.00	0.00	0.00	0.00
Cr_2O_3	0.00	0.00	0.00	0.00
Al_2O_3	18.84	18.75	18.86	19.98
Fe_2O_3	0.00	0.00	0.00	0.00
FeO	0.00	0.00	0.00	0.02
MnO	0.05	0.04	0.01	0.00
MgO	0.00	0.00	0.00	0.00
CaO	0.00	0.00	0.13	1.33
Na_2O	0.64	0.68	0.81	1.90
K_2O	16.04	15.89	15.65	12.89
Total	100.41	99.83	99.75	100.34
Cations (Fe^{2+}/Fe^{3+} charge balance)				
Si	2.980	2.979	2.970	2.937
Ti	0.000	0.000	0.000	0.000
Cr	0.000	0.000	0.000	0.000
Al	1.020	1.022	1.027	1.077
Fe^{3+}	0.000	0.000	0.000	0.000
Fe^{2+}	0.000	0.000	0.000	0.001
Mn	0.002	0.002	0.000	0.000
Mg	0.000	0.000	0.000	0.000
Ca	0.000	0.000	0.006	0.065
Na	0.057	0.061	0.073	0.168
K	0.940	0.937	0.923	0.752
Total	5.000	5.000	5.000	5.000
Endmembers				
$CaAl_2Si_2O_8$ (An)	0.000	0.000	0.006	0.066
$NaAlSi_3O_8$ (Alb)	0.057	0.061	0.073	0.171
$KAlSi_3O_8$	0.943	0.939	0.921	0.763
Total endmembers	1.000	1.000	1.000	1.000
Residuals and ratios				
Al_Fe3_deficit	0.020	0.022	0.021	0.011
Si deficit	–0.020	–0.021	–0.023	0.003
An/An+Ab	0.000	0.000	0.081	0.279
Fe3/Fetot	–	–	1.000	0.000
Charge deficit	0.017	0.017	0.028	–0.030
Sum feldspar	0.998	0.998	1.002	0.986

Table 3-4 (cont.). K-feldspar II (normalised to 32 charges and 8 cations).

	KLX03-11 kfc5	KLX03-11 kfc6	KLX03-11 kfc7	KLX03-11 kfr8	KLX03-11 kfr9	KLX03-11 kfr10
Weight %						
SiO_2	66.09	64.72	64.37	65.12	65.09	64.52
TiO_2	0.01	0.02	0.02	0.01	0.00	0.01
Cr_2O_3	0.00	0.00	0.05	0.01	0.03	0.00
Al_2O_3	19.68	18.83	20.06	19.00	18.83	18.89
Fe_2O_3	0.00	0.00	0.00	0.00	0.07	0.00
FeO	0.08	0.06	0.00	0.00	0.00	0.00
MnO	0.00	0.04	0.11	0.00	0.00	0.09
MgO	0.00	0.00	0.00	0.00	0.00	0.01
CaO	1.59	0.02	1.06	0.00	0.00	0.00
Na_2O	2.48	0.89	2.13	0.86	0.76	0.63
K_2O	11.15	15.37	12.37	15.68	15.85	16.09
Total	101.08	99.94	100.17	100.67	100.63	100.24
Cations (Fe^{2+}/Fe^{3+} charge balance)						
Si	3.002	2.986	2.947	2.982	2.984	2.970
Ti	0.000	0.001	0.001	0.000	0.000	0.000
Cr	0.000	0.000	0.002	0.000	0.001	0.000
Al	1.053	1.024	1.083	1.026	1.018	1.025
Fe^{3+}	0.000	0.000	0.000	0.000	0.002	0.000
Fe^{2+}	0.003	0.002	0.000	0.000	0.000	0.000
Mn	0.000	0.001	0.004	0.000	0.000	0.003
Mg	0.000	0.000	0.000	0.000	0.000	0.000
Ca	0.077	0.001	0.052	0.000	0.000	0.000
Na	0.218	0.079	0.189	0.076	0.068	0.056
K	0.646	0.905	0.723	0.916	0.927	0.945
Total	5.000	5.000	5.000	5.000	5.000	5.000
Endmembers						
$CaAl_2Si_2O_8$ (An)	0.082	0.001	0.054	0.000	0.000	0.000
$NaAlSi_3O_8$ (Alb)	0.232	0.080	0.196	0.077	0.068	0.056
$KAlSi_3O_8$	0.686	0.919	0.750	0.923	0.932	0.944
Total endmembers	1.000	1.000	1.000	1.000	1.000	1.000
Residuals and Ratios						
Al_Fe3_deficit	–0.029	0.023	0.029	0.026	0.020	0.025
Si deficit	0.084	–0.013	0.001	–0.018	–0.016	–0.030
An/An+Ab	0.262	0.010	0.216	0.000	0.000	0.000
Fe3/Fetot	0.000	0.000	–	–	1.000	–
Charge deficit	–0.194	–0.015	–0.069	0.001	0.007	0.035
Sum feldspar	0.941	0.985	0.963	0.992	0.994	1.001

kfc: centre of K-feldspar crystal.

kfr: rim of K-feldspar crystal.

Table 3-4 (cont.). Diopside (normalised to 12 charges).

	KLX03-11 cpx6	KLX03-11 cpx7	KLX03-11 cpx10	KLX03-11 cpx1	KLX03-11 cpx2	KLX03-11 cpx3
Weight %						
SiO_2	52.84	53.24	53.05	52.07	51.48	52.36
TiO_2	0.18	0.15	0.11	0.14	0.14	0.14
Cr_2O_3	0.02	0.07	0.03	0.02	0.14	0.18
Al_2O_3	1.16	0.93	0.94	0.95	1.11	0.93
Fe_2O_3	0.15	0.00	0.00	0.99	1.31	0.77
FeO	9.03	8.97	9.35	10.35	9.55	10.16
MnO	0.43	0.50	0.71	0.79	0.88	0.77
MgO	12.93	13.11	12.89	11.88	11.75	11.72
CaO	23.02	22.88	22.56	22.38	22.55	22.90
Na_2O	0.31	0.31	0.33	0.40	0.41	0.41
K_2O	0.00	0.01	0.01	0.00	0.03	0.01
Total	100.06	100.17	99.99	99.97	99.34	100.35
Cations (according to Lindsley, with AFe3+)						
Si	1.978	1.988	1.988	1.975	1.966	1.977
Ti	0.005	0.004	0.003	0.004	0.004	0.004
Cr	0.000	0.002	0.001	0.001	0.004	0.005
Al	0.051	0.041	0.041	0.042	0.050	0.041
Fe^{3+}	0.004	0.000	0.000	0.028	0.038	0.022
Fe^{2+}	0.283	0.280	0.293	0.328	0.305	0.321
Mn	0.014	0.016	0.023	0.026	0.028	0.025
Mg	0.721	0.729	0.720	0.672	0.669	0.659
Ca	0.923	0.915	0.906	0.909	0.923	0.926
Na	0.022	0.023	0.024	0.029	0.031	0.030
K	0.000	0.000	0.001	0.000	0.002	0.000
Total	4.002	3.998	4.000	4.014	4.019	4.011
Ratios and site activities						
Al4	0.022	0.012	0.012	0.025	0.034	0.023
Al6	0.029	0.029	0.030	0.017	0.016	0.018
xMg(Fe^{2+})	0.718	0.723	0.711	0.672	0.687	0.673
xMg(Fetot)	0.715	0.723	0.711	0.653	0.661	0.658
Fe^{3+}/Fe(tot)	0.015	0.000	0.000	0.079	0.110	0.064
Endmembers						
$NaFeSi_2O_6$ (acm)	0.004	0.000	0.000	0.028	0.032	0.022
$NaAlSi_2O_6$ (jad)	0.018	0.023	0.024	0.001	0.000	0.008
$CaTiAl_2O_6$	0.005	0.004	0.003	0.004	0.004	0.004
$CaCrAlSiO_6$	0.000	0.002	0.001	0.001	0.004	0.005
$CaFeAlSiO_6$	0.000	0.000	0.000	0.000	0.006	0.000
$CaAl2SiO_6$ (CaTs)	0.011	0.002	0.005	0.016	0.016	0.010
$Ca_{0.5}AlSi_2O_6$ (esc)	0.000	0.004	0.000	0.000	0.000	0.000
$Mg_2Si_2O_6$ (enst)	0.361	0.365	0.360	0.336	0.334	0.330
$Fe_2Si_2O_6$	0.141	0.140	0.147	0.164	0.152	0.160
$Mn_2Si_2O_6$	0.007	0.008	0.011	0.013	0.014	0.012
$Ca_2Si_2O_6$	0.453	0.453	0.449	0.444	0.446	0.454
Total endmembers	1.001	1.000	1.000	1.007	1.009	1.005
Total diopside	0.643	0.644	0.624	0.582	0.596	0.595

Table 3-4 (cont.). Amphibole (normalised to 46 charges and 2OH).

	KLX03-11 amp4	KLX03-11 amp5	KLX03-11 amp8	KLX03-11 amp9	KLX03-11 amp11	KLX03-11 amp12
Weight %						
SiO_2	59.90	54.76	50.15	57.57	54.30	51.31
TiO_2	0.01	0.10	0.78	0.11	0.15	0.69
Cr_2O_3	0.00	0.00	0.00	0.00	0.01	0.15
Al_2O_3	0.95	1.45	5.15	1.92	2.16	4.42
Fe_2O_3	0.00	0.00	0.00	0.00	0.00	0.00
FeO	11.85	13.26	15.37	11.45	13.08	14.87
MnO	0.47	0.52	0.55	0.42	0.44	0.34
MgO	12.93	14.36	12.68	14.11	15.01	13.49
CaO	11.13	12.48	11.90	11.62	12.51	12.21
Na_2O	0.14	0.15	0.68	0.22	0.24	0.53
K_2O	0.03	0.04	0.45	0.09	0.11	0.29
H_2O	2.05	2.06	2.03	2.07	2.08	2.06
Total	99.45	99.17	99.73	99.57	100.09	100.34
Cations (Fe^{2+}/Fe^{3+} charge balance)						
Si	8.764	7.987	7.392	8.359	7.828	7.469
Ti	0.001	0.011	0.086	0.011	0.017	0.076
Cr	0.000	0.000	0.000	0.000	0.001	0.017
Al	0.164	0.249	0.894	0.328	0.367	0.758
Fe^{3+}	0.000	0.000	0.000	0.000	0.000	0.000
Fe^{2+}	1.449	1.617	1.895	1.391	1.576	1.810
Mn	0.058	0.064	0.068	0.052	0.054	0.041
Mg	2.819	3.122	2.785	3.052	3.225	2.926
Ca	1.745	1.950	1.879	1.807	1.932	1.904
Na	0.039	0.041	0.195	0.061	0.066	0.149
K	0.005	0.008	0.085	0.017	0.021	0.053
H	2.000	2.000	2.000	2.000	2.000	2.000
Total	15.044	15.049	15.279	15.078	15.087	15.202
Ratios and site activities						
Al4	0.000	0.013	0.608	0.000	0.172	0.531
Al6	0.164	0.236	0.287	0.328	0.195	0.227
xMg(Fe^{2+})	0.660	0.659	0.595	0.687	0.672	0.618
xMg(Fetot)	0.660	0.659	0.595	0.687	0.672	0.618
xFe^{3+}	0.000	0.000	0.000	0.000	0.000	0.000
NaM4	0.000	0.000	0.000	0.000	0.000	0.000
NaA	0.039	0.041	0.195	0.061	0.066	0.149
NaK (A)	0.044	0.049	0.279	0.078	0.087	0.202

Table 3-4 (cont.). Biotite (normalised to 44 charges, 16 cations and 4OH).

	KLX 03-11 bt1	**KLX 03-11 bt2**	**KLX 03-11 bt3**	**KLX 03-11 bt4**	**KLX 03-11 bt5**	**KLX 03-11 bt6**	**KLX 03-11 bt7**	**KLX 03-11 bt8**	**KLX 03-11 bt9**	**KLX 03-11 bt10**
Weight %										
SiO_2	36.88	37.02	37.00	37.00	37.11	37.05	36.85	37.25	36.92	37.04
TiO_2	2.69	2.61	3.22	3.01	3.01	2.80	3.10	2.90	3.59	3.53
Cr_2O_3	0.01	0.06	0.02	0.00	0.00	0.00	0.00	0.12	0.05	0.02
Al_2O_3	14.81	14.92	14.57	14.70	15.31	15.40	15.08	14.91	14.79	14.75
Fe_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FeO	19.78	20.31	21.01	20.75	19.39	19.83	19.15	19.70	19.56	19.41
MnO	0.25	0.24	0.25	0.16	0.12	0.25	0.22	0.22	0.18	0.20
MgO	10.94	11.05	10.71	10.78	10.93	11.08	10.77	11.03	11.03	11.23
CaO	0.00	0.00	0.02	0.02	0.00	0.01	0.05	0.00	0.02	0.00
Na_2O	0.09	0.08	0.11	0.09	0.08	0.10	0.09	0.12	0.10	0.09
K_2O	9.89	9.79	9.86	9.81	10.00	10.01	9.86	9.99	9.83	9.89
H_2O	3.83	3.86	3.87	3.85	3.86	3.88	3.82	3.87	3.85	3.86
F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cl	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	99.17	99.94	100.63	100.17	99.79	100.38	98.99	100.10	99.92	100.01
F,Cl=O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	99.17	99.94	100.63	100.17	99.79	100.38	98.99	100.10	99.92	100.01
General Cations										
Cations (Fe^{2+}/Fe^{3+} charge balance)										
Si	5.773	5.755	5.739	5.756	5.769	5.724	5.780	5.777	5.747	5.753
Ti	0.317	0.305	0.375	0.353	0.351	0.325	0.366	0.338	0.421	0.412
Cr	0.001	0.007	0.002	0.000	0.000	0.000	0.000	0.014	0.006	0.002
Al	2.733	2.734	2.665	2.695	2.806	2.804	2.789	2.725	2.713	2.700
Fe^{3+}	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Fe^{2+}	2.590	2.640	2.725	2.699	2.520	2.562	2.512	2.555	2.546	2.521
Mn	0.033	0.032	0.033	0.021	0.016	0.032	0.029	0.029	0.024	0.026
Mg	2.553	2.561	2.476	2.499	2.532	2.550	2.517	2.550	2.558	2.601
Ca	0.000	0.000	0.003	0.004	0.000	0.001	0.008	0.000	0.004	0.000
Na	0.027	0.024	0.033	0.028	0.023	0.029	0.027	0.037	0.031	0.026
K	1.974	1.942	1.950	1.946	1.983	1.972	1.972	1.976	1.951	1.960
H	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000	4.000
F	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cl	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	16.000	16.000	16.000	16.000	16.000	16.000	16.000	16.000	16.000	16.000
Ratios and Site activities										
xMg(Fe^{2+})	0.496	0.492	0.476	0.481	0.501	0.499	0.501	0.499	0.501	0.508
xMg(Fetot)	0.496	0.492	0.476	0.481	0.501	0.499	0.501	0.499	0.501	0.508
xFe^{3+}	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table 3-4 (cont.). Prehnite (normalised to 22 charges, 7 cations and 2OH).

	KLX03-11 prh5	KLX03-11 prh6	KLX03-11 prh7	KLX03-11 prh8	KLX03-11 prh9	KLX03-11 prh19
Weight %						
SiO_2	43.16	43.36	43.24	43.14	42.83	43.17
TiO_2	0.31	0.25	0.36	0.10	0.32	1.24
Cr_2O_3	0.02	0.00	0.00	0.00	0.02	0.04
Al_2O_3	21.76	22.14	21,.41	22.37	21.51	20.72
Fe_2O_3	0.00	0.00	0.00	0.00	0.00	0.00
FeO	3.35	2.94	3.97	2.90	4.53	3.57
MnO	0.11	0.00	0.03	0.00	0.00	0.09
MgO	0.00	0.00	0.00	0.00	0.33	0.00
CaO	26.18	26.53	26.41	26.56	25.70	26.07
Na_2O	0.03	0.01	0.01	0.02	0.00	0.01
K_2O	0.01	0.02	0.02	0.01	0.01	0.01
H_2O	4.29	4.31	4.30	4.31	4.29	4.27
Total	99.22	99.55	99.74	99.40	99.52	99.20
General cations						
Cations (Fe^{2+}/Fe^{3+} charge balance)						
Si	3.019	3.018	3.014	3.004	2.991	3.034
Ti	0.016	0.013	0.019	0.005	0.017	0.065
Cr	0.001	0.000	0.000	0.000	0.001	0.002
Al	1.794	1.817	1.759	1.837	1.770	1.717
Fe^{3+}	0.000	0.000	0.000	0.000	0.000	0.000
Fe^{2+}	0.196	0.171	0.232	0.169	0.264	0.210
Mn	0.006	0.000	0.002	0.000	0.000	0.005
Mg	0.000	0.000	0.000	0.000	0.034	0.000
Ca	1.962	1.978	1.972	1.981	1.922	1.963
Na	0.004	0.001	0.001	0.002	0.000	0.002
K	0.001	0.001	0.002	0.001	0.001	0.001
H	2.000	2.000	2.000	2.000	2.000	2.000
Total	7.000	7.000	7.000	7.000	7.000	7.000
Ratios and site activities						
xMg(Fe^{2+})	0.000	0.000	0.000	0.000	0.114	0.000
xMg(Fetot)	0.000	0.000	0.000	0.000	0.114	0.000
xFe^{3+}	0.000	0.000	0.000	0.000	0.000	0.000

Table 3-4 (cont.). Vesuvianite (normalised to Ca + Na + K + Ba + Sr = 19).

Comment	KLX03-11 prh14	KLX03-11 prh16	KLX03-11 prh17	KLX03-11 pre5	KLX03-11 pre6	KLX03-11 pre7	KLX03-11 pre8
Weight %							
SiO_2	34.63	34.54	35.07	34.81	35.52	35.42	34.84
TiO_2	1.18	3.32	0.24	1.92	1.70	1.62	1.77
Cr_2O_3	0.00	0.04	0.04	0.00	0.02	0.00	0.00
Al_2O_3	9.22	8.90	10.71	11.36	10.87	10.55	11.35
FeO	15.96	14.11	15.04	12.95	13.47	13.86	12.64
MnO	0.01	0.01	0.00	0.03	0.01	0.00	0.03
MgO	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CaO	36.08	36.05	35.76	35.96	36.16	36.37	35.68
Na_2O	0.00	0.01	0.01	0.00	0.00	0.01	0.00
K_2O	0.01	0.00	0.01	0.02	0.00	0.01	0.02
H_2O	2.73	2.75	2.73	2.76	2.78	2.78	2.74
Total	99.81	99.73	99.61	99.81	100.53	100.62	99.06
Normalised to Ca+K+Na+Ba+Sr=19							
Si	17.019	16.983	17.380	17.157	17.419	17.256	17.309
Ti	0.435	1.228	0.090	0.713	0.626	0.593	0.661
Cr	0.000	0.015	0.015	0.000	0.006	0.000	0.000
Al	5.337	5.159	6.253	6.600	6.284	6.058	6.647
Fe^{2+}	6.559	5.800	6.232	5.337	5.521	5.649	5.250
Mn	0.003	0.002	0.000	0.013	0.003	0.001	0.011
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ca	18.994	18.991	18.984	18.987	18.996	18.987	18.989
Na	0.000	0.009	0.012	0.000	0.004	0.009	0.000
K	0.006	0.000	0.004	0.013	0.001	0.005	0.011

Table 3-4 (cont.). Magnetite (mgt, normalised to 8 charges) and Sphene (tit, normalised to 10 charges).

Comment	KLX03-11 mgt1	KLX03-11 mgt2	KLX03-11 tit3
Weight %			
SiO_2	0.02	0.02	27.76
TiO_2	0.04	0.04	37.90
Cr_2O_3	0.11	0.16	0.00
Al_2O_3	0.02	0.02	1.53
Fe_2O_3	0.00	0.00	0.00
FeO	93.21	92.95	7.02
MnO	0.04	0.00	1.19
MgO	0.00	0.01	0.00
CaO	0.03	0.05	24.69
Na_2O	0.03	0.02	0.01
K_2O	0.00	0.00	0.01
Total	93.51	93.28	100.11
General oxygen			
Cations (Fe^{2+}/Fe^{3+} Input)			
Si	0.001	0.001	0.934
Ti	0.002	0.002	0.959
Cr	0.004	0.007	0.000
Al	0.001	0.001	0.061
Fe^{3+}	0.000	0.000	0.000
Fe^{2+}	3.981	3.978	0.198
Mn	0.002	0.000	0.034
Mg	0.000	0.001	0.000
Ca	0.002	0.003	0.890
Na	0.003	0.002	0.001
K	0.000	0.000	0.000
Total cations	3.996	3.994	3.077
Ratios and site activities			
$xMg(Fe^{2+})$	0.000	0.000	0.000
xMg(Fetot)	0.000	0.000	0.000
xFe^{3+}	0.000	0.000	0.000

Table 3-5. Fluid inclusion data of quartz.

Abbreviations:

Sample KLX03-11 FI-x: – thick section with several quartz grains
FI-No: – number of inclusion in thick section
T_nIce: – nucleation temperature of ice
T_mIce: – melting of ice
T_nCla: – nucleation temperature of clathrate
T_mCla: – melting temperature of clathrate
T_hCO_2: – homogenisation temperature of clathrate

Sample KLX03-11 FI-1

FI-No[1)]	$T_n$ice [°C]	$T_m$ice [°C]	T_nCla [°C]	T_mCla [°C]	T_hCO_2 [°C]	NaCl eq-wt %	Comments
1			–37	+1.2	+27.7→L	14.2	3-phase: pure CO_2 (L+V), salt solution
2			–37	+1.4	+29.5→L	14.0	3-phase: CO_2 with little N_2 (L+V), salt solution; calcite inclusion
3	–41	–1.9				3.2	
4	–40	–1.8				3.1	
5	–72	–23.6		+0.7		> 24	CO_2 calcite and rutile inclusions
6	–43	–2.5				4.2	
7	–55	–18.8		Cla?		21.8	CO_2
8			–35	+3.0	+26.3→L	11.9	3-phase: CO_2 (L+V), salt solution; calcite inclusion
9	–61	–12.6				16.6	
10	–61	–12.7				16.7	T_m hydrohalite = –27.0°C
11	–71	–22.2				> 24	
12	–59	–12.4				16.4	
13	–60	–11.9				16.0	
14	–86	–44.3				> 24	$T_n$ice prograde, calcite and biotite inclusions
15	–60	–12.2				16.2	
16	–44	–3.8				6.1	
17	–59	–21.8				> 24	T_mCla = –14.8°C, CO_2
18	–70	–18.1				21.3	
19	–39	–0.7				1.2	
20	–40	–1.3				2.2	
21	–41	–1.4				2.4	

[1)] FI-No 1 to 15 are fluid inclusions in quartz with solid inclusions of rutile and biotite, FI-No 16 to 20 are fluid inclusions in quartz free of solid inclusions.

Table 3-5. (continued).

Sample KLX03-11 FI-2 FI-No	$T_n$ice[°C]	$T_m$ice [°C]	NaCl eq-wt %	Comments
1	–62	–14.1	18.0	quartz free of solid inclusions
2	–61	–14.0	17.9	quartz free of solid inclusions
3	–64	–14.7	18.5	quartz free of solid inclusions
4	–42	–3.2	5.3	quartz free of solid inclusions
5	–43	–3.3	5.4	quartz free of solid inclusions
6	–41	–2.4	4.0	quartz free of solid inclusions
7	–42	–2.5	4.2	quartz free of solid inclusions
8	–66	–16.2	19.8	quartz free of solid inclusions
9	–64	–15.0	18.8	quartz free of solid inclusions
10	–50	–6.7	10.1	quartz free of solid inclusions
11	–49	–6.3	9.6	quartz free of solid inclusions
12	–33	–4.0	6.4	quartz free of solid inclusions
13	–65	–16.2	19.8	quartz free of solid inclusions
14	–40	–1.9	3.2	quartz free of solid inclusions
15	–46	–4.6	7.3	quartz free of solid inclusions
16	–42	–2.6	4.3	quartz free of solid inclusions
17	–47	–5.1	8.0	quartz free of solid inclusions
18	–42	–2.4	4.0	quartz free of solid inclusions
19	–46	–4.6	7.3	quartz free of solid inclusions
20	–41	–1.8	3.1	quartz free of solid inclusions

Sample KLX03-11 FI-3 FI-No	$T_n$ice[°C]	$T_m$ice [°C]	NaCl eq-wt %	Comments
1	–45	–4.3	6.9	quartz free of solid inclusions
2	–40	–0.9	1.6	quartz free of solid inclusions
3	–35	–4.6	7.3	N_2 detected, no CO_2, quartz free of solid inclusions
4	–46	–4.2	6.7	quartz free of solid inclusions
5	–59	–11.7	15.8	quartz free of solid inclusions
6	–59	–12.0	16.0	quartz free of solid inclusions
7	–43	–2.8	4.6	quartz free of solid inclusions
8	–47	–4.6	7.3	quartz free of solid inclusions
9	–45	–4.2	6.7	quartz free of solid inclusions
10	–50	–10.9	14.9	N_2 detected, no CO_2, quartz free of solid inclusions
11	–60	–12.4	16.4	quartz free of solid inclusions
12	–41	–1.4	2.4	quartz free of solid inclusions
13	–31	–1.1	1.9	quartz free of solid inclusions
14	–40	–1.2	2.1	quartz free of solid inclusions
15	–62	–13.0	17.0	quartz free of solid inclusions
16	–42	–2.8	4.6	quartz free of solid inclusions
17	–47	–4.8	7.6	quartz free of solid inclusions
18	–48	–5.6	8.7	quartz free of solid inclusions
19	–54	–12.1	16.1	N_2 detected, no CO_2, quartz free of solid inclusions
20	–51	–12.2	16.2	quartz free of solid inclusions
21	–40	–1.7	2.9	quartz free of solid inclusions

Sample KLX03-11 FI-3				
FI-No	$T_n$ice[°C]	$T_m$ice [°C]	NaCl eq-wt %	Comments
22	–40	–1.2	2.1	quartz free of solid inclusions
23	–61	–12.8	16.8	quartz free of solid inclusions
24	–42	–2.5	4.2	quartz free of solid inclusions
25	–42	–2.6	4.3	quartz free of solid inclusions
26	–60	–14.3	18.2	quartz free of solid inclusions
27	–43	–2.3	3.9	quartz free of solid inclusions
28	–33	–1.6	2.7	quartz free of solid inclusions
29	–40	–1.1	1.9	quartz free of solid inclusions

Sample KLX03-11 FI-4				
FI-No	$T_n$ice[°C]	$T_m$ice [°C]	NaCl eq-wt %	Comments
1	–44	–3.3	5.4	quartz with solid inclusions
2	–49	–6.0	9.2	quartz with solid inclusions
3	–49	–5.7	8.8	quartz with solid inclusions
4	–44	–3.4	5.6	quartz with solid inclusions
5	–48	–10.0	14.0	quartz with solid inclusions
6	–55	–10.3	14.3	quartz with solid inclusions
7	–66	–15.4	19.1	quartz with solid inclusions
8	–60	–12.2	16.2	quartz with solid inclusions
9	–71	–18.8	21.8	quartz with solid inclusions
10	–57	–10.7	14.7	quartz with solid inclusions
11	–42	–2.0	3.4	quartz with solid inclusions
12	–54	–9.0	12.9	quartz with solid inclusions
13	–45	–3.3	5.4	quartz with solid inclusions
14	–44	–3.0	4.9	quartz with solid inclusions
15	–70	–18.0	21.2	quartz with solid inclusions
16	–43	–3.0	4.9	quartz with solid inclusions
17	–27	–0.4	0.7	quartz with solid inclusions
18	–34	–0.4	0.7	quartz with solid inclusions
19	–43	–2.8	4.6	quartz free of solid inclusions
20	–45	–4.3	6.9	quartz free of solid inclusions
21	–44	–3.9	6.3	quartz free of solid inclusions
22	–63	–14.7	18.5	quartz free of solid inclusions
23	–62	–13.8	17.7	quartz free of solid inclusions
24	–64	–16.3	19.9	quartz free of solid inclusions
25	–67	–16.9	20.4	quartz free of solid inclusions
26	–45	–3.8	6.1	quartz free of solid inclusions
27	–45	–3.7	6.0	quartz free of solid inclusions
28	–41	–1.8	3.1	quartz free of solid inclusions
29	–62	–13.5	17.5	quartz free of solid inclusions
30	–62	–13.1	17.1	quartz free of solid inclusions

Table 3-6. Bulk and grain density and physical porosity of samples from borehole KLX03.

Laboratory sample No	Lithology	Bulk density dry[1)] (g/cm³)	Grain density[2)] (g/cm³)	Physical porosity (vol.–%)	Mass of sample (g)	Bulk density wet[3)] (g/cm³)
KLX03-1	Avrö granite				1015.640	2.72
KLX03-2					1028.960	2.72
KLX03-3					1227.891	2.71
KLX03-4					1031.454	2.72
KLX03-5					1028.396	2.75
KLX03-6					1007.473	2.74
KLX03-7					1027.610	2.76
KLX03-8					1015.631	2.74
KLX03-9					1002.790	2.73
KLX03-10	quartz-monzo-diorite				982.509	2.73
KLX03-11		2.800	2.825	0.93	1036.704	2.79
KLX03-12					1050.850	2.78
KLX03-13					1053.568	2.80
KLX03-14					1044.860	2.80
KLX03-15					1041.053	2.81
KLX03-16					1047.565	2.80

[1)] determined by Hg-displacement on dry rock sample.

[2)] determined by He-pycnometry on dry rock sample.

[3)] determined from mass and volume of saturated (wet) drillcore sample used for out-diffusion experiment.

Table 3-7. Average water content by drying at 105°C and water-content (connected) porosity of rock samples from borehole KLX03.

Laboratory sample No	Lithology	Number of samples	Water content average (wt.–%)	Water content 1 σ (wt.–%)	WC-porosity average (vol.–%)	WC-porosity 1 σ (vol.–%)
KLX03-1	Avrö granite	3	0.217	0.014	0.588	0.038
KLX03-2		3	0.214	0.004	0.581	0.012
KLX03-3		3	0.242	0.019	0.661	0.051
KLX03-4		3	0.369	0.040	0.997	0.108
KLX03-5		3	0.212	0.016	0.582	0.044
KLX03-6		3	0.173	0.005	0.471	0.014
KLX03-7		3	0.276	0.051	0.757	0.139
KLX03-8		3	0.375	0.073	1.019	0.198
KLX03-9		1	0.190	–	0.51	–
KLX03-10	quartz-monzo-diorite	1	0.068	–	0.186	–
KLX03-11		3	0.122	0.006	0.339	0.018
KLX03-12		3	0.258	0.010	0.715	0.027
KLX03-13		3	0.103	0.012	0.287	0.032
KLX03-14		3	0.083	0.010	0.232	0.027
KLX03-15		3	0.089	0.022	0.249	0.063
KLX03-16		3	0.094	0.023	0.263	0.064

Table 3-8. Chemical data and modelling results of aqueous leaching experiments.

SAMPLE DESCRIPTION						
Borehole		KLX03	KLX03	KLX03	KLX03	KLX03
Sample		KLX03-11A	KLX03-11B	KLX03-11C	KLX03-11D	KLX03-11E
Type of Sample		Aq. Extract	Aq. Extract	Aq. Extract	Aq. Extract	Aq. Extract
Laboratory Extract		RWI, UniBe	RWI, UniBe	RWI, UniBe	RWI, UniBe	RWI, UniBe
Extraction Date		May 05	May 05	May 05	May 05	May 05
Conditions Extraction		ambient	ambient	ambient	ambient	ambient
Extraction Time		24 hours	24 hours	24 hours	24 hours	24 hours
S:L ratio		1:1	1:1	1:1	2:1	2:1
Grain Size		> 63 μm	0.14–0.8 mm	0.8–2 mm	2–4 mm	> 4 mm
MISCELLANEOUS PROPERTIES						
pH (lab)	-log(H+)	9.56	9.58	9.49	9.31	9.55
Sample Temperature	°C	20	20	20	20	20
DISSOLVED CONSTITUENTS						
Cations						
Sodium (Na^+)	mg/l	50.9	24.6	18.9	26.5	15.5
Potassium (K^+)	mg/l	65.8	10.8	4.6	4.7	3.8
Magnesium (Mg^{+2})	mg/l	0.2	< 0.1	< 0.1	< 0.1	< 0.1
Calcium (Ca^{+2})	mg/l	3.3	1.5	2.1	2	1.4
Strontium (Sr^{+2})	mg/l	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1
Anions						
Fluoride (F^-)	mg/l	2.1	0.4	0.2	0.3	0.2
Chloride (Cl^-)	mg/l	38.8	9.2	5	8.2	3.6
Bromide (Br^-)	mg/l	0.3	0.1	0.1	0.1	< 0.1
Sulfate (SO_4^{-2})	mg/l	14.5	3.9	4.9	9	1.6
Nitrate (NO_3^-)	mg/l	0.9	0.4	0.2	0.3	0.3
Total Alkalinity	meq/l	2.21	1.03	0.69	0.92	0.66
Tot. Alkal. as HCO_3	mg/l	134.8	62.8	42.1	56.1	40.3
PARAMETERS CALCULATED FROM ANALYTICAL DATA						
Sum of Anal. Constit.	mg/l	312	114	78	107	67
Charge Balance:	%	4.39	0.77	4.84	0.44	1.88
Ion-ion ratios						
Br/Cl molal	molar	3.431	4.823	8.874	5.411	–
Na/Cl molal	molar	2.023	4.124	5.829	4.984	6.640
K/Na molal	molarl	0.760	0.258	0.143	0.104	0.144
SO_4/Cl molal	molar	0.138	0.156	0.362	0.405	0.164
CARBONATE SYSTEM						
Calculated using measured values						
TIC from alkalinity	mol/kg	1.869e-03	8.647e-04	5.895e-04	8.284e-04	5.537e-04
Calcite saturation index		0.48	–0.07	–0.13	–0.17	–0.27
log p(CO_2)		–4.61	–4.95	–5.01	–4.67	–5.10
Isotopes						
δ^{37}Cl (‰ V-SMOC)		0.23				
$^{87}Sr/^{86}Sr$		0.738873		0.722539		0.723003
$^{87}Sr/^{86}Sr$ error		0.000030		0.000034		0.000050

Table 3-9. $\delta^{18}O$ and $\delta^{2}H$ of standard solutions used for the isotope diffusive exchange method and the out-diffusion experiments.

Standard No	Date	$\delta^{18}O$ ‰ V-SMOW	$\delta^{2}H$ ‰ V-SMOW	Sample KLX03-isotope diffusive exchange	Sample KLX03-out-diffusion
STD-LAB 1	16.06.2004	–11.13	–78.2	1–6	
STD-LAB 2	24.06.2004	–11.20	–80.6	7	
STD-LAB 3	21.07.2004	–11.05	–78.1		
STD-LAB 4	04.09.2004	–11.94	–84.2	8–12	
STD-LAB 5	25.09.2004	–11.32	–80.0	13–16	
STD-LAB 6	25.09.2004	–11.14	–79.2		
STD-TEW 1	16.06.2004	–109.76	425.5	1–6	1–6
STD-TEW 2	24.06.2004	–109.79	425.7	7	7
STD-TEW 3	21.07.2004	–109.86	425.5		
STD-TEW 4	04.09.2004	–109.85	425.8	8–12	8–12
STD-TEW 5	25.09.2004	–109.84	425.3	13–16	13–16
STD-TEW 6	25.09.2004	–109.68	426.9		

Table 3-10. Chemical composition of solutions from out-diffusion experiments at steady state conditions.

Out-Diffusion Experiment Solution	Units	KLX03-1	KLX03-2	KLX03-3	KLX03-4	KLX03-5	KLX03-6	KLX03-7	KLX03-8	KLX03-9
SAMPLE DESCRIPTION										
Vertical Depth	m	159.22	202.66	253.72	303.10	355.66	411.70	462.76	524.63	590.12
Rock Type										
Water-Rock Ratio		0.118	0.106	0.091	0.105	0.111	0.086	0.108	0.110	0.116
Experiment Temperature	°C	20	45	45	45	45	45	45	45	45
Experiment Time	days	190	100	100	100	100	100	99	90	90
MISC. PROPERTIES										
Chemical Type	Na-HCO_3-(F)-(Cl)	Na-HCO_3-Cl)	Na-HCO_3	Na-HCO_3-(F)-(Cl)	Na-HCO_3	Na-HCO_3-(Cl)	Ca-Na-SO_4-(HCO_3)	Na-Ca-Cl-HCO_3-SO_4	Na-Ca-Cl-HCO_3-SO_4	Na-HCO_3-(F)-(Cl)
pH (lab)	-log(H+)	8.02	7.89	8.15	7.55	7.85	7.88	7.27	7.34	7.36
Electrical Conductivity	µS/cm	390	475	637	353	625	446	1303		983
Sample Temperature	°C	20	20	20	20	20	20	20	20	20
CATIONS										
Sodium (Na^+)	mg/L	93.3	116	166	87.2	145	101	145	173	167
Potassium (K+)	mg/L	1.8	2.2	1.5	1.3	5.5	4.1	12.6	7.3	4.8
Magnesium (Mg^{+2})	mg/L	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	1.2	0.8	< 0.5
Calcium (Ca^{+2})	mg/L	3.2	3.6	3.4	2.4	9.3	6.7	149	140	42.5
Strontium (Sr^{+2})	mg/L	0.012	0.053	0.047	0.097	0.13	0.1	1.7	1.8	0.68
ANIONS										
Fluoride (F^-)	mg/L	11.7	6.6	7.4	10.4	5.2	2.8	2.4	2.1	4.7
Chloride (Cl^-)	mg/L	16	16.2	14.3	13.8	12.9	15.5	35.8	198	142
Bromide (Br^-)	mg/L	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	1.3	0.58
Sulfate (SO_4^{-2})	mg/L	7.8	8.1	16.4	11.8	21.7	9.3	506	347	100
Nitrate (NO_3^-)	mg/L	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	1.4	< 0.5
Total Alkalinity as HCO_3^-	mg/L	171.5	213.6	307.5	123.9	309.4	211.7	100.1	98.8	137.3
CALC. PARAMETERS										
Total dissolved solids	mg/L	305	366	517	251	509	351	954	969	599
Charge Balance	%	2.71	8.30	9.23	10.28	5.78	6.46	3.24	3.32	5.14

Table 3-10. (continued).

Out-Diffusion Experiment Solution	Units	KLX03-10	KLX03-11	KLX03-12	KLX03-13	KLX03-14	KLX03-15	KLX03-16	Standard Solution
SAMPLE DESCRIPTION									
Vertical Depth	m	643.14	695.95	803.21	841.15	894.53	942.47	979.78	
Rock Type									
Water-Rock Ratio		0.109	0.109	0.101	0.106	0.107	0.110	0.111	
Experiment Temperature	°C	45	45	45	20	45	45	45	
Experiment Time	days	90	90	90	149	89	89	89	
MISC. PROPERTIES									
Chemical Type		Na-Ca-HCO_3-Cl	Na-Ca-HCO_3	Na-(Ca)-HCO_3-Cl		Na-Ca-HCO_3-Cl		Na-Ca-HCO_3-Cl	
pH (lab)	-log(H+)	7.43	7.4	7.32	7.45	7.26	7.32	7.27	
Electrical Conductivity	µS/cm		328	830		486		400	14
Sample Temperature	°C	20	20	20		20		20	20
CATIONS									
Sodium (Na^+)	mg/L	57.3	40.1	158		70.3		69.9	0.2
Potassium (K^+)	mg/L	5	8.4	8.6		8.9		6.3	< 0.1
Magnesium (Mg^{+2})	mg/L	0.5	< 0.5	0.8		0.8		< 0.5	0.3
Calcium (Ca^{+2})	mg/L	15.6	28.3	23.6		37		19.2	0.1
Strontium (Sr^{+2})	mg/L	0.081	0.16	0.19		0.25		0.12	
ANIONS									
Fluoride (F^-)	mg/L	0.4	0.9	3.9		1.1		1	< 0.1
Chloride (Cl^-)	mg/L	15.9	6.8	120		30.3		41.4	1.1
Bromide (Br^-)	mg/L	0.23	< 0.1	0.59		< 0.1		0.18	< 0.1
Sulfate (SO_4^{-2})	mg/L	9.8	4.9	16.2		10.9		9.5	< 0.1
Nitrate (NO_3^-)	mg/L	0.7	4	6.3		< 0.5		< 0.5	
Total Alkalinity as HCO_3^-	mg/L	138.5	172.7	220.3	159.9	189.2	160.5	136.7	< 0.1
CALC. PARAMETERS									
Total dissolved solids	mg/L	243	262	552		349		284	< 2
Charge Balance	%	7.16	2.11	3.95		10.21		6.42	2.57

Table 3-11. δ18O and δ2H of pore-water and water content derived from isotope diffusive exchange method.

Laboratory sample No	Average vertical depth (m)	δ18O[1)] pore-water (‰ V-SMOW)	δ2H[1)] pore-water (‰ V-SMOW)	Water content[1)] (wt.-%)
KLX03-1	159.22	–12.26	–90.1	0.1767
KLX03-2	202.66	–11.44	–92.5	0.2417
KLX03-3	253.72	–11.43	–116.8	0.2799
KLX03-4	303.10	–[2)]	–	–
KLX03-5	355.66	–13.12	–78.2	0.2197
KLX03-6	411.70	–11.58	*–161.2*	0.1445
KLX03-7	462.76	–7.51	–83.9	0.2702
KLX03-8	524.63	–13.64	*–54.9*	*0.4226*
KLX03-9	590.12	—[2)]	—	—
KLX03-10	643.14	—	—	—
KLX03-11	695.95	–9.38	*–28.3*	*0.1420*
KLX03-12	803.21	–10.94	–58.6	0.3333
KLX03-13	841.15	–	–	–
KLX03-14	894.53	–5.14	*–1.9*	*0.0704*
KLX03-15	942.47	–	–	–
KLX03-16	979.78	–6.56	–28.7	0.1020

1) light shaded areas: indications for slight evaporation during experiment with lab water, true calculated δ18O and δ2H values might be more negative,
dark shaded areas with data in italics: analysis of traced test water with larger than standard error (possibly memory effect during 2H mass spectrometric measurement) and calculated values are less reliable.

2) – : experimental solutions not analysed; — : not enough material to perform experiment.

Table 3-12. Isotopic composition of solutions from out-diffusion experiments at steady state conditions.

Laboratory sample No	Vertical depth (m)	δ18O[1)] ‰ V-SMOW	δ2H[1)] ‰ V-SMOW	δ37Cl ‰ V-SMOC	Sr[3)] ppm	87Sr/86Sr	87Sr/86Sr 1 σ
KLX03-1	159.22			b.d.[2)]	0.024	0.715469	0.000029
KLX03-2	202.66	*69*	*–205*	2.47[2)]	0.034	0.714463	0.00002
KLX03-3	253.72	*157*	*–858*	b.d.[2)]	0.034	0.714416	0.000024
KLX03-4	303.10	*–12*	*60*				
KLX03-5	355.66	*–589*	*87*	b.d.[2)]	0.068	0.714817	0.000032
KLX03-6	411.70			1.89	0.088	0.714955	0.000021
KLX03-7	462.76						
KLX03-8	524.63			1.47	1.851	0.708281	0.00002
KLX03-9	590.12			2.13	0.74	0.709984	0.000027
KLX03-10	643.14						
KLX03-11	695.95			b.d.[2)]	0.139	0.71908	0.000027
KLX03-12	803.21			0.64	0.272	0.717795	0.000037
KLX03-13	841.15			b.d.[2)]			
KLX03-14	894.53			1.53[3)]	0.203	0.721149	0.000023
KLX03-15	942.47						
KLX03-16	979.78			0.61	0.166	0.717054	0.000034

1) calculated data in italics are meaningless and not used for further interpretation (see text).

2) b.d. = below detection or very small signal and not used for further interpretation.

3) analyses by mass spectrometry.spectrometry.

Table 3-13. Chloride concentration of pore-water calculated from out-diffusion solutions and the water content of the samples.

Laboratory sample No	Average vertical depth (m)	Pore-water Cl mg/kg H_2O	Pore-water Cl +error[1)] mg/kg H_2O	Pore-water Cl –error[1)] mg/kg H_2O
KLX03-1	159.22	806	55	48
KLX03-2	202.66	765	16	15
KLX03-3	253.72	503	41	35
KLX03-4	303.10	374	44	35
KLX03-5	355.66	613	49	42
KLX03-6	411.70	730	22	21
KLX03-7	462.76	1,377	305	210
KLX03-8	524.63	5,674	1,334	897
KLX03-9	590.12	8,578	938	767
KLX03-10	643.14	2,260	249	204
KLX03-11	695.95	513	28	25
KLX03-12	803.21	4,691	177	164
KLX03-13	841.15	–	–	–
KLX03-14	894.53	3,828	510	402
KLX03-15	942.47	–	–	–
KLX03-16	979.78	4,739	1,498	915

[1)] error based on the standard deviation of multiple water-content measurements except for samples KLX03-9 and KLX03-10 where an error of ± 10% for the single water-content measurement was assumed.

4 Acknowledgements

Much appreciation is given to Thomas Kisiel (SKB) for the on-site selection and packaging and rapid dispatching of the drillcore samples to the University of Bern. The support and patience of Liselotte Ekström (SKB) throughout the study was much appreciated. We are grateful for the analytical support by Dr Y Krüger and Prof L W Diamond (fluid inclusions), PD Dr E Gnos (mineral chemical analysis), Prof J Kramers (Sr-isotope analysis) and R Maeder (aqueous extraction chemistry), all at the Institute of Geological Sciences, University of Bern.

5 References

Laaksoharju, M (Ed.), 2006. Hydrogeochemical evaluation. Preliminary site description. Laxemar subarea – version 1.2. SKB R-06-12, Svensk Kärnbränslehantering AB.

Rogge T, 1997. Eine molekular-diffusive Methode zur Bestimmung des Porenwassergehaltes und der Zusammensetzung von stabilen Isotopen im Porenwasser von Gestein. Unpubl. Diploma Thesis, Institut für Umweltphysik, Unversity of Heidelberg.

Rübel A P, 2000. Stofftransport in undruchlässigen Gesteinsschichten – Isotopenuntersuchungen im Grund- und Porenwasser. PhD Thesis, Institut für Umweltphysik, Unversity of Heidelberg, Der Andere Verlag, Osnabrück, Germany.

Rübel A P, Sonntag Ch, Lippmann J, Pearson F J, Gautschi A, 2002. Solute transport in formations of very low permeability: Profiles of stable isotope and dissolved noble gas contents of pore-water in the Opalinus Clay, Mont Terri, Switzerland. Geochim. Cosmochim. Acta, 1311–1321.

Smellie J A T, Waber H N, Frape S K, 2003. Matrix fluid chemistry experiment, Final Report. SKB TR-03-18, Svensk Kärnbränslehantering AB.

Waber H N, Smellie J A T, 2004. Oskarshamn site investigations Borehole KSH02: Characterisation of matrix pore-water (Feasibility Study). SKB P-04-249, Svensk Kärnbränslehantering AB.

Waber H N, Smellie J A T, 2005. SKB Site Investigations Forsmark. Borehole KFM06: Characterisation of pore-water. Part I: Diffusion experiments. SKB P-05-196, Svensk Kärnbränslehantering AB.