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TECHNICAL REPORT 23-01

Sorption of Cs, Ni, Eu, Th and U on Drill Core Samples of Opalinus Clay and Confining Geological Units from Deep Boreholes in the Potential Siting Regions Nördlich Lägern, Zürich Nordost and Jura Ost:

Measurements and Predictive Sorption Modelling

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Abstract

In Stage 2 of the Sectoral Plan for Deep Geological Repositories (SGT), three regions, namely Jura Ost (JO), Nördlich Lägern (NL) and Zürich Nordost (ZNO) have been identified as suitable to host the deep geological repository for radioactive waste. To assess the potential of radionuclide (RN) retention and perform safety analyses during SGT Stage 3, sorption data bases covering the various combinations of porewater and mineralogical composition for the argillaceous rock formations in these three regions are required.

Because radionuclide sorption in complex geologic rock formations is inherently complex to be easily predicted by considering all processes, a methodology that accounts for the major retention pathways is needed. The simplified component additive modelling approach, known as the "bottom-up" approach, assumes that retention in clay-mineral-rich environments is controlled by sorption onto 2:1 clay minerals (*e.g.*, montmorillonite, illite or illite/smectite mixed layers). This approach allows the derivation of solid-liquid distribution coefficients (R_d values) for argillaceous rocks over a wide range of porewater and mineralogical compositions, using thermodynamic sorption models specifically developed for individual clay minerals.

In this report, the predictive capability of the ClaySor model, which is an upgraded version of the generalised Cs sorption (GCS) model and the 2-site protolysis non-electrostatic surface complexation and cation exchange (2SPNE SC/CE) model developed for illite is assessed on experimental sorption data obtained on rock samples from the three siting regions. Sorption isotherms for Cs(I), Ni(II), Eu(III), Th(IV) and U(VI) were measured on drill core samples from the boreholes Bözberg-1-1 in JO, Bülach-1-1 in NL and Trüllikon-1-1 in ZNO in their corresponding porewater compositions and compared to the R_d values calculated with the bottom-up approach. A total of 100 sorption isotherms were measured. For each of these isotherms, a blind prediction was calculated by scaling the ClaySor model, in which the GCS and 2SPNE SC/CE models together with the updated PSI/Nagra thermodynamic data base (TDB) 2020 were implemented to the 2:1 clay mineral content, considering the aqueous speciation of the RNs in the porewater. A comparison between measured and predicted R_d values for each case was then made.

For most clay-mineral-rich samples, the prediction and experimental data for Cs, Eu and Th agree well. The sorption of Ni is, however, mostly overestimated in the Ni equilibrium concentration below $10^{-5.5}$ M, probably due to the presence of competing cations such as Fe(II) or Mn(II). This was not considered in the modelling of the experimental data since the analytical determination of the competing cations, particularly Fe(II), was inconsistent. In contrast, the sorption of U is systematically underestimated, which was not the case in previous studies. The main reason is that the formation constant for $Ca_2UO_2(CO_3)_{3(aq)}$ (major aqueous U complex in the porewaters) leading to U sorption reduction in the modelling, was an order of magnitude lower in the previous studies compared to the one selected in the most recent PSI/Nagra TDB 2020. Another explanation could be the reduction of small amounts of U(VI) to U(IV) by Fe(II)-containing trace minerals, which would also lead to increased sorption. In clay-mineral-poor rocks, other minerals, especially calcite, might (partly) control the retention of given radionuclides.

All in all, the bottom-up approach provides a good and conservative methodology to predict the sorption on argillaceous rocks of several radionuclides, with oxidation states from I to IV and VI. In the cases where the blind prediction underestimates the observed sorption data, the bottom-up approach gives mostly conservative R_d values for the safety assessment.

Zusammenfassung

In Etappe 2 des Sachplans geologische Tiefenlager (SGT) wurden die drei Regionen Jura Ost (JO), Nördlich Lägern (NL) und Zürich Nordost (ZNO) als geeignete Standorte für ein geologisches Tiefenlager für radioaktive Abfälle identifiziert. Für die Auswahl des am besten geeigneten Standorts in SGT-Etappe 3 werden für die Sicherheitsanalysen Sorptionsdatenbanken (SDB) für die wichtigsten Gesteinsformationen dieser drei Regionen benötigt, die die verschiedenen möglichen Varianten der Porenwässer und die mineralogischen Zusammensetzungen der Gesteine einschliessen.

Da die Sorption von Radionukliden in geologischen Gesteinsformationen grundsätzlich zu komplex ist, um sie anhand der Berücksichtigung aller Prozesse leicht vorhersagen zu können, ist eine Methode erforderlich, die die wichtigsten Rückhaltungspfade heranzieht. Der vereinfachte «Bottom-up»-Ansatz der additiven Komponenten geht davon aus, dass die Rückhaltung in tonmineralreichen Umgebungen durch Sorption an 2:1 Tonmineralen (z. B. Montmorillonit, Illit oder Illit-/Smektit-Wechsellagerungen) gesteuert wird. Dieser Ansatz ermöglicht die Ableitung von Feststoff-Flüssigkeit-Verteilungskoeffizienten (R_d-Werte) für tonhaltige Gesteine für eine Bandbreite von Porenwässern sowie von mineralogischen Zusammensetzungen auf der Grundlage von thermodynamischen Sorptionsmodellen, die für die bestimmten Tonminerale entwickelt wurden.

Dieser Bericht beurteilt die Vorhersagefähigkeit des ClaySor-Modells, einer aktualisierten Version des «generalised Cs sorption» (GCS) Modells sowie des für Illit entwickelten «2-site protolysis non-electrostatic surface complexation and cation exchange» (2SPNE SC/CE) Modells. Die Bewertung erfolgt anhand experimenteller Sorptionsdaten, die an Gesteinsproben aus den drei Regionen gewonnen wurden. Sorptionsisotherme für Cs(I), Ni(II), Eu(III), Th(IV) und U(VI) wurden an Bohrkernproben aus den Tiefbohrungen Bözberg-1-1 (BOZ1-1) in JO, Bülach-1-1 (BUL1-1) in NL und Trüllikon-1-1 (TRU1-1) in ZNO in den jeweiligen Porenwässern gemessen und mit den nach dem Bottom-up-Ansatz berechneten Sorptionswerten verglichen. In dieser Studie wurden insgesamt 100 Sorptionsisotherme gemessen. Für jedes dieser Isotherme wurde eine Blindvorhersage berechnet, indem das ClaySor-Modell, das das GCS-Modell, die 2SPNE-SC/CE-Modelle und die aktualisierte thermodynamische PSI/Nagra Datenbank 2020 umfasst, auf den 2:1 Tonmineralgehalt skaliert und die wasserhaltige Speziation der Radionuklide im Porenwasser berücksichtigt wurden. Anschliessend wurde für alle Sorptionsisotherme ein Vergleich zwischen den gemessenen und vorhergesagten R_d-Werten durchgeführt.

Bei den meisten tonmineralreichen Proben stimmen für Cs, Eu und Th die Vorhersagen und die experimentellen Daten weitgehend überein. Die Sorption von Ni wird jedoch bei der Ni-Gleichgewichtskonzentration unter $10^{-5.5}$ M meist überschätzt, was wahrscheinlich auf das Vorhandensein von konkurrierenden Kationen wie Fe(II) oder Mn(II) zurückzuführen ist. Dies wurde bei der Modellierung der experimentellen Daten nicht berücksichtigt, da die analytische Bestimmung der konkurrierenden Kationen, insbesondere Fe(II), nicht immer einheitlich war. Im Gegensatz dazu wird die Sorption von U systematisch unterschätzt, was in früheren Studien nicht der Fall war. Der Grund dafür ist, dass die Bildungskonstante für $Ca_2UO_2(CO_3)_{3(aq)}$ (wichtigster wässriger U-Komplex in den Porenwässern), die in der Modellierung zu einer Verringerung der U-Sorption führt, in früheren Studien um eine Grössenordnung niedriger war als in der neuesten PSI/Nagra thermodynamischen Datenbank (TDB). Eine weitere Erklärung könnte die Reduktion geringer Mengen von U(VI) zu U(IV) durch Fe(II)-haltige Spurenelemente sein, was ebenfalls zu einer erhöhten Sorption führen könnte. In tonmineralarmen Gesteinen können andere Mineralien, insbesondere Kalzit, die Rückhaltung bestimmter Metalle (teilweise) steuern.

Grundsätzlich bietet der Bottom-up-Ansatz eine gute und konservative Methode zur Vorhersage der Sorption mehrerer Metalle in tonmineralreichen Gesteinen mit Oxidationsstufen von I bis IV und VI. Wo die Blindvorhersage die beobachteten Sorptionsdaten unterschätzt, gibt der Bottom-up-Ansatz meist konservative R_d-Werte für die Sicherheitsbeurteilung vor.

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List of Acronyms

2SPNE SC/CE	2-site protolysis non-electrostatic surface complexation and cation exchange
BOZ1-1	Bözberg-1-1 (deep borehole in the Jura Ost siting region)
BUL1-1	Bülach-1-1 (deep borehole in the Nördlich Lägern siting region)
CA	Component additive
CE	Cation exchange
CEC	Cation exchange capacity
CRZ	Containment-providing rock zone
EM	End-member
FES	Frayed edge sites
GCS	Generalised caesium sorption
GEMS	Gibbs energy minimisation software
ISML	Illite/smectite mixed layers
JO	Jura Ost (siting region)
NAGRA	National cooperative for the disposal of radioactive waste
NEA	Nuclear Energy Agency of the OECD
NL	Nördlich Lägern (siting region)
NTB	Nagra Technical Report (*Nagra Technischer Bericht*)
PS	Planar sites
PSI	Paul Scherrer Institute
PW	Porewater
RN	Radionuclide
RBG	General licence application (*Rahmenbewilligungsgesuch*)
RWI	Rock water interaction
SA	Safety assessment
SC	Surface complexation
SCC	Surface complexation constant
SDB	Sorption data base
SGT	Sectoral Plan for Deep Geological Repositories (*Sachplan geologische Tiefenlager*)
S/L	Solid/liquid
SPW	Synthetic porewater

T2S	Type II sites
TBO	Deep drilling (*Tiefbohrung*)
TDB	Thermodynamic data base
TIC	Total inorganic carbon
TRU1-1	Trüllikon-1-1 (deep borehole in the Zürich Nordost siting region)
ZNO	Zürich Nordost (siting region)

1 Introduction

The disposal of radioactive waste in deep geological argillaceous rock formations aims at retarding the migration of the radionuclides (RNs) into the biosphere for many hundreds of thousands of years. The transport of radionuclides in clay-rich sedimentary host rocks is mainly controlled by the diffusive properties of the formations and by retention processes such as the sorption along the migration path on, for example, mineral constituents of the host rock.

As part of the Swiss Sectoral Plan for Deep Geological Repositories (SGT) (BFE 2008), the National Cooperative for the Disposal of Radioactive Waste (Nagra) carried out an extensive deep borehole campaign in the Jura Ost (JO), Nördlich Lägern (NL) and Zürich Nordost (ZNO) siting regions to characterise in detail the site-specific rock properties. The sorption properties of the selected host rock Opalinus Clay and its containment-providing rock zone (CRZ) (*i.e.,* confining geological units), among others, are key parameters for the safety analysis and provide valuable information on the geochemical performance of the potential site (Leupin et al. 2017).

Since the sorption properties cannot be determined experimentally for all types of rock compositions, thermodynamic models must be developed and validated to ensure their capability to reliably predict sorption of radionuclides over a large range of geochemical conditions. The safety assessment (SA) for the general licence application (RBG) relies on calculated state-of-the-art sorption data bases (SDBs) (containing solid-liquid partition coefficients, R_d) for the relevant radionuclides in the different potential host rock formations. The simplified component-additive (CA) approach, the so-called "bottom-up" approach, is used to derive R_d values for argillaceous rocks at a wide range of porewater (PW) and mineralogical compositions. In general, the predictive CA approach considers all minerals constituting the natural system with their unique sorption properties, requiring sorption models for each single mineral component of the assemblage (Davis et al. 1998, OECD/NEA 2012).

However, CA modelling can be substantially simplified when one mineral component is assumed to dominate sorption (Payne et al. 2013). The underlying hypothesis of this approach is that the uptake of radionuclides in complex mineral/PW systems can be quantitatively predicted based on the understanding of the mechanistic sorption processes on single minerals, and the models developed to describe them. In the case of argillaceous rocks, the 2:1 clay minerals illite, smectite and illite-smectite mixed layers are assumed to be the preferential sorbents. Scaling the sorption models, *i.e.*, the site capacities, to the 2:1 clay mineral content of the rock, and including the element speciation in the PWs, the sorption isotherms in the natural rocks can be calculated. The applicability of this approach to clay mineral rich rocks has been demonstrated for different types of radionuclides on many types of sedimentary rocks and their corresponding PWs (Bradbury & Baeyens 2011, Chen et al. 2014, Marques Fernandes & Baeyens 2021, Marques Fernandes et al. 2015).

In the last two decades, "in-house" mechanistic thermodynamic sorption models have been extensively developed for a wide range of key elements, such as Cs(I), Ra(II), Ni(II), Co(II), Pb(II), Eu(III), Am(III), Th(IV), Sn(IV), Np(V), Pa(V) and U(VI). For the quantitative description of sorption on illite, two different models have been developed, namely the generalised Cs sorption (GCS) model (Bradbury & Baeyens 2000) and the 2-site protolysis non-electrostatic surface complexation and cation exchange (2SPNE SC/CE) model (Bradbury & Baeyens 2009a, Bradbury & Baeyens 2009b).

The 2SPNE SC/CE model has been implemented in Gibbs energy minimisation software (GEMS) (Kulik et al. 2013), which was developed and distributed at PSI (https://gems.web.psi.ch), under the name ClaySor model (Kulik et al. 2018). However, in the ClaySor thermodynamic SDB, surface complexation (SC) and cation exchange (CE) reactions with standard thermodynamic properties were compiled for montmorillonite and illite using the older thermodynamic data for

aqueous species collected from several literature sources, without uncertainty estimates for the thermodynamic constants. Since then, the standard thermodynamic data of relevant radionuclides have been revised in the PSI/Nagra chemical thermodynamic data base (TDB) 2020 (Hummel & Thoenen 2023), and the ClaySor model was updated accordingly. The update of the ClaySor model and of the data base consists of the implementation of the GCS model (Bradbury & Baeyens 2000) and the revision of the standard equilibrium constants of sorption species to ensure consistency with the most recent TDB data, along with the derivation of parameter confidence intervals which are compiled in Marinich et al. (2024). The latter are then used for evaluating the model uncertainty in predicting the uptake of relevant radionuclides in repository safety assessments (SA) for a given composition of PW and clay rock mineralogy. The R_d values are calculated directly by GEMS, including aqueous speciation, solubility and concentration-dependent sorption of each element for each defined argillaceous rock/PW system.

The overall aim of this study was to experimentally investigate the sorption properties of the rock formations of the JO, NL and ZNO siting regions and to test the predictive capability of the so-called "bottom-up" approach, towards sorption. For this purpose, sorption isotherms of the key nuclides Cs(I), Ni(II), Eu(III), Th(IV) and U(VI), which cover a wide range of relevant oxidation states, were measured on drill core samples from the deep boreholes Bözberg-1-1 (BOZ1-1) in JO, Bülach-1-1 (BUL1-1) in NL and Trüllikon-1-1 (TRU1-1) in ZNO. The sorption was blind-predicted with two sorption models developed for illite (GCS model and 2SPNE SC/CE model), implemented in the ClaySor model, and compared to the experimental data.

Ensuring that the argillaceous rocks possess the assumed sorption properties and validating the bottom-up approach are critical to justify their applicability for the SA of the deep geological repository for radioactive waste.

2 Materials and methods

2.1 Geographic origin of rock samples

The rock samples investigated for their sorption properties originate from the geological siting regions JO, NL, and ZNO, and are sub-samples from drill cores recovered from the deep boreholes (TBO) BOZ1-1, BUL1-1, and TRU1-1. An overview of the geographical location of these boreholes is given Fig. 2-1 in comparison with the other boreholes.

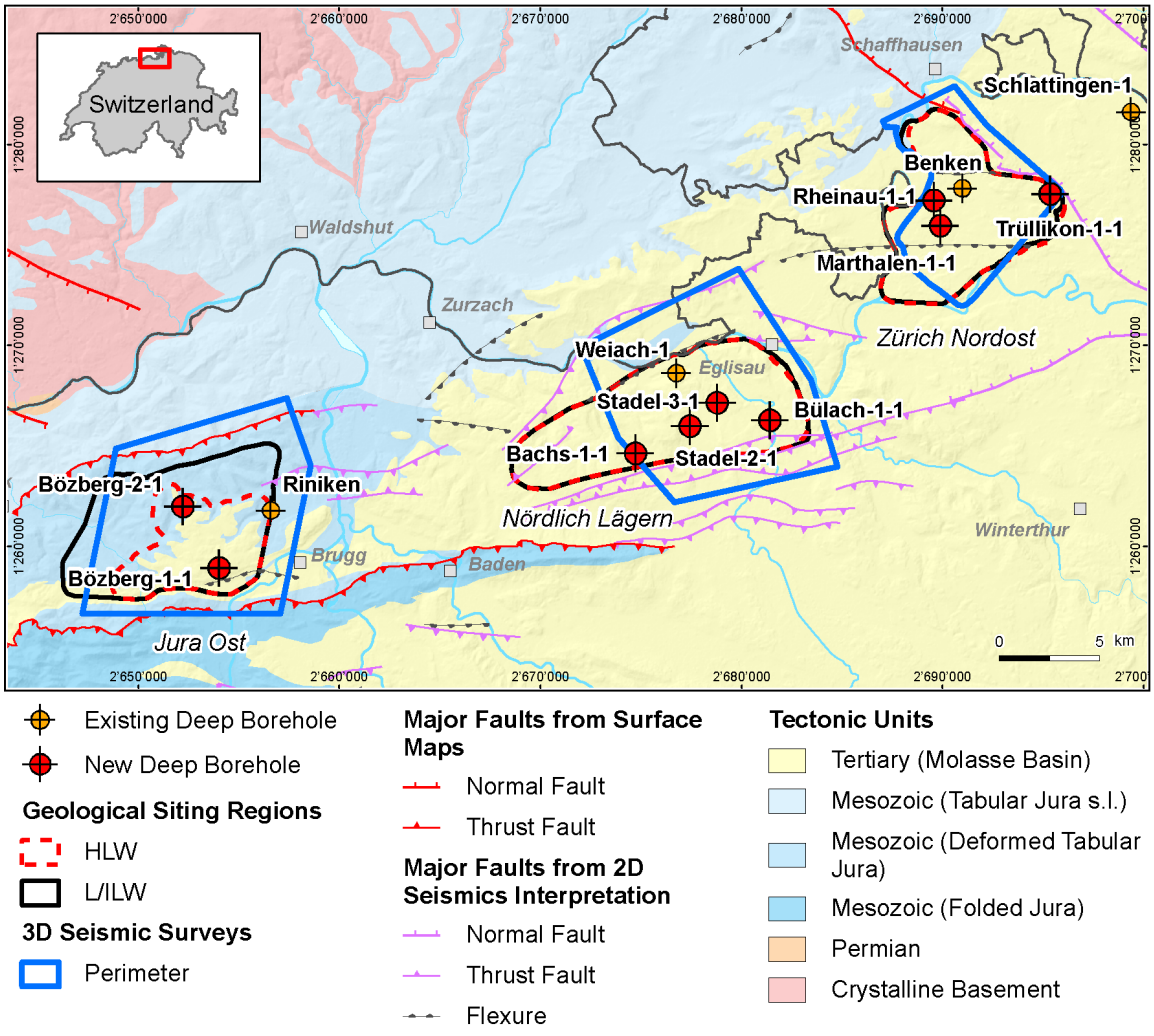

Fig. 2-1: Map of the three siting regions JO, NL, and ZNO, with the locations of the TBO boreholes, including the ones sampled for this study (BOZ-1-1, BUL-1-1, TRU-1-1)

2.2 Mineralogy

The sorption experiments were carried out on a total of 21 samples with different mineralogical compositions from cores recovered from the TBO BOZ1-1, BUL1-1, and TRUL1-1. In general, the samples were selected to ensure the determination of the sorption of the host rock (*i.e.*, Opalinus Clay) for the deep geological repository as well as of the upper and lower CRZ.

The mineralogical analysis of the rock samples was performed by the Rock Water Interaction (RWI) group of the University of Bern by X-ray diffraction on sub-samples of the same or close depth sample but not exactly on the samples used in the present study. The detailed mineralogical analyses for BOZ1-1, BUL1-1, and TRUL1-1 rock samples are shown in Tab. 2-1, Tab. 2-2 and Tab. 2-3, respectively. Key minerals with respect to this study are the illite end-member (EM) and smectite EM contents and are denoted throughout this report as illite and smectite, respectively. These tables also show the main lithographic groups and formations (Marques Fernandes et al. 2024b) and their Füchtbauer names (Füchtbauer 1988) for each rock sample investigated in this report.

The total clay mineral content of the studied rock samples varies from 1 wt.% (BUL1-845) to 79.2 wt.% (BOZ1-681). Most of the samples are argillaceous with total clay mineral contents ranging from ~ 30 - 60 wt.%. In all cases, illite is the dominant clay mineral followed by kaolinite, smectite and chlorite. Generally, the clay mineral rich samples have low calcite contents whereas the clay mineral poor samples have very high calcite contents (*e.g.,* up to 98 wt.% for BUL1-845).

For BOZ1-1, sorption was measured on four samples from the upper confining Wildegg, Klingnau and Passwang formations (BOZ1-323, -440, -493, -521). The illite/smectite content ranged from 11 to 36.6 wt.% with calcite contents from 81 to 16 wt.% (Tab. 2-1). Two additional samples, one Opalinus Clay sample (BOZ1-572) and one from the underlying Staffelegg Formation (BOZ1-681) were also examined. BOZ1-572 and BOZ1-681 contained 25.4 wt.% and 56.9 wt.% illite/ smectite, respectively.

From BUL1-1, eight samples from different depths and lithologies were investigated. These include three samples from Opalinus Clay formation (BUL1-921, -955 and -995) and one from Wedelsandstein (BUL1-861) with illite/smectite content varying between 25.5 – 43.7 wt.% and low calcite content (≤ 14 wt.%) (Tab. 2-2). Additionally, two clay-mineral-poor but calcite-rich samples were taken from the upper «Herrenwis Unit», *i.e.,* BUL1-845 and -851 with 0.9 and 6 wt.% illite/smectite, respectively, as well as two samples from the lower Staffelegg Formation (BUL1-1002 and -1017) with similar illite/smectite contents of about 25 wt.% but with BUL1-1002 being calcareous. It should be noted that the clay-mineral-poor sample BUL1-851 was only used for the U sorption experiments due to insufficient material of the BUL1-845 sample.

For TRU1-1, sorption experiments were carried out on seven samples. Three samples from the Opalinus Clay (TRU1-831, -882 and -923) had comparable illite/smectite contents of about 31.7 to 36.5 wt.% and low calcite content. The other four samples, three samples from the overlying units (TRU1-748, -794 and -815), and one from the underlying Staffelegg Formation (TRU1-938), had illite/smectite contents between 15.9 to 33.9 wt.% and calcite contents between 14 to 43 wt.% (Tab. 2-3).

Cation exchange capacities (CEC) measurements (in meq/kg) of the rock samples from JO, NL, and ZNO were obtained using the nickeltriethylenediamine (Ni-en) method (Marques Fernandes et al. 2024b) and the results are included in Tab. 2-1, Tab. 2-2 and Tab. 2-3, respectively. The dominant clay minerals in most of the rock samples sample are illite and kaolinite EMs. The former contributes significantly to the overall CEC, whereas the latter contributes much less due to the very low CEC of kaolinite. The study of Marques Fernandes et al. (2024) showed a very good agreement between the experimentally determined Ni-en CEC and clay mineral content.

Tab. 2-1: Mineralogical composition (wt.%) and CEC values of the BOZ1-1 rock samples from JO

Rock sample	**BOZ-323**	**BOZ-440**	**BOZ-493**	**BOZ-521**	**BOZ-572**	**BOZ-681**
Lithographic Group	Malm	Dogger	Dogger	Dogger	Dogger	Lias
Formation	Wildegg	Klingnau	Passwang	Passwang	Opalinus Clay	Staffelegg
Füchtbauer name	Limestone	Calcareous marl	Sandy/ silty marl	Very sandy/ silty claystone	Very sandy/ silty claystone	Claystone
Depth (m)	-323.16	-440.55	-493.15	-521.50	-572.43	-681.57
Mineral	(wt.%)					
C(org)	0.36	0.40	0.60	0.60	0.68	0.87
Quartz	3	6	22	31	31	9
K-feldspar	2	2	5	5	5	0
Plagioclase	0	0	2	4	3	0
Calcite	81	55	35	16	15	8
Dolomite/Ankerite	2	7	0	0	0	0
Siderite	-	-	-	3	5	3
Anhydrite	0	0	0	0	3	0
Pyrite	0.6	0.6	1.2	1.4	0.6	3.0
Illite EM	8.4	12.5	23.3	29.5	22.1	49.1
Smectite EM	2.5	1.8	7.8	7.1	3.3	7.8
Kaolinite EM	0.3	7.9	2.0	2.4	13.5	15.5
Chlorite EM	0.1	6.9	2.2	2.4	4.0	6.8
Total clay minerals	11.3	29.1	35.3	41.4	42.9	79.2
Ni-en CEC	(meq/kg)					
	57.9	56.7	136.8	136.5	84.5	163.9

Tab. 2-2: Mineralogical composition (wt.%) and CEC values of the BUL1-1 rock samples from NL

Rock sample	**BUL-845**	***BUL-851**	**BUL-861**	**BUL-921**	**BUL-955**	**BUL-995**	**BUL-1002**	**BUL-1017**
Lithographic Group	Dogger	Dogger	Dogger	Dogger	Dogger	Dogger	Lias	Lias
Formation	«Herrenwis Unit»	«Herrenwis Unit»	Wedel-sandstein	Opalinus Clay	Opalinus Clay	Opalinus Clay	Staffelegg	Staffelegg
Füchtbauer name	Limestone	Limestone	Very sandy/ silty claystone	Very sandy/ silty claystone	Claystone	Claystone	Calcareous marl	Very argillaceous sandstone/ siltstone
Depth (m)	-845.05	-851.50	-861.00	-921.43	-955.62	-995.09	-1002.19	-1017.33
Mineral	(wt.%)							
C(org)	0.10	0.18	0.56	0.85	1.01	0.98	4.03	0.67
Quartz	1	3	27	28	15	16	9	37
K-feldspar	-	-	6	5	4	5	3	5
Plagioclase	-	-	3	3	3	3	2	4
Calcite	98	90	14	10	4	9	47	7
Dolomite/Ankerite	-	-	-	-	-	-	-	2
Siderite	-	-	-	3	3	2	-	2
Pyrite	-	0.2	1.1	1.2	0.5	1.1	2.0	0.3
Illite EM	0.7	5.4	36.9	22.9	33.3	29.0	21.2	21.2
Smectite EM	0.2	0.6	6.8	2.6	3.9	3.4	3.1	2.2
Kaolinite EM	0.0	0.4	2.7	17.7	25.5	23.4	5.9	12.5
Chlorite EM	0.1	0.4	2.1	5.3	6.6	7.1	3.1	6.1
Total clay minerals	1.0	6.8	48.5	57.6	69.3	62.9	33.3	42.0
Ni-en CEC	(meq/kg)							
	0	7.0	140.0	86.9	110.4	106.3	60.2	68.9

* Sample BUL-851 is only used for the sorption experiments of U.

Tab. 2-3: Mineralogical composition (wt.%) and CEC values of the TRU1-1 rock samples from ZNO

Rock sample	**TRU-748**	**TRU-794**	**TRU-815**	**TRU-831**	**TRU-882**	**TRU-923**	**TRU-938**
Lithographic Group	Dogger	Dogger	Dogger	Dogger	Dogger	Dogger	Lias
Formation	Parkinsoni-Württenberg	Wedelsandstein	Wedelsandstein	Opalinus Clay	Opalinus Clay	Opalinus Clay	Staffelegg
Füchtbauer Name	Argillaceous marl	Very sandy/ silty claystone	Sandstone/ siltstone	Very sandy/ silty claystone	Very sandy/ silty claystone	Claystone	Calcareous marl
Depth (m)	-748.98	-794.56	-815.28	-831.37	-882.36	-923.34	-938.9
Mineral	(wt.%)						
C(org)	0.76	0.66	0.43	1.27	1.10	1.01	4.65
Quartz	16	27	42	19	22	15	10
K-feldspar	5	5	6	5	5	5	3
Plagioclase	2	3	4	3	3	3	2
Calcite	27	14	23	5	7	6	43
Dolomite/Ankerite	4	1	1	-	-	-	-
Siderite	-	-	-	3	5	3	-
Pyrite	-	-	-	-	-	-	-
Illite EM	27.4	31.2	14.2	31.6	28.9	33.2	24.2
Smectite EM	2.2	2.9	1.9	3.2	2.8	3.3	2.8
Kaolinite EM	10.4	9.7	4.9	20.9	18.2	20.6	5.3
Chlorite EM	3.5	4.9	2.6	7.6	6.8	8.6	3.2
Total clay minerals	43.5	48.7	23.6	63.3	56.7	65.7	35.5
Ni-en CEC	(meq/kg)						
	88.6	111.1	50.9	117.2	110.5	119.4	92.7

2.3 Synthetic porewater composition

The sorption of Cs(I), Ni(II), Eu(III), Th(IV) and U(VI) on the different rock samples were measured in well-defined synthetic porewaters (SPW). The redox state of these five elements remains constant in all sorption experiments and will be omitted throughout this report. The composition of the PWs used in the experiments was defined by the RWI Group of the University of Bern and are summarised in Tab. 2-4. For each borehole, one single PW composition was used. It should be noted that the SPW compositions are not representative of in-situ PW conditions in terms of pε, pH and pCO_2. The partial pressure of CO_2 is a very important parameter that affects the pH, the aqueous speciation and consequently the SC behaviour of certain elements (*e.g.*, Eu, U). The PWs were chosen in equilibrium with atmospheric pCO_2 ($10^{-3.4}$ bar) to avoid experimental problems (*e.g.*, pH drift, potential intrusion of atmospheric CO_2) and to establish well-constrained experimental systems for the modelling. The main difference between the three SPWs is their ionic strength ranging from 0.505 M to 0.190 M. This difference in salinity is expected to essentially affect the retention of Cs, as it adsorbs through CE. The relatively small variation of total inorganic carbon (TIC) of the three SPWs is caused by the slight pH variation at constant pCO_2. The TIC is expected to influence essentially the cations which adsorb via SC, and which form strong aqueous carbonate complexes with *e.g.*, UO_2^{2+}.

Tab. 2-4: SPW compositions used in the sorption experiments with the samples from BOZ1-1 (JO), BUL1-1 (NL), and TRU1-1 (ZNO)

Element	**BOZ1-1 (JO)**	**BUL1-1 (NL)**	**TRU1-1 (ZNO)**
Na (M)	$1.40 \cdot 10^{-1}$	$3.43 \cdot 10^{-1}$	$2.44 \cdot 10^{-1}$
K (M)	$7.76 \cdot 10^{-4}$	$1.91 \cdot 10^{-3}$	$1.64 \cdot 10^{-3}$
Ca (M)	$9.24 \cdot 10^{-3}$	$3.83 \cdot 10^{-2}$	$2.22 \cdot 10^{-2}$
Mg (M)	$3.94 \cdot 10^{-3}$	$1.76 \cdot 10^{-2}$	$1.56 \cdot 10^{-2}$
Sr (M)	$1.15 \cdot 10^{-4}$	$3.33 \cdot 10^{-4}$	$2.89 \cdot 10^{-4}$
Cl (M)	$8.28 \cdot 10^{-2}$	$4.02 \cdot 10^{-1}$	$2.72 \cdot 10^{-1}$
S (as SO_4) (M)	$4.21 \cdot 10^{-2}$	$2.75 \cdot 10^{-2}$	$2.43 \cdot 10^{-2}$
TIC (as HCO_3) (M)	$7.05 \cdot 10^{-4}$	$4.13 \cdot 10^{-4}$	$4.87 \cdot 10^{-4}$
pH pCO_2 (bar) I (M)	7.90 $10^{-3.4}$ 0.190	7.56 $10^{-3.4}$ 0.505	7.68 $10^{-3.4}$ 0.354

2.4 Experiments

The CEC and sorption measurements were performed on crushed rock samples. Vacuumed samples (2×3 cm^3 cubes) from the different drill cores were provided by the Institute of Geological Sciences (University of Bern). Once at PSI, the vacuumed samples were transferred into an N_2-flooded glove box ($O_2 < 1$ ppm) for crushing and storage. The samples were first crushed by hand in an agate mortar to pieces < 1 cm^3. Further grinding (< 1 mm) was carried out in a Retsch mortar. The samples were stored in the glove box in closed, well-labelled containers.

2.4.1 Cation exchange capacity experiments

The CECs of the rock samples were determined using the high-selective divalent Ni-en complex radiolabelled with ^{63}Ni (Peigneur 1976). These measurements were carried out and replicated once or twice under ambient air conditions. As a measure of the total negative charge, the CEC predominantly results from the presence of 2:1 phyllosilicates. CEC is directly correlated with the wt.% content and type of clay minerals in the rock samples, and consequently to the sorption properties towards radionuclides.

The procedure consists essentially of a sorption experiment with ^{63}Ni labelled Ni-en. The high-selectivity complex was prepared by adding uncharged ethylenediamine to an $Ni(NO_3)_2$ solution to obtain a stable Ni-triethylenediamine complex. 30 mL of the ^{63}Ni-en solution were added to ~1 g of rock sample, pre-weighed into polypropylene centrifuge tubes, to give an S:L ratio of ~32 g/L. The tubes were closed, shaken end-over-end for 1 day, centrifuged, and the supernatant solutions were radio-assayed using a Packard Tri-Carb liquid scintillation counter. The CEC experiments were carried out in duplicate or triplicate. The pH of the supernatant was measured after phase separation.

The Ni-en adsorbed ($Ni\text{-}en_{ads}$) in meq/kg (equal to the CEC) is calculated from the redistribution of the radiotracer between the solid and liquid phases and is calculated from:

$$Ni\text{-}en_{ads} = \frac{A_{in} - A_{final}}{A_{in}} \cdot Ni\text{-}en_{in}$$

where A_{in} = initial ^{63}Ni activity (cpm) in the liquid phase; A_{final} = final ^{63}Ni activity (cpm) in the liquid phase and $Ni\text{-}en_{in}$ = initial amount of Ni-en (in meq/kg). The average results of the CEC measurements for the samples from JO, NL and ZNO are summarised in Tab. 2-1, Tab. 2-2 and Tab. 2-3, respectively. These CEC values are in good agreement with the CEC values expected when considering the clay mineralogy (Marques Fernandes et al. 2024b).

2.4.2 Sorption experiments

The sorption of Cs, Ni, Eu, Th and U on the different rock samples was quantified by radiochemical assay using the corresponding radioisotopes. ^{134}Cs ($t_{1/2}$ = 2.06 y), ^{63}Ni ($t_{1/2}$ = 100 y), ^{152}Eu ($t_{1/2}$ = 13.3 y) and ^{228}Th ($t_{1/2}$ = 1.913 y) were purchased from Eckert and Ziegler Nuclitec GmbH (Braunschweig, Germany) and Isotope Products Laboratories (Burbank, California, USA). For ^{233}U, an in-house source solution ($4 \cdot 10^{-3}$ M) in 1 M HCl was used. The isotopic composition of the used tracer was provided by the manufacturer. In the case of U, the stable carrier concentration was determined in-house by ICP-MS.

The PW preparation, the conditioning of the rock samples with the corresponding SPWs and the sorption experiments were carried out under anoxic conditions in a glovebox (MBraun, Munich, Germany). The glovebox was filled with a mixture of N_2 and CO_2. The CO_2 concentration was 400 ± 10 ppm, reflecting atmospheric conditions. The O_2 concentration in the glovebox was < 0.1 ppm. The average temperature in the glovebox was 26.7 ± 0.8 °C.

The three SPWs were prepared by dissolving Ca-, Mg-, Na- and K-salts in Milli-Q water to achieve the corresponding composition given in Tab. 2-4. Prior to use, the Milli-Q water was degassed by boiling and by purging with N_2 for 2 hours. The water was then transferred to a glovebox where it was left to equilibrate with the box atmosphere for 2 days. After this time period, given amounts of salt were dissolved in a given volume. After one day, the pH of the solution was adjusted to the target value by adding small amounts of a 1 M NaOH solution.

Conditioning of rock samples: Prior to the sorption measurements, the crushed rock samples were conditioned to the corresponding SPW given in Tab. 2-4. The procedure was the same for all rock samples. The conditioning of the samples and the sorption experiments were carried out in equilibrium with atmospheric pCO_2. Dialysis bags were washed with de-ionised water before being filled with crushed rock and SPW. The bags were sealed so that an air pocket was trapped inside, which promoted a good mixing during end-over-end shaking. The dialysis bags were placed in a 2-litre polyethylene flask filled with SPW and then shaken for 24 hours. After this time, the equilibrated solutions in the flasks were replaced by fresh SPW and the bottles were again shaken for 24 hours. This procedure was repeated four times. Finally, each rock suspension inside the dialysis bags was emptied into a quantity of the last equilibrated SPW to yield sorbent concentrations of ~ 30 to 50 g/L. The exact rock content in the final suspensions was determined by heating aliquots weighed to constant weight at 105 °C and correcting for the salt content. The concentrations of the major elements Na, K, Mg, Ca, Sr, Si and S (SO_4^{2-}) in the liquid phase of the last equilibration step of the rock batches were quantified by ICP-OES. The analysis of TIC was carried out using a Dohrmann Carbon Analyser. The results of the cation/anion analyses in the liquid phase of the conditioned rock suspensions were very similar to the corresponding SPWs given in Tab. 4.2.

Batch sorption experiments: Sorption isotherms of Cs, Ni, Eu, Th and U were measured on the rock samples from the three siting regions in their corresponding conditioned SPWs at the corresponding pH. The sorption measurements with Th could only be carried out at trace concentrations because of aqueous solubility limits under the given chemical conditions of the PW (Hummel & Thoenen 2023). The detailed experimental results (*i.e.*, solid/liquid (S/L) ratio, pH, radionuclide concentration range) for Cs, Ni, Eu, Th and U are given in the appendices App. A, App. B, App. C, App. D and App. E., respectively.

Standard solutions covering the respective element concentration ranges were prepared in the conditioned SPWs for each element and were labelled with the corresponding radioisotope. Aliquots of rock suspensions and the appropriately labelled standard solutions were transferred into 40 mL centrifuge tubes and shaken end-over-end for 1 week. After the selected equilibration period, phase separation was obtained using a Beckman Coulter Avanti™ J30i High-Performance Centrifuge (1 hour at 95,000 *g* max.) and aliquots of the supernatant solutions were taken for radio assay. The sorption measurements were carried out in duplicate or triplicate. The pH of the supernatant of each sample was measured after phase separation using a Metrohm combined electrode. The electrode was calibrated against commercial Merck™ buffers for pH 4, 7 and 10. Radiochemical assays were performed using either a Canberra Packard TRI-CARB 2750 TR/LL liquid scintillation counter (^{63}Ni, ^{233}U) or a Canberra Packard Cobra Quantum γ-counter (^{134}Cs, ^{152}Eu, ^{228}Th).

The sorption of RNs is usually quantified by the solid liquid distribution ratio R_d (L/kg), which is defined as:

$$R_d = \frac{RN_{ads}}{RN_{aq}}$$

Where RN_{ads} are the moles of RN adsorbed on the solid phase per unit mass (mol/kg) and RN_{aq} is the equilibrium RN aqueous concentration (M).

The results of the sorption isotherms (experimental and modelling) for Cs, Ni, Eu, Th and U in this report are graphically presented as the logarithm of R_d ($\log_{10} R_d$ in L/kg) *vs.* the logarithm of RN_{aq} ($\log_{10} RN_{aq}$ in M).

3 Predictive sorption modelling with ClaySor model

3.1 Sorption models for illite

The modelling calculations are carried out using GEMS (Kulik et al. 2013) together with the most recent PSI/Nagra TDB 2020 (Hummel & Thoenen 2023).

The 2SPNE SC/CE model for illite and the GCS model used for the calculation of the radionuclide sorption on the argillaceous samples are briefly described in the following section. Both models were implemented in GEMS under the name ClaySor model (Kulik et al. 2018). Recently, the standard thermodynamic data of relevant radionuclides were revised in the PSI/Nagra TDB 2020, requiring an upgrade of the ClaySor thermodynamic SDB since the surface complexation constants (SCCs) as well as the sorption calculations are directly correlated to the metal aqueous speciation. To be consistent with the new PSI/Nagra TDB 2020, all sorption data used to develop the 2SPNE SC/CE model for illite were refitted to derive consistent SCCs. In addition, for the SCCs, confidence intervals were determined allowing to evaluate the model uncertainty in predicting the uptake of relevant radionuclides in repository SA for a given composition of PW and rock mineralogy. It should be noted that uncertainties were estimates only for the element-specific parameters such as the SCCs and selectivity constants (K_c), not for clay mineral specific model parameters such as site capacities and protolysis constants. Details on the estimate of the uncertainties with the GEMSFIT code (Miron et al. 2015) and all the refitted SCCs and the K_c values are given in Marinich et al. (2024).

3.1.1 2SPNE SC/CE model

The surfaces of 2:1 clay mineral platelets carry a permanent negative charge arising from isomorphous substitution of lattice cations by cations of a lower valence. Charge neutrality is maintained by the presence of an excess of cations in solution held electrostatically in close proximity around the outside of the Si-Al-Si clay mineral units. The electrostatically bound cations, which constitute the electrical double layer, can undergo stoichiometric exchange with the cations in solution (Grim 1953, van Olphen 1964). The total permanent negative charge of a clay mineral is defined as the CEC.

A second category of reactive sites associated with clay minerals are surface hydroxyl groups (≡SOH) situated along the edges of the clay platelets, "edge" or "broken bond" sites. These sites protonate and deprotonate as a function of pH and form surface complexes with aqueous metal species.

The 2:1 clay minerals such as illite, smectite and illite/smectite mixed layers (ISML) are of prime importance because of their high reactivity and their ubiquity in argillaceous rocks. The sorption properties of illite were investigated in terms of its protolysis (titration measurements) and retention (sorption edge and isotherm measurements) behaviour. From these data, a multi-site mass action sorption model combining protolysis, SC and CE was developed, without an electrostatic term, to quantitatively describe the uptake of aqueous metal species illite (Bradbury & Baeyens 2009a, Bradbury & Baeyens 2009b). Titration measurements were modelled with reactions on two types of weak sites (≡S^{W1}OH and ≡S^{W2}OH), both having similar capacities. To describe pH-dependant trace metal sorption data and metal-concentration-dependent sorption data, weak types of sites (≡S^{W1}OH) and strong type of sites (≡S^{S}OH) were necessary. The ≡S^{S}OH type sites have a much smaller capacity but form considerably stronger SCs with metals and dominate the sorption at trace concentrations. Within the application of the bottom-up approach to SC reactions, it is assumed that ISML have essentially the same sorption characteristics as illite. This can be justified by the similar sorption characteristics of metals on illite and montmorillonite (see *e.g.*, Baeyens & Marques Fernandes 2018). A summary of the different site types, site

capacities and corresponding protolysis constants for illite are given in Tab. 3-1. These model-specific parameters and their associated values are fixed in all modelling calculations provided later.

Tab. 3-1: Summary of the 2SPNE SC/CE model parameters (site types, site capacities and protolysis constants) for illite implemented in GEMS

(From Bradbury & Baeyens 2009a).

Site type	Capacity (mol/kg)	
$\equiv S^{S}OH$ (strong) $\equiv S^{W1}OH$ (weak 1) $\equiv S^{W2}OH$ (weak 2)	$2.0 \cdot 10^{-3}$ $4.0 \cdot 10^{-2}$ $4.0 \cdot 10^{-2}$	
Protolysis reactions	log K ($\equiv S^{S/W1}OH$)	log K ($\equiv S^{W2}OH$)
$\equiv SOH + H^+ \Leftrightarrow \equiv SOH_2^+$ $\equiv SOH \Leftrightarrow \equiv SO^- + H^+$	4.0 -6.2	8.5 -10.5

CE reactions occurring on the planar sites (PS) are often expressed in terms of a selectivity coefficient. There are different approaches for describing CE equilibria, with the two most common ones being the Gaines and Thomas (K_c) (Gaines & Thomas 1953) and the Vanselow (K_v) (Vanselow 1932) conventions. K_c defines the fractional ion occupancies on the PS of clay minerals by an equivalent concentration scale whereas K_v uses the molar scale in the mass action equation.

The CE reaction of a metal B, of valence z_B, exchanging with a metal A, of valence z_A, on a clay mineral in the A-form, can be written as:

$$z_B A^{z_A} - clay + z_A B^{z_B} \Leftrightarrow z_A B^{z_B} - clay + z_B A^{z_A}$$

Following the Gaines & Thomas (1953) convention, a selectivity coefficient, ${}^{B}_{A}K_c$, for reaction (1) can be defined by the following mass action law as:

$${}^{B}_{A}K_c = \frac{(N_B)^{z_A}}{(N_A)^{z_B}} \cdot \frac{[A]^{z_B}}{[B]^{z_A}} \cdot \frac{(\gamma_A)^{z_B}}{(\gamma_B)^{z_A}}$$

N_A and N_B = equivalent fractional occupancies, defined as the equivalents of A (or B) adsorbed per kg of clay mineral divided by the CEC expressed in eq/kg. A and B = aqueous concentrations (M). γ_A and γ_B = aqueous phase activity coefficients.

A SC reaction used for surface edge binding can be written as:

$$\equiv S^{\overline{S}}_{W1}OH + Me^{z} + y\,H_2O \Leftrightarrow \equiv S^{\overline{S}}_{W1}OMe(OH)_y^{z-(y+1)} + (y+1)\,H^+$$

Me is a metal with valence z, and y an integer. For $y = 0$, the surface complex is $\equiv S^{\overline{W1}}OMe^{(z-1)}$. In a non-electrostatic model, the SCC corresponding to reaction (3), K_y can be expressed as:

$$K_y = \frac{\left[\equiv S^{\overline{W1}}OMe(OH)_y^{z-(y+1)}\right]}{\left[\equiv S^{\overline{W1}}OH\right]} \cdot \frac{\{H\}^{(y+1)}}{\{Me^z\}}$$

where [ ] terms are concentrations and { } terms are aqueous activities.

It should be noted that the 2SPNE SC/CE model was developed in simple background electrolytes ($NaCl/NaClO_4$) and only free cationic, neutral and positively hydrolysed species are considered to adsorb by SC. The SC reactions and corresponding SCCs for Ni, Eu, Th and U and their associated uncertainties implemented in GEMS (Marinich et al. 2024, Bradbury & Baeyens 2017) are summarised in Tab. 3-2.

In addition to SC on the edge site, CE on the PS of illite is included in the modelling for Ni, Eu and U. For the hydrolysed $Th(OH)_4^0$ species at the pH of the SPW, CE is not considered. Tab. 3-3 summarises the CE reactions, selectivity coefficients and associated uncertainties for Ni, Eu and U.

Tab. 3-2: SCCs for Ni, Eu, Th and U on illite

From Marinich et al. (2024).

Surface complexation reaction	**log ^{S}K**	**log ^{W1}K**
$\equiv S^{S/W1}OH + Ni^{2+} \Leftrightarrow \equiv S^{S/W1}ONi^{+} + H^{+}$	0.65 ± 0.04	-1.92 ± 0.12
$\equiv S^{S/W1}OH + Ni^{2+} + H_2O \Leftrightarrow \equiv S^{S/W1}ONiOH^{0} + 2H^{+}$	-7.92 ± 0.15	
$\equiv S^{S/W1}OH + Eu^{3+} \Leftrightarrow \equiv S^{S/W1}OEu^{2+} + H^{+}$	2.47 ± 0.4	1.00 ± 0.19
$\equiv S^{S/W1}OH + Eu^{3+} + H_2O \Leftrightarrow \equiv S^{S/W1}OEuOH^{+} + 2H^{+}$	-4.28 ± 0.17	
$\equiv S^{S/W1}OH + Eu^{3+} + 3H_2O \Leftrightarrow \equiv S^{S/W1}OEu(OH)_3^{-} + 4H^{+}$	-21.34 ± 0.17	
$\equiv S^{S}OH + Th^{4+} \Leftrightarrow \equiv S^{S}OTh^{3+} + H^{+}$	6.73 ± 1.61	
$\equiv S^{S}OH + Th^{4+} + H_2O \Leftrightarrow \equiv S^{S}OTh(OH)^{2+} + 2H^{+}$	2.41 ± 0.91	
$\equiv S^{S}OH + Th^{4+} + 3H_2O \Leftrightarrow \equiv S^{S}OTh(OH)_3^{0} + 4H^{+}$	-9.12 ± 1.56	
$\equiv S^{S}OH + Th^{4+} + 4H_2O \Leftrightarrow \equiv S^{S}OTh(OH)_4^{-} + 5H^{+}$	-15.20 ± 0.13	
$\equiv S^{S/W1}OH + UO_2^{2+} \Leftrightarrow \equiv S^{S/W1}OUO_2^{+} + H^{+}$	2.37 ± 0.17	-0.83 ± 0.23
$\equiv S^{S/W1}OH + UO_2^{2+} + H_2O \Leftrightarrow \equiv S^{S/W1}OUO_2OH^{0} + 2H^{+}$	-4.43 ± 0.82	-5.60 ± 0.13
$\equiv S^{S/W1}OH + UO_2^{2+} + 2H_2O \Leftrightarrow \equiv S^{S/W1}OUO_2(OH)_2^{-} + 3H^{+}$	-11.07 ± 0.26	-12.32 ± 0.15
$\equiv S^{S/W1}OH + UO_2^{2+} + 3H_2O \Leftrightarrow \equiv S^{S/W1}OUO_2(OH)_3^{2-} + 4H^{+}$	-19.29 ± 0.18	

Tab. 3-3: CE reactions and the corresponding selectivity coefficient values (log K_c) for Ni, Eu and U on Na-illite

(From Marinich et al. 2024).

Log K_c (U-Na) was taken from Bradbury & Baeyens (2017).

Exchange reaction	Selectivity coefficient (log K_c)
$2Na^+$-clay + Ni^{2+} ⇔ Ni^{2+}-clay + $2Na^+$	0.73 ± 0.37
$3Na^+$-clay + Eu^{3+} ⇔ Eu^{3+}-clay + $3Na^+$	1.78 ± 0.63
$2Na^+$-clay + UO_2^{2+} ⇔ UO_2^{2+}-clay + $2Na^+$	0.65

3.1.2 Generalised Cs sorption model

The GCS model is taken from the work of Bradbury & Baeyens (2000) where a detailed model description can be found. The sorption of Cs on illite is purely based on CE reactions and is assumed to take place on three different site types, denoted as frayed-edge sites (FES), type II sites (T2S) and PS, each having a given site capacity and affinity for Cs. The relations between these site capacities as fixed percentages of the CEC of illite and the capacities of these sites are given in Tab. 3-3. An integral assumption in the model concept is that the relationship between the three different sites is valid for different types of illite irrespective of their origin, as shown by Bradbury & Baeyens (2000). It should be noted that FES and T2S are not present in smectites and their presence in soils and sediments can be used as a fingerprint for Cs sorption onto illite. Selectivity coefficients for Cs and the main competing cations (K, Ca and NH_4) were converted from experimental sorption data on illite taken from literature (Brouwer et al. 1983, Wick et al. 2018, Marinich et al. 2024). The K_c for the CE equilibria on the three site types of illite for Cs, K, and Ca w.r.t. Na, considered generally valid for all illite clay minerals, are listed in Tab. 3-4.

In illite and argillaceous rock systems, at Cs equilibrium concentrations ($Cs_{aq} < 10^{-3}$ M), only the Cs uptake on FES and T2S is important (Marques Fernandes & Baeyens 2021). These sites are predominantly accessible to cations with low hydration energies (*e.g.*, K and NH_4) which compete most effectively with Cs. Na may also compete, but only when the concentration is many orders of magnitude greater than that of Cs and/or K. Divalent cations such as Mg, Ca and Sr, with relatively large hydration energies, are effectively non-competitive for steric reasons (Brouwer et al. 1983). FES exhibit the strongest affinity for Cs and are the main sorption sites at concentrations $< 10^{-8}$ M, where the sorption is linear. In the concentration range up to ~ 10^{-4} M, T2S dominate, and the sorption is non-linear. Non-linear sorption behaviour extends to even higher concentrations due to contributions from the PS and site saturation effects.

Tab. 3-4: Summary of GCS model parameters (site types and capacities) and K_c for the CE equilibria on the three site types of illite for Cs, K, and Ca w.r.t. Na on illite with a CEC = 225 meq/kg

Log K_c (Cs-Na) was taken from Marinich et al. (2024)

Log K_c (K-Na) was taken from Brouwer et al. (1983)

Log K_c (Ca-Na) was taken from Wick et al. (2018) and log K_c values for Mg-Na and Sr-Na are assumed to be the same as for Ca-Na

Site type (% of CEC*)	**FES (0.25%)**	**T2S (20%)**	**PS (~80%)**
Site capacity (meq/kg)	0.5625	45	180
Exchange reaction	log K_c		
$Cs^+ + Na^+$-illite ⇔ Cs^+-illite + Na^+	6.64 ± 0.05	3.03 ± 0.85	1.49 ± 0.74
$K^+ + Na^+$-illite ⇔ K^+-illite + Na^+	2.4	2.1	1.1
$Me^{2+} + 2Na^+$-illite ⇔ Me^{2+}-illite + $2Na^+$	0.2	0.0	0.4

3.2 Predictive modelling: bottom-up approach

To blindly predict the sorption of Cs, Ni, Eu, Th and U on the rock samples from JO, NL and ZNO, a simplified CA or "bottom-up" approach was used. Briefly, this approach is based on the hypothesis that the uptake of cations in argillaceous rocks is predominantly controlled by sorption on the major clay mineral components. Conservative quantitative predictions are then possible based on the knowledge and understanding of the mechanistic sorption processes on these clay minerals, and the models developed to describe them. The 2:1 clay minerals illite, smectite and ISML minerals are major components of the rock samples investigated in this study. The mineralogical composition and weight contents for BOZ1-1, BUL1-1 and TRU1-1 samples are given in Tab. 2-1, Tab. 2-2 and Tab. 2-3, respectively. The 1:1 clay mineral kaolinite is also ubiquitous in many of the investigated rock samples, however, since there is no complete sorption model available for this clay mineral, its contribution to sorption is not considered in the modelling. A further assumption is that ISML minerals have similar sorption behaviour on the amphoteric edge site as illite (towards cation-adsorbing via SC). This assumption cannot be confirmed unambiguously because sorption data for these ISML minerals are very sparse in the open literature. However, the similarities in terms of SC behaviour for many cations on illite and montmorillonite are evidenced in Baeyens & Marques Fernandes (2018). In this study, the total 2:1 clay mineral content is considered for the modelling of sorption by SC for Ni, Eu, Th and U. In contrast, for the modelling of Cs sorption, only the illite content is considered. The bottom-up approach using the 2SPNE SC/CE sorption model for montmorillonite and illite and the GCS model for illite has been applied on many occasions to predict sorption of radionuclides on different clay-mineral-rich rocks (Bradbury & Baeyens 2011, Marques Fernandes & Baeyens 2021, Marques Fernandes et al. 2015).

In the present report, the GCS and 2SPNE SC/CE models for illite implemented in GEMS as the ClaySor model are used to blindly predict sorption isotherms measured on samples from the three study regions in their corresponding SPW (Tab. 2-4). For all samples, predictive modelling was performed at the experimentally determined pH.

Cs is retained essentially by CE. Its sorption on the rock samples is modelled by scaling the capacity of the CE sites (*i.e.*, FES, T2S and PS) (Tab. 3-4**)** only to the illite content of the rock samples according to the GCS model (Bradbury & Baeyens 2000). Since FES and T2S are not

present in smectites, retention of Cs at trace and medium concentration is solely governed by sorption on these two sites. The competitive exchange on FES and T2S with elements from the SPW such as Na, K, Mg and Ca is considered.

The sorption of Ni, Eu, Th and U, which essentially undergo SC under most PW conditions, is modelled by scaling the capacity of the SC sites of the ClaySor model for illite (Tab. 3-1) to the 2:1 clay mineral content (illite, ISML) of the respective rock sample and by considering the aqueous speciation for each element in the associated PWs. The conservative modelling approach applied here assumes the sorption of each specific element as the only uptake mechanism.

The potential influence of competing divalent cations such as ferrous iron on the sorption of divalent Ni as shown in a recent study (Marques Fernandes & Baeyens 2020) could not be fully considered in the present modelling exercise since Fe(II) concentration in the experiments was difficult to quantify. Most experiments were set up within experimental conditions (*i.e.*, pH, cation concentrations) where the precipitation of known solubility-limiting phases was avoided.

As already mentioned, the aqueous speciation of the radionuclide plays a very important role in calculating its sorption values. The correctness and completeness of the TDB used in the calculations are critical. The calculations were performed using ClaySor with the most recent updated PSI/Nagra TDB 2020 (Hummel & Thoenen 2023).

3.3 Uncertainties

Uncertainties in the results presented in this study can have various sources and are not always easy to quantify. In case of the application of the bottom-up approach to blindly predict sorption on natural rock samples, the most important sources of uncertainties are related to:

(i) the experimental errors;

(ii) the assumption that only 2:1 clay minerals (illite, smectite, ISML) act as sorbents;

(iii) the sorption model and its intrinsic non-adjustable parameters (*i.e.*, site capacities, protolysis constants, SCCs, and selectivity coefficients);

(iv) the heterogeneity of the natural rock samples (*e.g.*, uncertainties on the mineralogical composition, uncertainties on the sorption properties of the different clay minerals compared to the reference clay minerals used in the model development);

(v) the uncertainty in the aqueous complexation constants; and

(vi) the intrinsic trace metal inventory of the sedimentary rocks which can compete with the investigated radionuclides.

Experimental measurements are subject to some uncertainty or error, which can be formally estimated by considering the maximum error in each experimental operation step (Baeyens & Bradbury 1995a, Baeyens & Bradbury 1995b). Over the years, numerous batch sorption experiments have been carried out within our research group on different rock batches, by different technicians, for various elements and at different experimental conditions (*e.g.*, high/low sorption and high/low S/L ratio). Considering most of these potential sources of error, an uncertainty of ± 60% for the R_d seems to be a realistic value (Marques Fernandes & Baeyens 2021, Baeyens et al. 2014). This value was generally applied to all experimental data presented in this study.

As mentioned before, the SCCs and K_c values in the ClaySor model for illite and montmorillonite have recently been extended with uncertainties (Marinich et al. 2024, Miron et al. 2015). The model, however, does not have intrinsic uncertainties associated to the fixed model-specific parameters (*i.e.*, site capacities, protolysis constants).

The uncertainty range associated to the predictive modelling provided in this report only considers the uncertainty related to the SCCs and K_c values. Uncertainties in the aqueous speciation (related to the uncertainties in the aqueous complexation constants) or in the mineralogical composition are not considered. In that sense, the presented uncertainties related to the modelling are underestimated. Aqueous speciation, particularly in natural environments, plays an important role for the sorption of radionuclides on sorbents. The 2SPNE SC/CE model was developed in simple background electrolytes ($NaCl/NaClO_4$), and only the sorption of free cationic, neutral and positively hydrolysed species is considered. The presence of inorganic ligands (*e.g.*, chloro, sulphato and carbonato complexes) can considerably influence sorption. Since these complexes are assumed to be non-sorbing, their formation in the PW can reduce sorption. Depending on the strength of the thermodynamic complexation constant and the associated uncertainty, the influence of speciation could be very high. Also, the choice of the aqueous thermodynamic constants, particularly with ligands which might reduce the sorption (*e.g.*, $Ca_nUO_2(CO_3)_3^{(4-2n)-}$ (n = 1;2) complexes), can greatly affect the modelling (see Section 4.5).

Several studies have shown that competitive sorption can affect the uptake of trace metals on the clay-mineral edge sites (Marques Fernandes & Baeyens 2019, Marques Fernandes & Baeyens 2020, Orucoglu 2022). Competitive effects for sorption via SC were not considered in this study, since the SPWs used do not contain elements that could compete with the investigated radionuclides. The presence of competing trace elements in the natural rock system can, however, not be excluded but is difficult to quantify (Bradbury & Baeyens 2005). In the development of the SDB for the RBG, however, competitive sorption is considered since the reference PWs contain competing cations such as Fe(II) and Mn(II).

4 Results and discussion

The experimental sorption and modelling results obtained for Cs, Ni, Eu, Th and U on TBO samples from JO, NL and ZNO are shown and discussed in this chapter. The results are presented graphically, with the experimental data shown as symbols and the model predictions as solid lines. The experimental conditions and results in form of tabulated values for Cs, Ni, Eu, Th and U are given in App. A, App. B, App. C, App. D and App. E, respectively.

4.1 Cs

The Cs isotherms measured on 20 rock samples from Bözberg, Bülach and Trüllikon in their corresponding SPWs (Tab. 2-4) are shown in Fig. 4-1, Fig. 4-2 and Fig. 4-3, respectively. The experimental conditions and sorption results are given in App. A. Each individual isotherm was modelled with the ClaySor model for illite (Bradbury & Baeyens 2000, Kulik et al. 2018, Marinich et al. 2024) as described in Section 3. The site capacities of the FES, T2S and PS are non-adjustable parameters in the modelling procedure. Cs cation exchange on smectite was not considered. The Cs isotherms were calculated by (i) scaling the site capacities to the illite content in each rock sample and (ii) in their corresponding SPW compositions.

In agreement with the GCS model (Tab. 3-4), the following site capacity scaling factors were applied for each sample.

$$Q_{FES} = F_{illite} \cdot CEC_{illite} \cdot 0.0025$$

$$Q_{T2S} = F_{illite} \cdot CEC_{illite} \cdot 0.2$$

$$Q_{PS} = F_{illite} \cdot CEC_{illite} \cdot 0.8$$

Where Q is the site capacity, F_{illite} = wt.% illite/100, CEC_{illite} = 225 meq/kg, and 0.0025, 0.2 and 0.8 are the fractions of FES, T2S and PS, respectively. As already mentioned in Section 3.1.2, FES and T2S are specific to illite and their non-adjustable parameter values are an excellent indicator of the presence of illite (see Fig. 4-1, Fig. 4-2 and Fig. 4-3) in sedimentary rocks. The competitive exchange with Na, K, Mg and Ca on PS, and Na, K (and NH_4) on FES and T2S, are controlled by the CE reactions and selectivity coefficients given in Tab. 3-4.

The Cs sorption measurements on six samples from the BOZ1-1 borehole from JO are shown in Fig. 4-1. The variation of the illite content is more pronounced compared to the BUL1-1 and TRU1-1 boreholes, ranging from 8 wt.% for the sample at the smallest depth to 49.1 wt.% for the sample at the greatest depth. Comparing the blind model predictions with the experimental data reveals that the isotherms in all cases are very well reproduced. Fig. 4-1 clearly shows that all the samples display significantly more pronounced sorption behaviour compared to those from the two other boreholes, even though they have similar illite contents. The lower K concentration in the SPWs (see Tab. 2-4) leads to higher Cs sorption since it is the main competitor for the sorption of Cs on FES and T2S.

The result of the Cs sorption measurements on the seven samples from the BUL1-1 borehole from NL is illustrated in Fig. 4-2. The agreement between the blind prediction and the experimental data is strikingly good for all samples, independent of the lithological origin of the samples or illite content. The six samples shown in Fig. 4-2b to Fig. 4-2g exhibit an illite content from 21 to 36 wt.%. This rather small range of illite content is reflected by the similar Cs sorption of these samples, *i.e.*, log R_d is ~ 3 L/kg at trace concentration and decreases to ~ 0.8 L/kg at the highest Cs_{aq} of ~ 10^{-2} M. The Cs isotherm shown in Fig. 4-2a for a very poor illite sample from the calcar-

eous «Herrenwis Unit» (see Tab. 2-1) exhibits a much less pronounced Cs sorption behaviour. At trace Cs_{aq}, the log R_d is ~ 1.7 L/kg and decreases to ~ - 1.5 L/kg at the highest Cs_{aq}. Even at this very low illite content (0.7 wt.%), the model prediction for this sample is remarkably good. This result illustrates that the Cs sorption at trace concentration on a rock sample for which no clay mineralogy is available can act as an indicator of the illite content present in the sample.

The results of the Cs sorption measurements on seven samples from the TRU1-1 borehole from the ZNO siting region are shown in Fig. 4-3. The illite content of these samples ranges from 14 and 33 wt.%, which is a relatively small variation (see Tab. 2-3). Consequently, the R_d values of the Cs isotherms are very similar and exhibit the same features as the six isotherms from the BUL1-1 borehole samples (Fig. 4-2b to Fig. 4-2g) regardless of the origin of the rock sample. This is primarily due to the similar K concentrations, the main competing cation for Cs on the FES and T2S, in both SPWs (Tab. 2-4).

In summary, the Cs sorption for all 20 rock samples is very consistent and is mainly governed by the illite content and the PW composition.

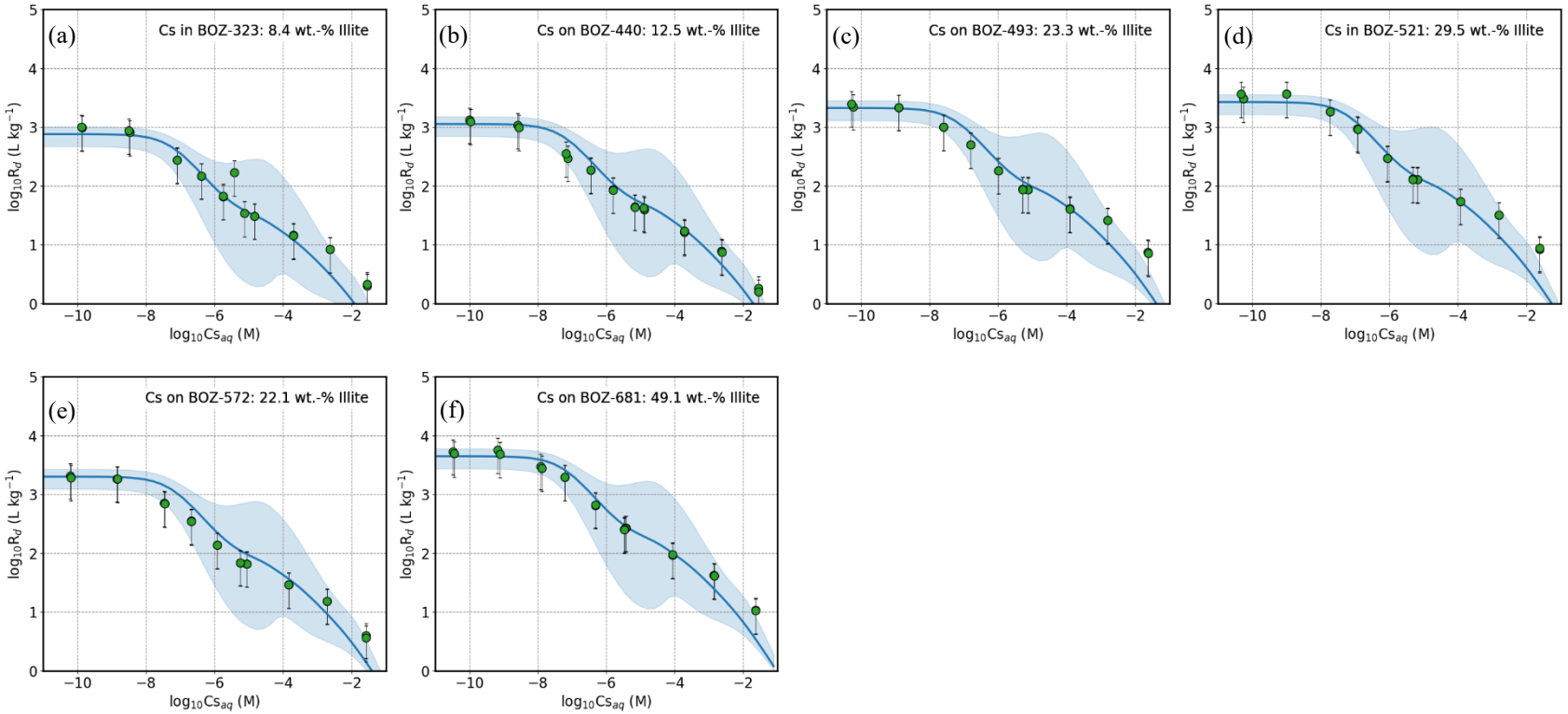

Fig. 4-1: Measured (green dots) and blindly predicted (blue line) sorption of Cs on the 6 rock samples from BOZ1-1 from JO siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with the selectivity coefficients of the ClaySor model (Tab. 3-4).

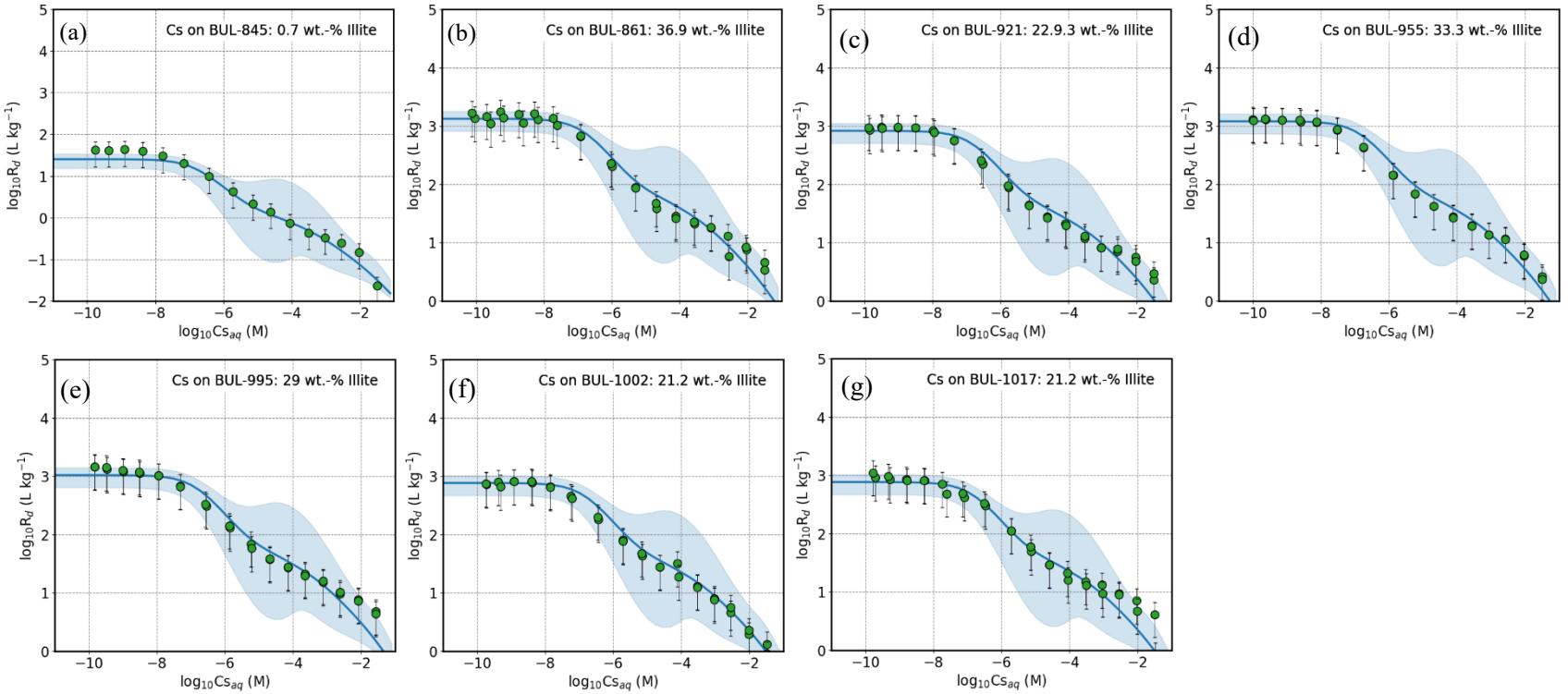

Fig. 4-2: Measured (green dots) and blindly predicted (blue line) sorption of Cs on the 7 rock samples from BUL1-1 from the NL siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with the selectivity coefficients of the ClaySor model (Tab. 3-4).

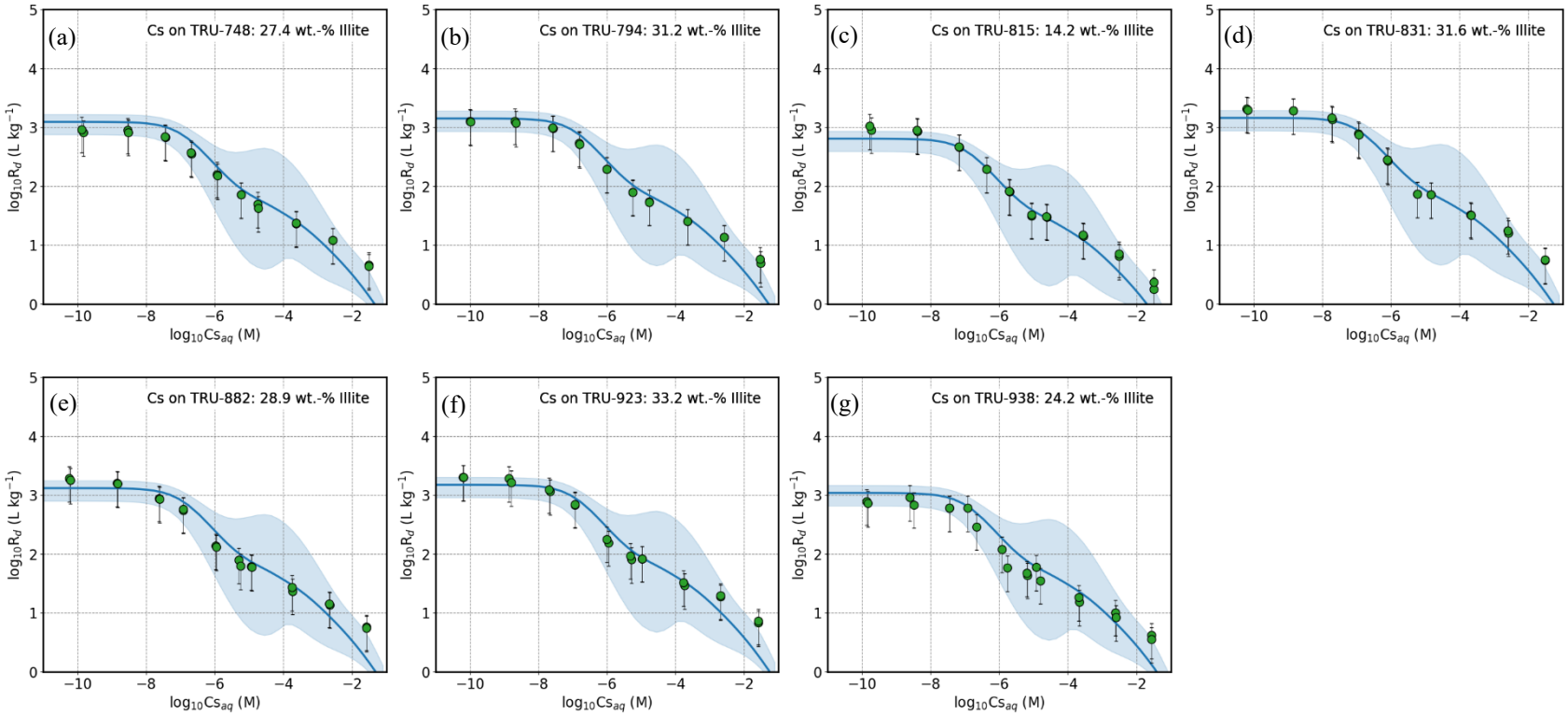

Fig. 4-3: Measured (green dots) and blindly predicted (blue line) sorption of Cs on the 7 rock samples from TRU1-1 from the ZNO siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with the selectivity coefficients of the ClaySor model (Tab. 3-4).

4.2 Ni

The Ni isotherms measured on 20 rock samples originating from JO (Tab. 2-1), NL (Tab. 2-2) and ZNO (Tab. 2-3) in their corresponding SPW (Tab. 2-4) and the predictive modelling using the ClaySor model on illite are summarised in this section. The experimental conditions and results for Ni on twenty rock samples are given in App. B. The sorption was calculated at the experimentally determined pH conditions and scaled to the illite/smectite content of each sample as described in Section 3.2. Ni essentially adsorbs by surface complexation in the rather narrow pH range of the SPWs. The contribution to Ni sorption from CE on the PS is negligible. The model, the associated parameters and the SC reactions and constants are summarised in Section 3.1. As already mentioned, the modelling uncertainty was estimated based on the uncertainty of the SCCs. Potential sorption competition (Marques Fernandes & Baeyens 2020) on the same strong sites between Ni and other divalent cations such as Fe^{2+} or Mn^{2+} naturally present in the rock samples (blocking the strong sites) was not considered in the modelling. This omission was due to the inability to reliably assess the inventory of these cations in the experiments. It should be noted that the SPWs used in this study do not contain competing cations.

Ni isotherms measured on the samples from JO, NL and ZNO covering Ni_{aq} from ~ 10^{-10} M to ~10^{-4} M are shown in Fig. 4-4, Fig. 4-5 and Fig. 4-6, respectively. Ni^{2+} and $NiSO_{4(aq)}$ are the dominating aqueous species in the three SPWs. The sorption of Ni on almost all rock samples is reduced compared to the Ni sorption on pure illite in simple NaCl background electrolyte (log R_d ~3.8 L/kg) under similar pH and Ni_{aq} conditions, except for the BOZ-440 sample (Fig. 4-4b). For all the other samples, Ni sorption values vary between log R_d ~ 1.5 and 3 L/kg at the lowest Ni_{aq}. Except for the sorption measured on the BOZ1-1 samples and BUL-955, the Ni sorption data show little scatter. Contrary to the model predictions, for most samples, Ni sorption only decreases slightly (saturation of strong sites) as a function of Ni_{aq}.

The predicted Ni sorption on BOZ1-1, BUL1-1 and TRU1-1 is illustrated by the solid blue lines in Fig. 4-4, Fig. 4-5 and Fig. 4-6, respectively. The small 95% confidence interval (blue-shaded area) reflects the small uncertainty on the dominating surface complexes, $\equiv S^SONi^+$ and $\equiv S^SONiOH$ up to Ni_{aq} ~ $10^{-6.5}$ M and $\equiv S^wONi^+$ at higher Ni_{aq} (Tab. 3-2). The decrease in the modelled sorption at $Ni_{aq} > 10^{-6.5}$ M reflects the saturation of the low-capacity strong sites (decrease of $\equiv S^SONi^+$ and $\equiv S^SONiOH$ contribution and increase of $\equiv S^wONi^+$ contribution to the overall sorption).

The discrepancy between the experimental data and the bottom-up modelling is smaller for BOZ1-1 samples from the JO siting region (Fig. 4-4) than for those from the boreholes in the other two siting regions. The sorption on BOZ-323 (Fig. 4-4a), and BOZ-572 (Fig. 4-4e) is well described except at high Ni_{aq} ~ $10^{-5.5}$ M, where experimental sorption data slightly increase. For BOZ-681 (Fig. 4-4f), sorption is satisfactorily reproduced. On BOZ-521 (Fig. 4-4d) experimental sorption is nearly constant and is clearly overpredicted in the low Ni_{aq} range by 0.6 log units. The clay mineral-poor BOZ-440 (Fig. 4-4b) is the only sample from the JO siting region where sorption is clearly underpredicted (by up to one log unit).

For the samples from the BUL1-1 borehole from NL (Fig. 4-5), only 2 out of 7 experimental data sets are well reproduced (shape and sorption value) by the bottom-up approach over almost the entire Ni_{aq} range, namely on the calcite-rich, clay mineral-poor BUL-845 sample (0.9 wt.% illite/ smectite) and on the Opalinus Clay BUL-995 sample (32.4 wt.%). For the other samples, Ni sorption is significantly underpredicted by up to 1 order of magnitude at low Ni_{aq} despite these samples being clay mineral-rich. The highest deviation is observed in BUL-861 sample (Fig. 4-5b), whereas the smallest deviation is seen in BUL-955 sample (Fig. 4-5e) (showing comparatively scattered data). At higher Ni_{aq}, the modelling curves converge with the experimental data.

The model calculations of the Ni sorption on the TRU1-1 samples from ZNO shows a similar trend as on BUL1-1. The calculated sorption diverges from the experimental data at low Ni_{aq} and converges at higher concentrations. Generally, the discrepancy between modelling and experimental data is less pronounced than for the BUL1-1 samples except for TRU-938 (Fig. 4-6g), where the sorption is nearly constant over the entire Ni_{aq} range and the modelling underpredicts sorption by a maximum of one order of magnitude. For TRU-831 sample (Fig. 4-6d), sorption values and shape of the isotherm are well reproduced. Generally, the discrepancy between modelling and experimental data for the ZNO samples is less pronounced than for the NL samples, except for TRU-938.

In 11 samples out of 21, the sorption modelling of Ni was overestimated in the low Ni_{aq} range and converged at $Ni_{aq} > 10^{-6}$ M where the weak sites are dominant. This overprediction could be explained by sorption competition between Ni and other divalent cation intrinsically present in the rock samples. Competing cations are expected to sorb on the same strong sites and to decrease the sorption of Ni according to the total divalent metal concentration along the isotherm. The high sorption of Ni on the clay mineral-poor BOZ-440 (Fig. 4-4b) sample could be due to the retention of Ni by calcite (55 wt.%), but this was not observed on the other calcium-rich samples.

In the present study, with the uncertainty on the divalent metal inventory, the bottom-up approach generally provides a conservative estimate of divalent Ni sorption. The in-situ PW for the three siting regions contains competing cations such as Fe and Mn, which will be considered in the development of the SDB for the RBG for divalent cations that undergo surface complexation. The SDB for the SA will be conservative for all these cases.

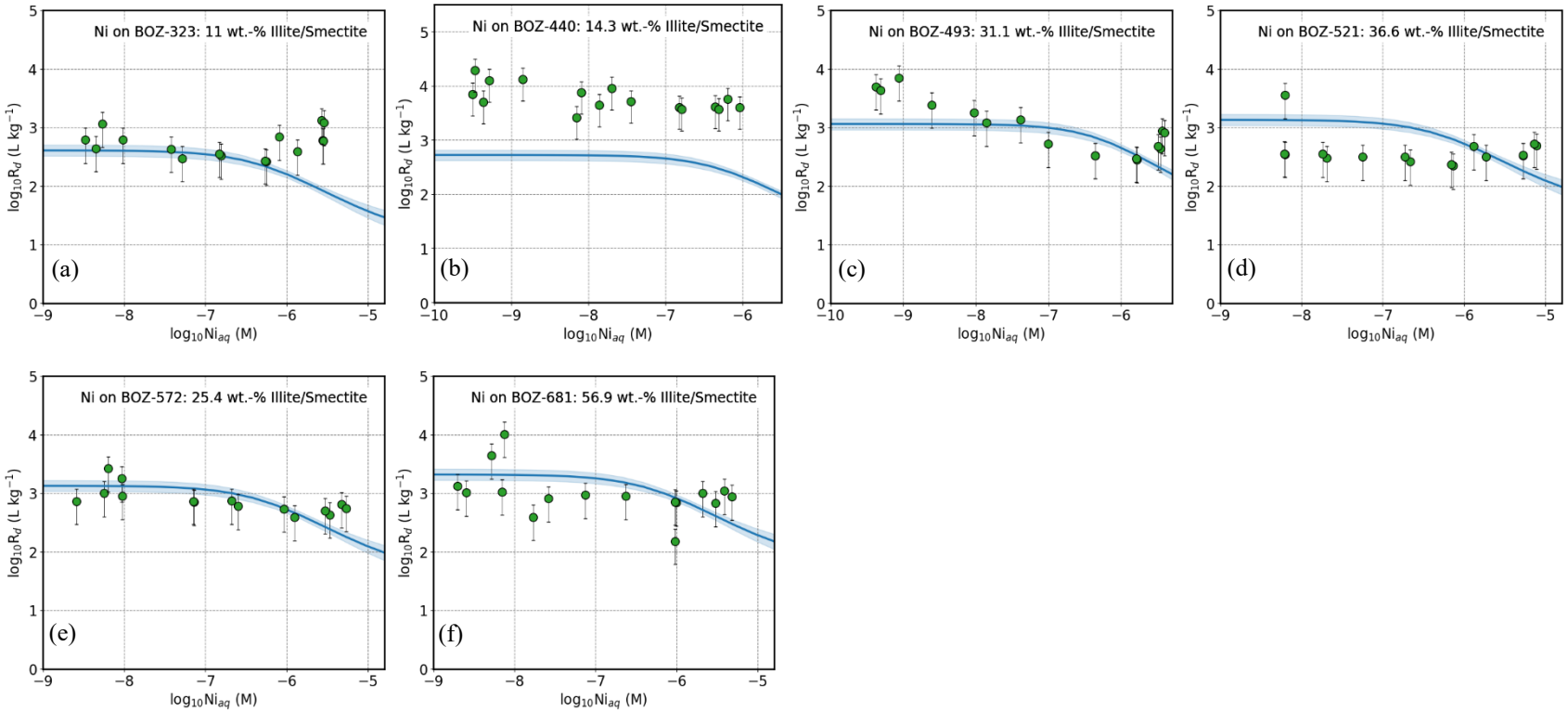

Fig. 4-4: Measured (green dots) and blindly predicted (blue line) sorption of Ni on the 6 rock samples from BOZ1-1 from the JO siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of Ni in the ClaySor model on illite (Tab. 3-2).

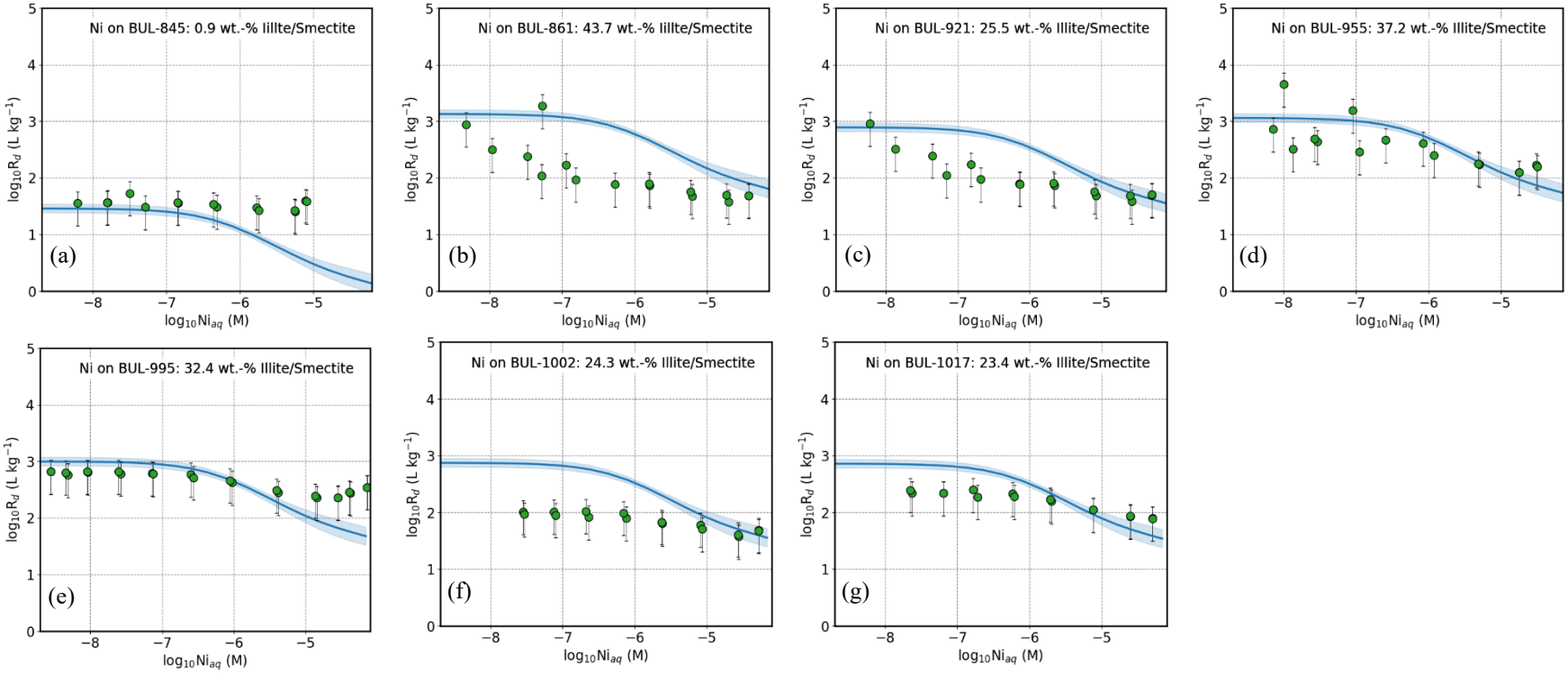

Fig. 4-5: Measured (green dots) and blindly predicted (blue line) sorption of Ni on the 7 rock samples from BUL1-1 from the NL siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of Ni in the ClaySor model on illite (Tab. 3-2).

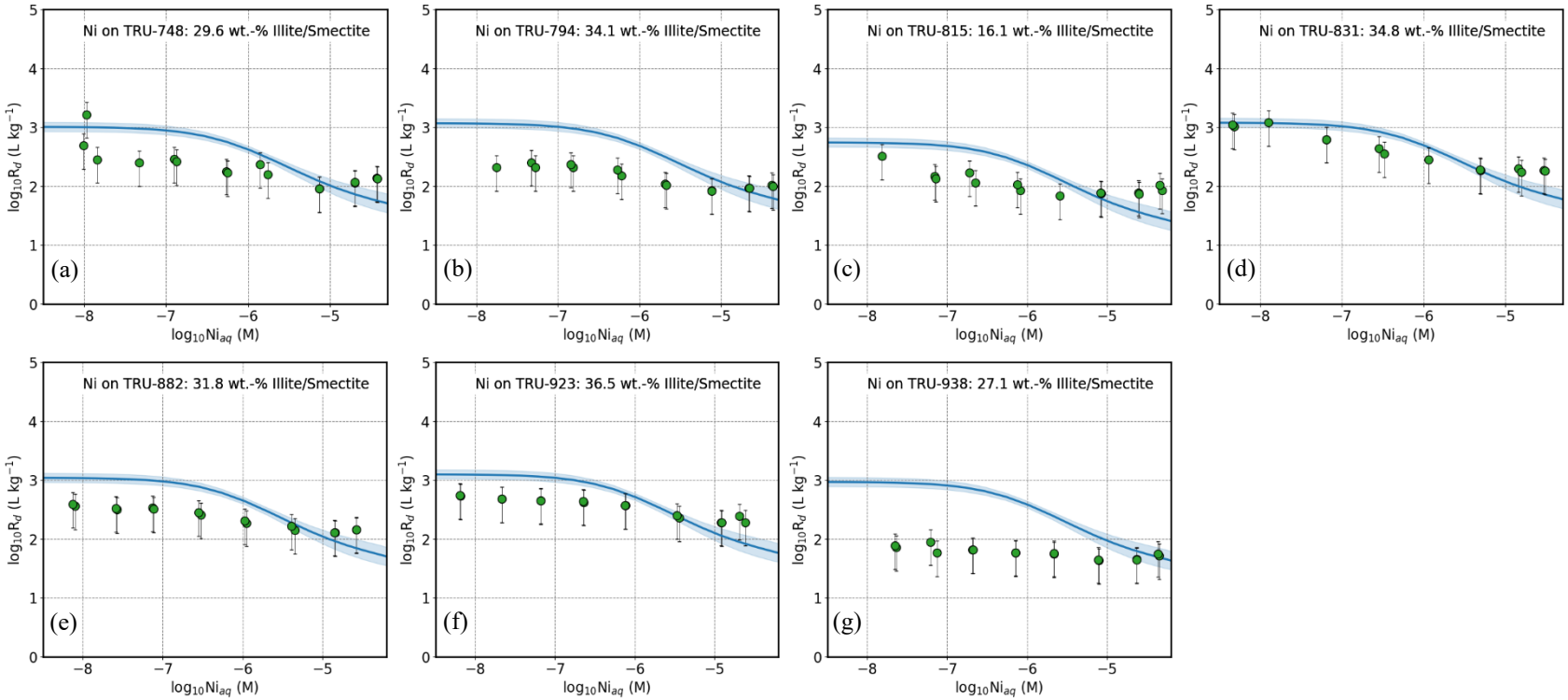

Fig. 4-6: Measured (green dots) and blindly predicted (blue line) sorption of Ni on the 7 rock samples from TRUL1-1 from the ZNO siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of Ni in the ClaySor model on illite (Tab. 3-2).

4.3 Eu

The Eu isotherms measurements on 20 rock samples from different lithologies from the JO, NL and ZNO siting regions in their corresponding SPWs together with the predictive modelling are shown in Fig. 4-7, Fig. 4-8 and Fig. 4-9, respectively. The experimental conditions and R_d values for Eu are given in App. C. The Eu sorption on all rock samples is generally high (log R_d > 4 L/kg) even for samples where the illite/smectite content (given in brackets) is small, *i.e.,* BOZ-323 (11 wt.%), BOZ-440 (14.4 wt.%), BUL-845 (0.9 wt.%) and TRU-815 (15.5 wt.%). The sorption behaviour of Eu on almost all rock samples is similar. In the Eu_{aq} range from 10^{-12} M to 10^{-8} M the sorption is linear with log R_d values between 4 L/kg and 5 L/kg and starts to decrease at $Eu_{aq} \geq \sim 10^{-8}$ M. This decrease is likely due to the saturation of the "strong sites" (low capacity, high affinity) of illite (Bradbury & Baeyens 2009a). The maximum Eu_{aq} concentration is constrained by the solubility of $EuOHCO_3(s)$ ($\log_{10}K^o = 21.7$) in the SPWs. If the solubility limit is reached, the Eu_{aq} concentration remains constant, the sorption of Eu will cease and an Eu solid phase will precipitate, which normally results in an increase of the R_d value. However, no precipitation was observed for any of the samples. On the limestone samples, with very high calcite contents (given in brackets), *i.e.*, BOZ-323 (81 wt.%), BOZ-440 (98 wt.%) and BUL-845 (98 wt.%), Eu sorption is remarkably high (log R_d > 4.5 L/kg) and remains constant over the entire Eu_{aq} range. For these samples, the high sorption does not reflect the low illite/smectite content. The sorption isotherm of the TRU-815 sample (Fig. 4.9c) with 23 wt.% calcite and 16.1 wt.% illite/smectite exhibits a similar non-linear shape as for the argillaceous rock samples and is well reproduced by the modelling.

The predictive sorption modelling for Eu is illustrated by the blue lines in the graphical presentations. As for Ni, the modelling considers only the illite/smectite content and only Eu^{3+} and positive and neutral hydrolysed Eu species are assumed to adsorb by SC on illite (Tab. 3-2). The modelling reproduces the shape and R_d values of most of the Eu isotherms very well, except for the clay mineral-poor/calcite-rich samples BOZ-323 (Fig. 4-7a), BOZ-440 (Fig. 4-7b), BOZ-572 (Fig. 4-7e) and BUL-845 (Fig. 4-8a). The experimental data points are mostly close to or in the 95% confidence interval.

For JO, two samples are calcareous with calcite contents of 81 and 55 wt.% for BOZ-323 (Fig. 4.7a) and BOZ-440 (Fig. 4.7b), respectively and with relatively low illite/smectite contents of 10.0 and 14.3 wt.%, respectively. The model calculations are clearly underpredicted by more than 1.2 log units as in the case of the limestone sample BUL-845 from NL (Fig. 4-8a). The four remaining samples have illite/smectite contents between 25.4 and 56.9 wt.% (Tab. 2-1). On the argillaceous rock samples BOZ-493, BOZ-521 and BOZ-681, the sorption and the shape of the isotherms are very well described by the bottom-up modelling approach. The sorption on the argillaceous sample BOZ-572 (Fig. 4-7e) is also underpredicted (~1 log unit) despite this sample being clay-rich and showing a sorption isotherm shape typical for argillaceous rocks. The reason for the more pronounced sorption of this sample is not clear. The experimentally determined CEC value (Tab. 2-1) supports the clay-mineral content of the samples, excluding some mineralogical sample inhomogeneities. Also, this sample does not contain significantly more kaolinite compared to samples from other regions. The plateau of the isotherm slightly differs from that of the other argillaceous samples, with sorption beginning to decrease at $Eu_{aq} \sim 10^{-9}$ M). Notably, this sample is the only rock sample that contains anhydrite, albeit only 3 wt.%.

The results for the NL siting region are summarised in Fig. 4-8. Six argillaceous rock samples with illite/smectite contents varying between 23.4 and 43.7 wt.% are very well described by the model. The predicted sorption on the limestone sample BUL-845 (Fig. 4-8a) is ~ 1.9 log units below the experimentally determined sorption, and the modelling reflects the very low illite/ smectite content of 0.9 wt.% of this limestone sample.

Figs. 4-9a to 4-9g show the results for the ZNO siting region. The illite and smectite content of the rock samples varies between 16.1 and 34.1 wt.% (Tab. 2-3) and the model calculations reproduce well the Eu sorption on all the samples. The experimental data points are in all cases close to the model prediction within the 95% confidence interval.

The considerable discrepancy between model predictions and experimental results obtained on the calcite-rich samples BOZ-323 (Fig. 4-7a), BOZ-440 (Fig. 4-7b) and BUL-845 (Fig. 4-8a) might be due to Eu uptake onto calcite (Lakshtanov & Stipp 2004). It is likely that the crushing of these calcareous samples has increased the specific reactive surface area of calcite. These results should, however, not be used to quantify the influence of calcite on sorption as they do not represent the reactivity of undisturbed, compacted calcareous rock.

From 20 investigated rock samples, Eu sorption could not be reproduced by the bottom-up approach using the ClaySor model for illite on only 4 limestone samples. The blind predictions for the remaining 16 samples agree with previous studies (Bradbury & Baeyens 2011, Marques Fernandes & Baeyens 2021, Marques Fernandes et al. 2015) and support the applicability of the bottom-up approach to argillaceous rocks for SA.

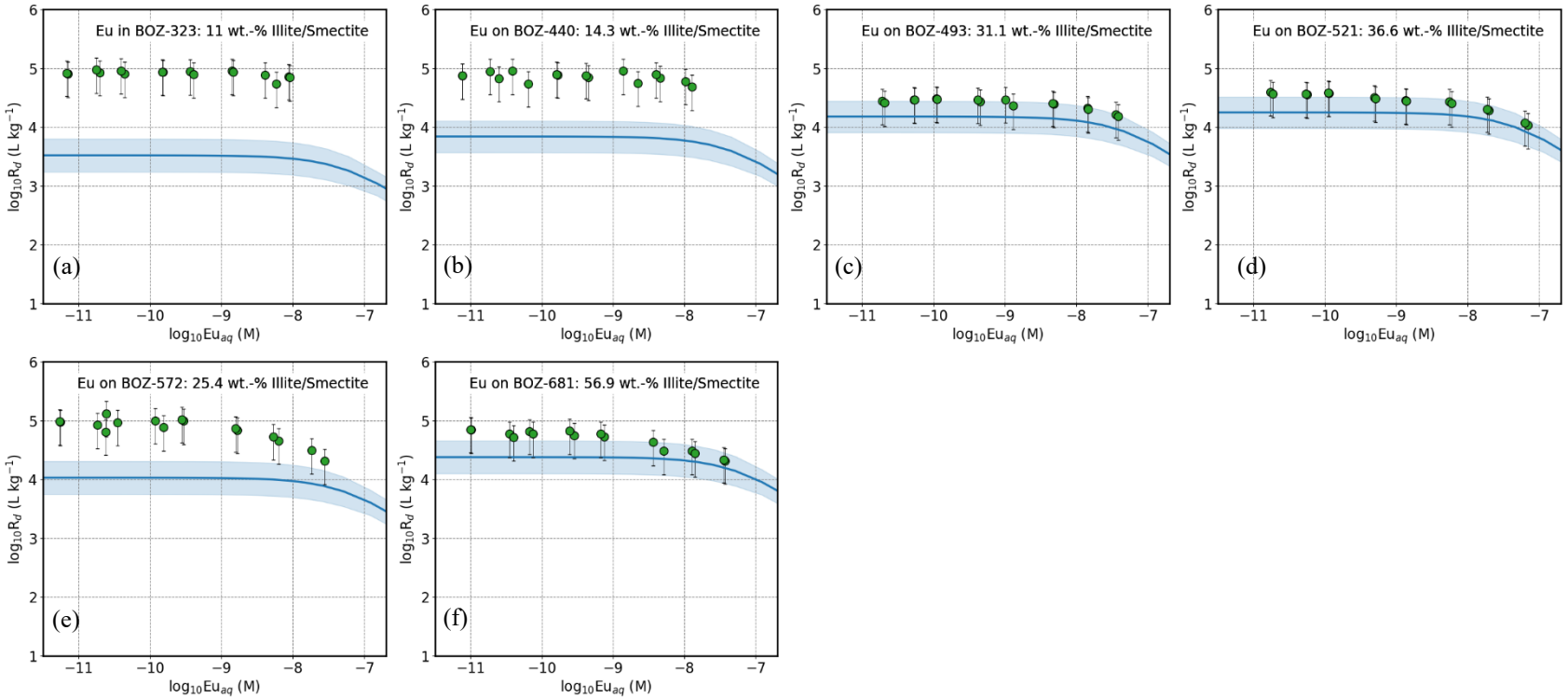

Fig. 4-7: Measured (green dots) and blindly predicted (blue line) sorption of Eu on the 6 rock samples from BOZ1-1 from JO in the corresponding SPW (cf. Tab. 2-4)

The blue shaded area represents the uncertainty on the modelling originating from the uncertainty associated to SCCs of Eu in the ClaySor model on illite (Tab.3-2).

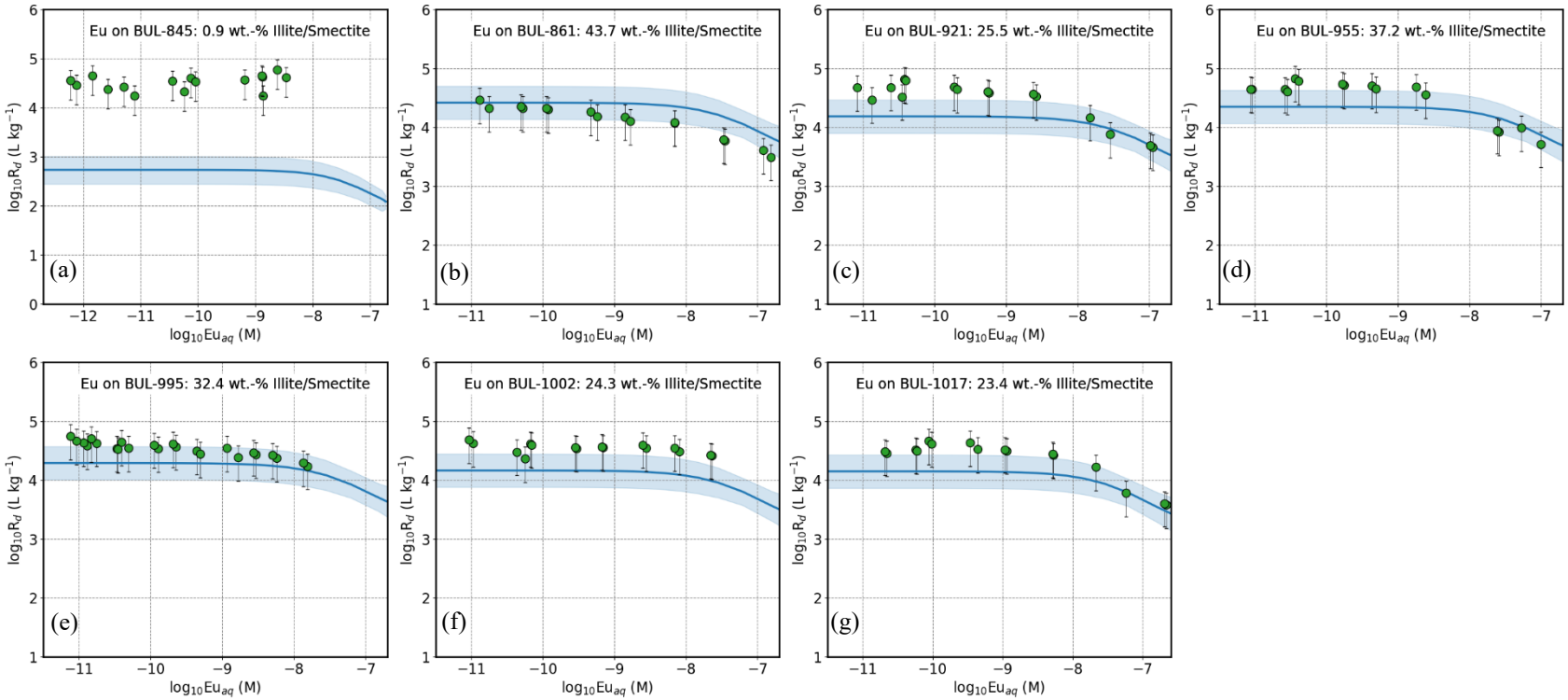

Fig. 4-8: Measured (green dots) and blindly predicted (blue line) sorption of Eu on the 7 rock samples from BUL1-1 from the NL siting region in the corresponding SPW (cf. Tab. 2-4)

The blue shaded area represents the uncertainty on the modelling originating from the uncertainty associated to SCCs of Eu in the ClaySor model on illite (Tab. 3-2).

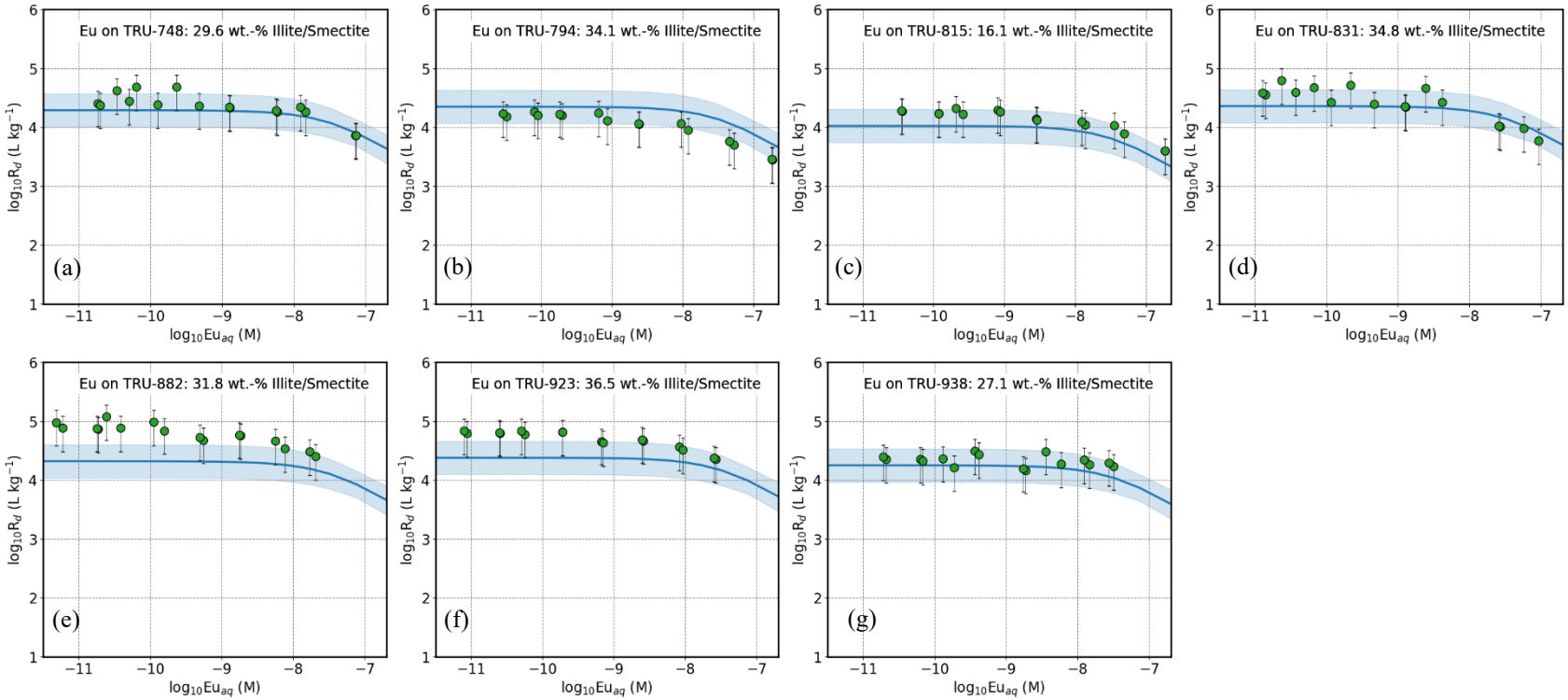

Fig. 4-9: Measured (green dots) and blindly predicted (blue line) sorption of Eu on the 7 rock samples from TRUL1-1 from the ZNO siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of Eu in the ClaySor model on illite (Tab. 3-2).

4.4 Th

Th isotherms measurements together with the predictive modelling on 20 rock samples from the JO, NL and ZNO siting regions are shown in Fig. 4-10, Fig. 4-11 and Fig. 4-12, respectively. The detailed experimental results are given in App. D. The sorption of tetravalent Th is very high and constant with log R_d values vary between 4 L/kg and 5.8 L/kg on all rock samples over the measured Th_{aq} range. The lowest and highest sorption is measured on the samples with the lowest (0.9 wt.%) and highest (56.7 wt.%) illite/smectite content, respectively. Due to the very low solubility of Th, isotherms were measured only over a narrow Th_{aq} range of 10^{-13} M to 10^{-9} M. None of the isotherms suggests precipitation of Th solid phases. Because of this concentration constraint, Th cannot reach the saturation of the strong sites on illite and consequently the sorption is expected to be constant. The measured R_d values are in good agreement with sorption data obtained on other argillaceous rock samples measured in similar SPW (Marques Fernandes & Baeyens 2021, Marques Fernandes et al. 2015, Baeyens et al. 2014, Bradbury & Baeyens 2011).

The sorption behaviour of Th is very similar on illite and montmorillonite (Baeyens & Marques Fernandes 2018). Therefore, the illite model could be used to predict Th sorption on rock samples that primarily contain illite with small amounts of smectite.

The predictive sorption modelling was carried out with the ClaySor model of Th for illite (Tab. 3-1 and Tab. 3-2) and the recent PSI/Nagra TDB 2020 (Hummel & Thoenen 2023) as described in Section 3.2. The calculated Th isotherms are illustrated by the blue lines in Fig. 4-10, Fig. 4-11 and Fig. 4-12. The blind predictions are in very good agreement with the experimental data for the 20 Th isotherms measured for the 3 different regions.

The relatively large 95% confidence interval is attributed to the significant uncertainty on the $\equiv S^{S}OTh(OH)_3^0$ SCC (Marinich et al. 2024). Overall, the predicted Th sorption is in very good agreement with the experimental data for almost all rock samples from the three siting regions. In a few cases, the predictions are slightly underpredicted, but in no instance does the model overpredict the experimental data.

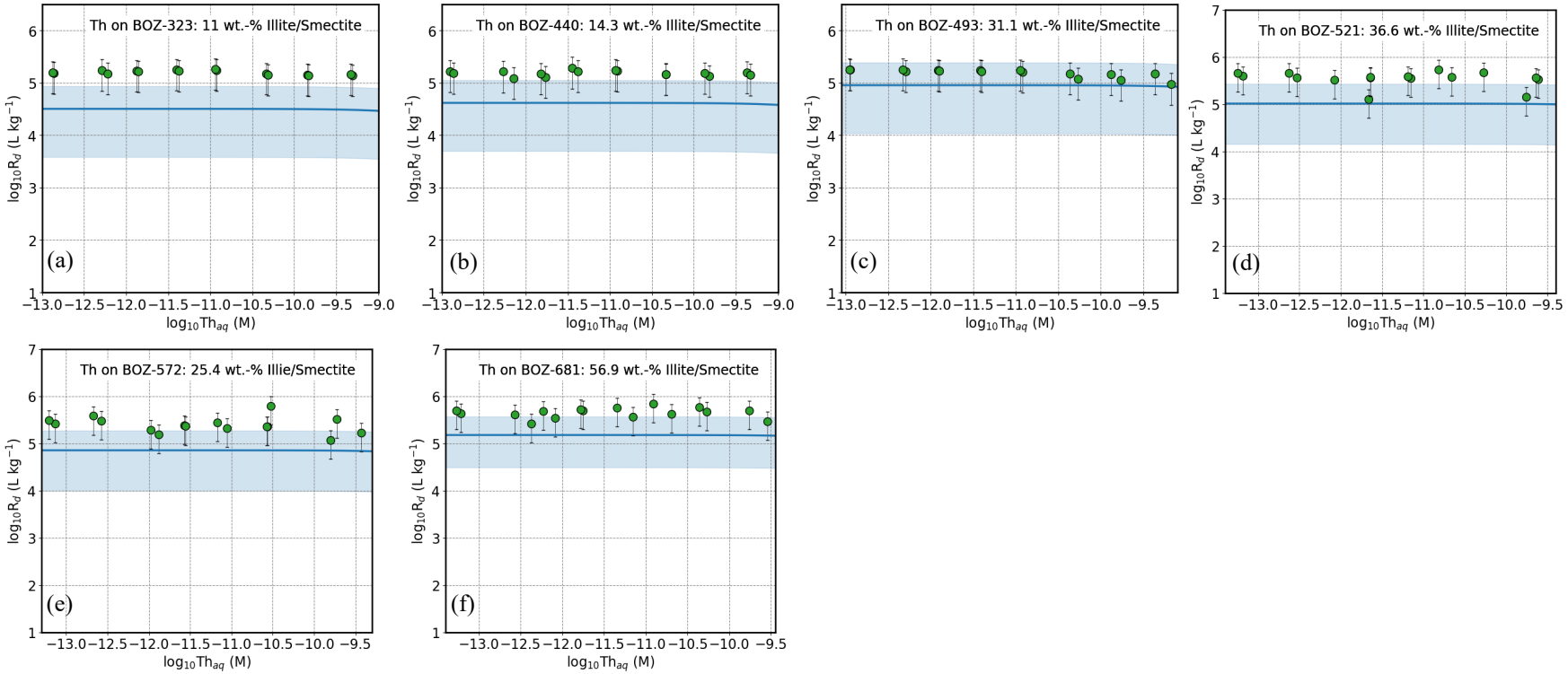

Fig. 4-10: Measured (green dots) and blindly predicted (blue line) sorption of Th on the 6 rock samples from BOZ1-1 from the JO siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of Th in the ClaySor model on illite (Tab. 3-2).

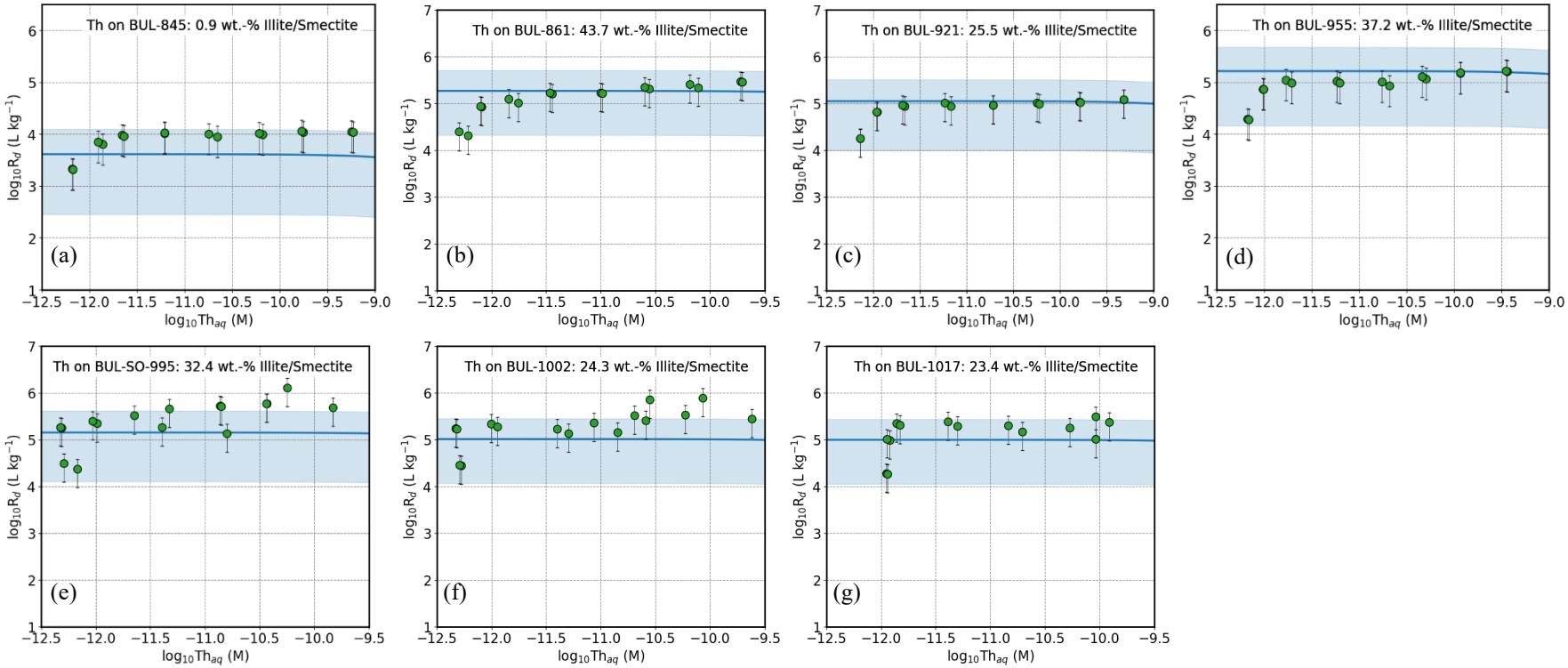

Fig. 4-11: Measured (green dots) and blindly predicted (blue line) sorption of Th on the 7 rock samples from BUL1-1 from the NL siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of Th in the ClaySor model on illite (Tab. 3-2).

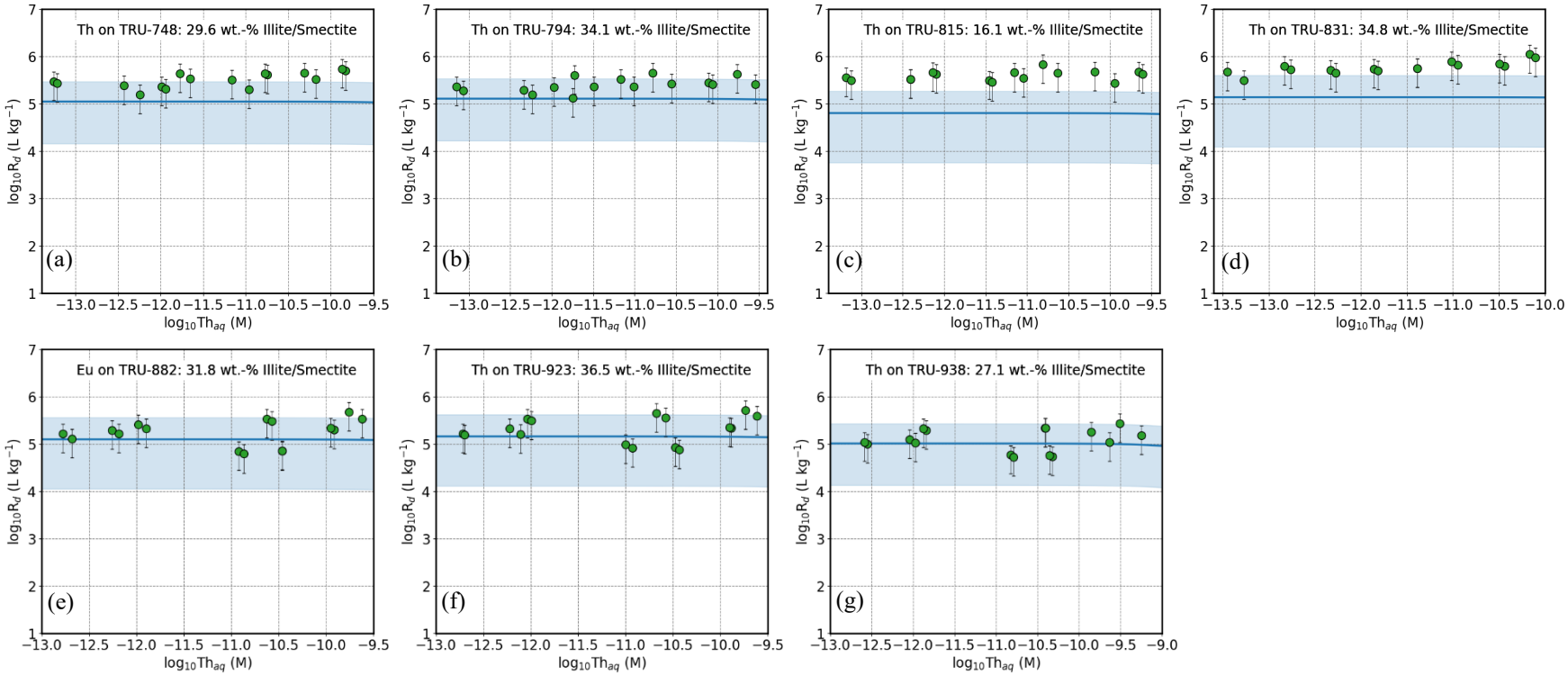

Fig. 4-12: Measured (green dots) and blindly predicted (blue line) sorption of Th on the 7 rock samples from TRU1-1 from the ZNO siting region in the corresponding SPW (cf. Tab. 2-4)

The blue-shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of Th in the ClaySor model on illite (Tab. 3-2).

4.5 U

The experimental sorption data and corresponding predictive modelling results for U on 20 rock samples originating from the three siting regions JO, NL and ZNO are shown in Fig. 4-13, Fig. 4-14 and Fig. 4-15, respectively.

The experimental conditions and R_d results for U on all rock samples are detailed in App. E. The sorption measurements generally show little scatter and as expected, the U sorption is considerably reduced by ~ 3 to 4 orders of magnitude compared to sorption on pure illite in a simple NaCl electrolyte at similar pH and U_{aq} conditions (Bradbury & Baeyens 2009a) for all rock samples regardless of mineralogy and SPW composition. The sorption of U compared to all other elements is extremely sensitive to the composition of the SPW, especially by the CO_3^{2-} /HCO_3^- concentrations and consequently to the pH (Bradbury & Baeyens 2011, Marques Fernandes & Baeyens 2021, Marques Fernandes et al. 2015). In the 3 SPWs used for the U isotherms, the uranyl aqueous speciation is dominated by complexation with carbonate species, mainly in the form of the strongly non-sorbing aqueous $Ca_2UO_2(CO_3)_3^0$ and $CaUO_2(CO_3)_3^{2-}$ complexes (> 90%).

The log R_d values at the lowest U_{aq} vary between 2 L/kg (for the clay mineral richest samples BOZ-681 (see Fig. 4-13f) and ~ 1 L/kg for the clay mineral poorest samples BUL-851 (Fig. 4-14a) and BOZ-323 (Fig. 4-13a). For the samples from NL and ZNO, the log R_d values lie in the range from ~ 1 to 1.8 at the lowest U_{aq}. It should be noted that the pH of the BUL samples varies between 7.2 and 7.7. Despite these relatively small pH variations, they have a significant influence on carbonate speciation. Most isotherms determined on the samples of JO, NL and ZNO, except on BUL-851 (Fig. 4-14a), BUL-1017 (Fig. 4-14g) and TRU-938 (Fig. 4-15g), show a slight decrease in sorption (~ 0.5 log units) as a function of U_{aq}. It should be noted that BUL-851 and TRU-938 are calcite-rich samples, with 90 and 43 wt.% calcite, respectively. On the other hand, BUL-1017, contains only 7 wt.% calcite. Despite being calcite-rich, too, U sorption on BUL-1002 (Fig. 4-14f) decreases slightly as a function U_{aq}. Sorption on the JO samples is generally less pronounced at similar illite/smectite contents compared to the samples from NL and ZNO, which reflects the slightly higher pH values ~ 8 and consequently higher TIC concentrations.

The model calculations for U were performed on each sample in the corresponding SPW at the experimentally determined pH value. Strikingly, the predictive modelling (blue solid line in Fig. 4-13, Fig. 4-14 and Fig. 4-15) underestimates all experimental data by about one order of magnitude, regardless of mineralogy and SPW composition. This systematic underprediction is unexpected, as uranyl sorption onto sedimentary rock samples in similar SPWs has generally been well described in the numerous studies performed in the past (Bradbury & Baeyens 2011, Marques Fernandes & Baeyens 2021, Marques Fernandes et al. 2015). The reasons for this systematic underprediction are not clear. The sorption of aqueous $UO_2CO_3^0$ complexes, which are not considered in the modelling approach, could potentially take place, and slightly increase the sorption. For Ca-free systems, however, studies have shown that the sorption of UO_2CO_3 complexes, if any, is rather low, especially at the pH and pCO_2 conditions currently investigated (Marques Fernandes et al. 2012, Stockmann et al. 2022, Tournassat et al. 2018). Another process that could lead to enhanced sorption would be the reduction of U(VI) to U(IV) by redox reactive mineral phases present in the sedimentary rock (*e.g.*, Fe(II)-bearing clays minerals or minerals such as pyrite (FeS_2) or siderite ($FeCO_3$)) (Fröhlich et al. 2012, Schacherl et al. 2023, Townsend et al. 2022). Small amounts of pyrite (ranging from 0.2 to 3 wt.%) are present in almost all samples from BOZ1-1 and BUL1-1 (see Tab. 2-1 and Tab. 2-2). Siderite is detected in small quantities in three samples from BOZ1-1 (< 5 wt.%), four samples from BUL1-1 (< 2 wt.%) and three samples from TRU1-1 (< 5 wt.%) (see Tab. 2-1 and Tab. 2-2). Only a few per cent of reduced U would be sufficient to increase the R_d values, owing to the strong sorption behaviour of tetravalent actinides (see Section 4.4 on Th). However, it is not expected that this would be the case for all the investigated samples, particularly not to a same systematic extent, but it could potentially play a role. It should be noted that in the previous mentioned published studies, pyrite and siderite were

also present in the argillaceous rock samples investigated. Sorption on kaolinite or other reactive mineral phases such as calcite can potentially also contribute to an increased sorption (Dong et al. 2005, Shi et al. 2022, Křepelová et al. 2006). This could be the case for the illite-/smectite-poor, calcite-rich samples BOZ-323, BOZ-440, BUL-851, TRU-815 and TRU-815. As discussed in Section 4.3, crushing the samples has increased the specific reactive surface area of calcite. However, these results should not be interpreted to extrapolate the influence of calcite on the sorption of U in undisturbed compacted rocks.

A major difference between the present and past modelling is the use of the updated aqueous formation constant of $Ca_2UO_2(CO_3)_3^0$ ($\log \beta = 30.8 \pm 0.4$) in the PSI/Nagra TDB 2020. This constant was recently revised and selected by NEA (OECD/NEA 2020) and was implemented in the most recent TDB by Hummel & Thoenen (2023). The $\log \beta = 29.22 \pm 0.25$ for $Ca_2UO_2(CO_3)_3^0$ selected in the previous PSI/Nagra TDB 2014 (Thoenen et al. 2014a) is 1.6 log units lower than the currently selected value. To visualise the effect of the log β value, the model calculations were repeated with the $\log \beta = 29.22$ constant and the results are illustrated by the dashed grey lines in Fig. 4-13, Fig. 4-14 and Fig. 4-15. The predictive modelling has clearly improved for all samples, but sorption remains underestimated for a number of cases, especially for the JO rock samples. Recently, Hennig & Kühn (2021) quantified the influence of the choice of stability constant on the simulation of the diffusion of uranium through the Opalinus Clay. A difference in the stability constant of 1.33 log units changes the migration lengths by 5 to 7 m. This example and the U sorption results of this study clearly illustrate the importance and influence of the thermodynamic constants of non-sorbing aqueous complexes. Presently, based on the chosen data base, the bottom-up approach seems to be very conservative with respect to the U sorption.

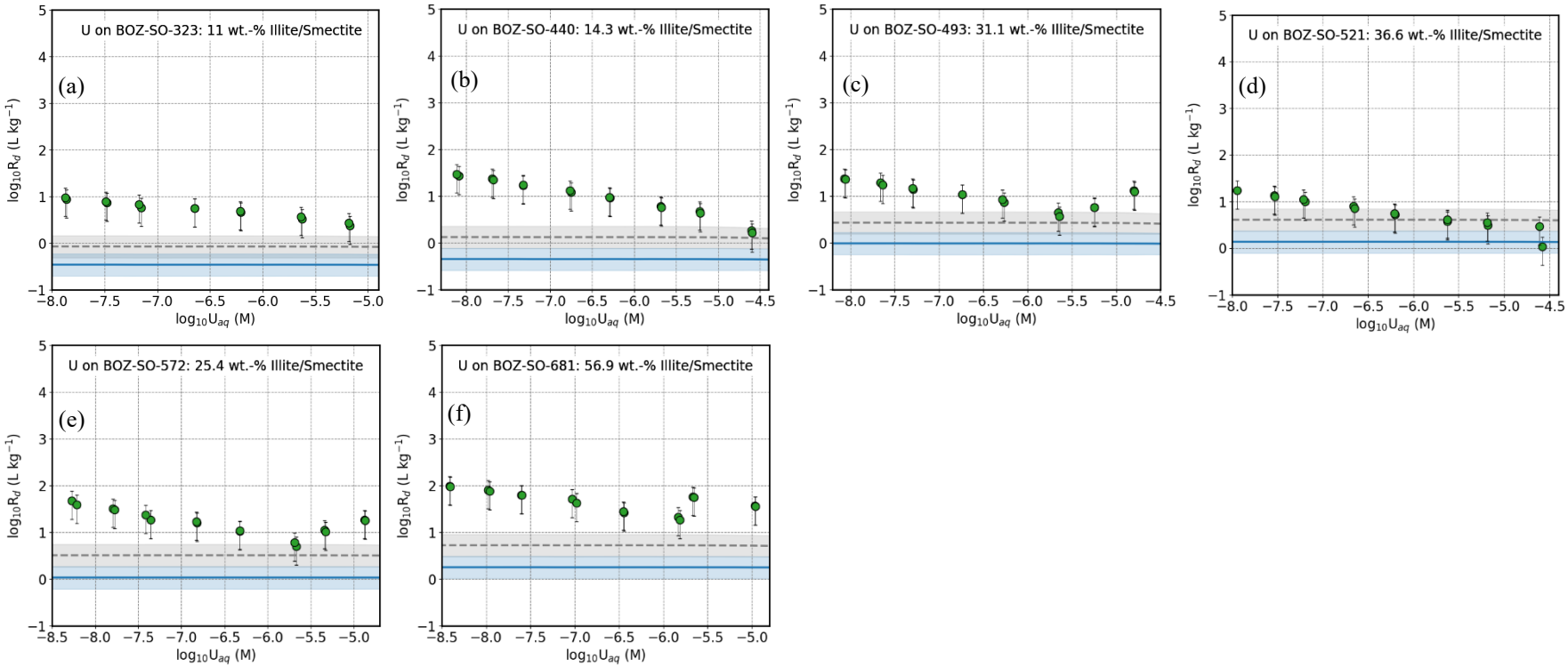

Fig. 4-13: Measured (green dots) and blindly predicted (blue and grey dashed lines) sorption of U on the 6 rock samples from BOZ1-1 from the JO siting region in the corresponding SPW (cf. Tab. 2-4)

The shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of U in the ClaySor model on illite (Tab. 3-2). The blue line is the modelling with the $Ca_2UO_2(CO_3)_{3(aq)}$ complexation constant (log K = 30.8 ± 0.4) selected in Hummel & Thoenen (2023), and the grey dashed line is the modelling with the $Ca_2UO_2(CO_3)_{3(aq)}$ complexation constant (log K = 29.22 ± 0.25) selected in Thoenen et al. (2014b).

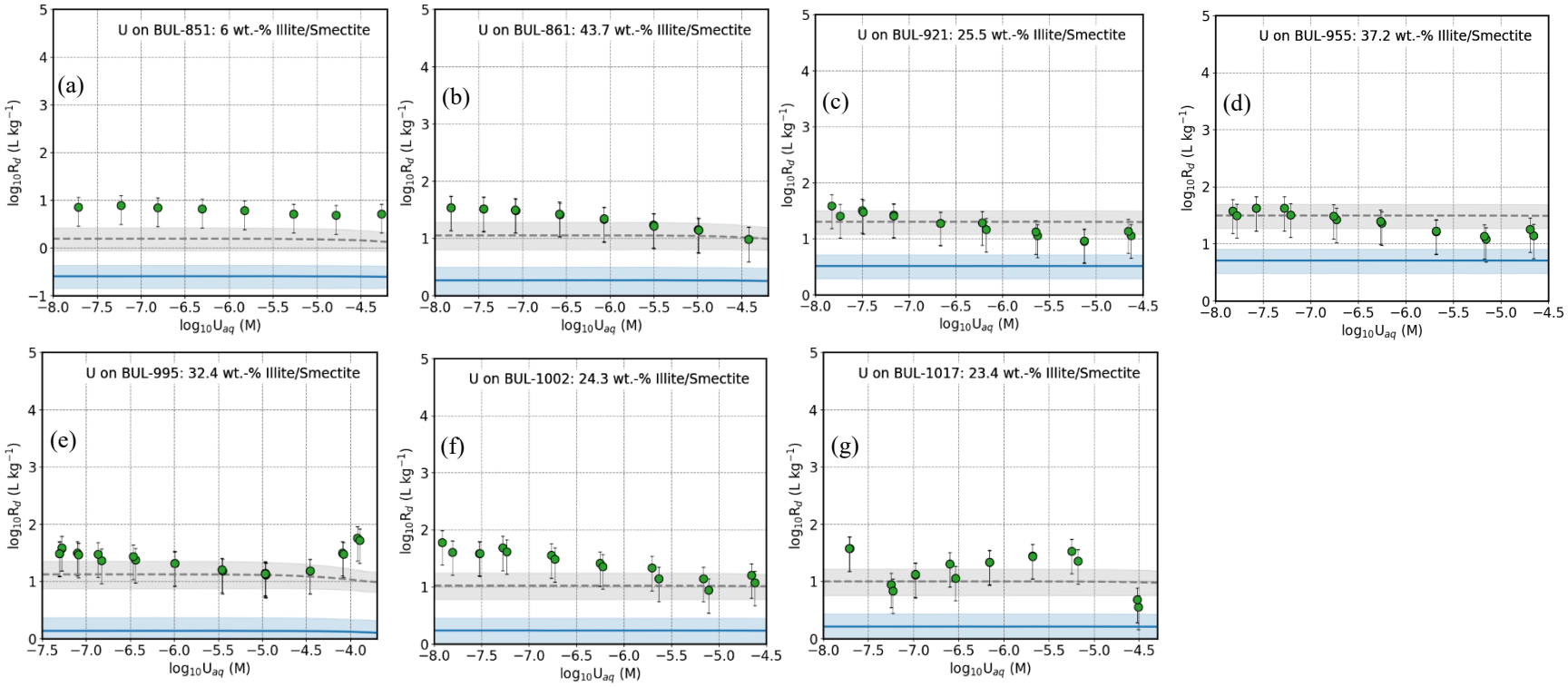

Fig. 4-14: Measured (green dots) and blindly predicted (blue and grey dashed lines) sorption of U on the 7 rock samples from BUL1-1 from the NL siting region in the corresponding SPW (cf. Tab. 2-4)

The shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of U in the ClaySor model on illite (Tab. 3-2). The blue line is the modelling with the $Ca_2UO_2(CO_3)_{3(aq)}$ complexation constant (log K = 30.8 ± 0.4) selected in Hummel & Thoenen (2023), and the grey-dashed line is the modelling with the $Ca_2UO_2(CO_3)_{3(aq)}$ complexation constant (log K = 29.22 ± 0.25) selected in Thoenen et al. (2014b).

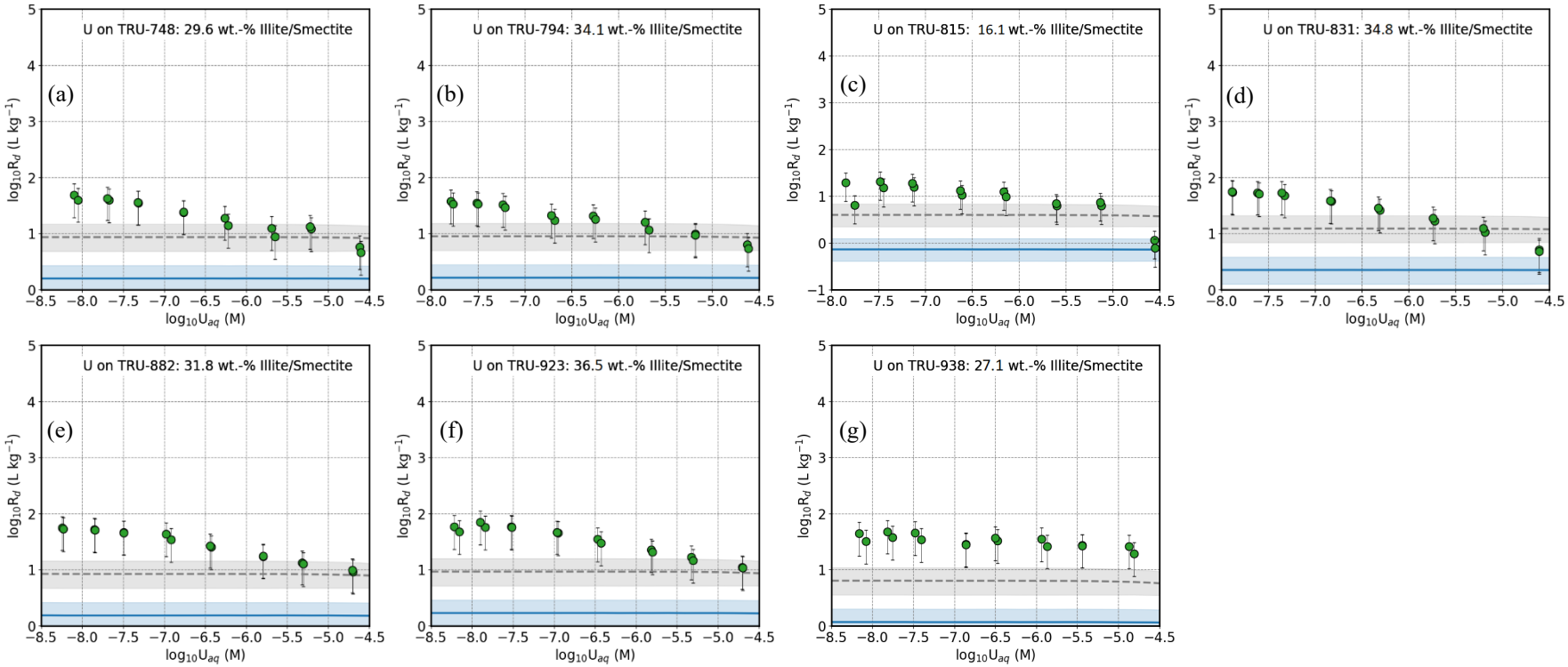

Fig. 4-15: Measured (green dots) and blindly predicted (blue and grey dashed lines) sorption of U on the 7 rock samples from TRU1-1 from the ZNO siting region in the corresponding SPW (cf. Tab. 2-4)

The shaded area represents the modelling uncertainty originating from the uncertainty associated with SCCs of U in the ClaySor model on illite (Tab. 3-2). The blue line is the modelling with the $Ca_2UO_2(CO_3)_{3(aq)}$ complexation constant (log K = 30.8 ± 0.4) selected in Hummel & Thoenen (2023), and the grey-dashed line is the modelling with the $Ca_2UO_2(CO_3)_{3(aq)}$ complexation constant (log K = 29.22 ± 0.25) selected in Thoenen et al. (2014b).

5 Summary and conclusions

The safety assessment of a deep geological repository for radioactive waste depends, among other things, on the ability to reliably predict the long-term fate of (radio-)contaminants under in-situ geochemical conditions. Sorption on mineral phases along the potential migration path is one of the main pillars on which the safety assessment is based. However, sorption on sedimentary rocks from geological formations identified as potential host rocks (and their confining geological rock units) in Switzerland and many other countries is inherently too complex to be easily predicted by sorption models due to the multi-mineral nature of these rocks.

For argillaceous rocks, the complexity of modelling can be reduced by considering only 2:1 clay minerals (bottom-up approach), given their high sorption properties. Under this assumption, it is crucial to understand the sorption processes on the pure clay minerals and to develop robust thermodynamic sorption models that can reliably predict the radionuclide sorption under a wider range of geochemical conditions.

Verifying and validating the applied bottom-up modelling approach is critical for justifying its use in calculating state-of-the-art SDBs required for the safety assessment in the RBG. The SDBs developed from existing sorption models allow direct calculation of the R_d values by accounting for aqueous speciation, sorption competition, solubility limits, and concentration-dependent sorption of each radionuclide for specific rock-porewater systems.

Nagra carried out an extensive deep borehole campaign in the JO, NL and ZNO siting regions as part of the SGT to investigate the site-specific rock properties. The sorption properties of the selected host rock Opalinus Clay as well as of the upper and lower CRZ (*i.e.,* confining geological units) are key parameters for the safety assessment and provide valuable information on the geochemical performance of the potential site.

This report has two main objectives. Firstly, to assess the sorption capacity of the three siting regions and verify their retention properties. For this, sorption isotherms of Cs(I), Ni(II), Eu(III), Th(IV) and U(VI) (covering different oxidation states) were determined on rock samples from drill cores obtained from the BUL1-1, TRU1-1 and BOZ1-1 boreholes (with different clay mineral contents) in the NL, ZNO and JO siting regions, respectively, in their corresponding SPWs. Secondly, to evaluate the effectiveness of the bottom-up approach using the ClaySor model for illite, scaled to the 2:1 clay mineral content, and considering the aqueous speciation of the radionuclides in the respective SPWs, in predicting the experimentally measured sorption isotherms.

The experimentally determined Cs, Ni, Eu, Th and U sorption isotherms revealed that the rock samples from the different regions showed similar effective sorption properties. Major factors influencing sorption include (i) the clay mineral (illite/smectite) content, (ii) the porewater composition (*i.e.,* pH, concentration of complexing ligands or competing cations), and (iii) the salinity. The illite/smectite content affects the sorption of all radionuclides, whereas salinity, under the defined in-situ pH conditions (circumneutral), primarily impacts the sorption of elements which sorb via CE such as Cs. The SPW composition, in particular the concentration of dissolved TIC, is critical for elements such as uranyl which form strong aqueous carbonate complexes. The sorption of divalent cations (*e.g.*, Ni) is likely influenced by competition for the strong sites with other divalent cations present in the porewater or inherently in the rock. Tetravalent cations (*e.g.*, Th) strongly hydrolyse and are less affected by porewater compositions.

In the case of Cs, the model predictions reproduce the experimental data extremely well on 20 different rock samples with varying illite contents. Even on the samples with very low illite content, down to 0.7 wt.%, the non-linear Cs sorption behaviour typical for illite (multi-site sorption) is very well reproduced, confirming that Cs sorption can be used as a fingerprint to quantify the illite content in rock samples.

The largest deviation between the prediction and the experimental data is observed for Ni, especially in the lower equilibrium concentration range. The modelling overpredicts the sorption of Ni on 7 rock samples out of 20 by up to one log unit in the lower Ni_{aq} range where the surface speciation is dominated by the strong sites. One possible explanation is the ubiquitous presence of divalent cations such as Fe and Mn in the natural rock system which can compete with Ni for sorption on the strong sites, and consequently decreases the sorption of Ni (Marques Fernandes & Baeyens 2020) In the development of the SDBs for the RBG, competitive sorption between divalent cations present in the porewater and the radionuclide of interest will be considered (Marques Fernandes et al. 2024a). In this study it could not be confirmed that calcite plays an important role in Ni retention.

Most of the Eu sorption isotherms are well reproduced by the shape and R_d value, except for the illite-/smectite-poor and calcite-rich samples and one Opalinus Clay sample where the model underpredicts the measured sorption. In the calcareous samples, the enhanced sorption could result from the partitioning of Eu into the crushed calcite. However, this uptake process does not reflect the influence of calcite on Eu sorption in undisturbed, compacted calcareous rock.

The modelling of Th sorption exhibits a high level of accuracy in replicating the experimental data. The modelled curves for most rocks align closely within or just above/below the uncertainty range, indicating a robust fit between the model and the actual experimental results.

In the case of U, the blind predictions consistently underestimate sorption on all rock samples, irrespective of the illite/smectite content, SPW composition or origin of the samples. It is crucial to highlight the significant impact of aqueous carbonato complexes on the sorption of uranyl, particularly the ternary uranyl-calcium-carbonato complexes, *i.e.*, $Ca_nUO_2(CO_3)_3^{(4-2n)-}$ (n = 1; 2), as these form strong non-sorbing complexes. The systematic underprediction observed in this study is not entirely clear, especially given that it has not been observed in previous studies. Further investigation is warranted to better understand the underlying factors contributing to this consistent underestimation. The reduction of U(VI) to U(IV) by redox-reactive mineral phases present in the sedimentary rock (*i.e.,* pyrite, siderite) could lead to enhanced U sorption. In addition, U sorption on minerals such as kaolinite or other reactive phases, *i.e.,* calcite could contribute to increased sorption. However, the varying content of these minerals does not reflect the systematic and consistent underprediction observed. The only notable difference between the present and past modelling calculations lies in the use of the updated stability constant for the aqueous $Ca_2UO_2(CO_3)_3^0$ complex. The former selected log β value in PSI/Nagra TDB 2014 (Thoenen et al. 2014a) is considerably lower (1.6 log units) than the currently selected value in PSI/Nagra TDB 2020 (Hummel & Thoenen 2023). Calculations using the former constant improved the modelling. The case of U highlights the critical importance and influence of the thermodynamic constants. Presently, based on the chosen data base, the bottom-up approach is conservative regarding U sorption. After the closure of the repository, reducing conditions and higher pCO_2 are expected to prevail in the near-field. Consequently, U will exist partly as tetravalent U, forming weak carbonato complexes and exhibiting strong sorption such as Th. Despite this, some U will be stabilised in its +VI form, primarily as the aqueous $Ca_2UO_2(CO_3)_3^0$ complex, due to the elevated pCO_2 levels, as well as the composition and pH of the PW. Overall, however, the reducing conditions lead to an increase in U sorption.

Considering the uncertainties inherent in the complexity of natural rocks and thermodynamic sorption modelling, the simplified bottom-up approach proves to be a fairly reliable tool for predicting the sorption behaviour of a range of metals (with oxidation states from I to IV and VI) in various sedimentary rocks. This approach, along with the underlying sorption model, can predict the uptake of radionuclides in geological environments, provided that sorption on 2:1 clay minerals is the predominant retention mechanism. In rocks with low clay mineral content, other minerals, particularly calcite, can control the retention of certain radionuclides.

Finally, this study makes an important contribution to demonstrating the reliability and robustness of the SDBs developed using the bottom-up approach, to assess the safety of the future deep geological repository.

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App. A Experimental data for caesium

A.1 Experimental data for Cs on BOZ1-1 samples

Tab. A-1: Experimental data for Cs on sample BOZ-323 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	32.00	$2.99 \cdot 10$	$2.81 \cdot 10$	-1.55	32.8	0.30	7.96
b	32.00	$2.99 \cdot 10$	$2.80 \cdot 10$	-1.55	32.8	0.33	8.02
2a	32.00	$2.99 \cdot 10^{-3}$	$2.35 \cdot 10^{-3}$	-2.63	32.8	0.92	7.95
b	32.00	$2.99 \cdot 10^{-3}$	$2.35 \cdot 10^{-3}$	-2.63	32.8	0.92	7.99
3a	32.00	$2.99 \cdot 10^{-4}$	$2.03 \cdot 10^{-4}$	-3.69	32.8	1.16	7.98
b	32.00	$2.99 \cdot 10^{-4}$	$2.04 \cdot 10^{-4}$	-3.69	32.8	1.15	8.05
4a	32.00	$2.99 \cdot 10^{-5}$	$1.49 \cdot 10^{-5}$	-4.83	32.8	1.49	8.08
b	32.00	$2.99 \cdot 10^{-5}$	$1.49 \cdot 10^{-5}$	-4.83	32.8	1.49	8.03
5a	32.00	$1.00 \cdot 10^{-5}$	$3.76 \cdot 10^{-6}$	-5.42	9.8	2.23	8.07
b	32.00	$1.00 \cdot 10^{-5}$	$7.50 \cdot 10^{-6}$	-5.13	9.8	1.54	8.08
6a	32.00	$2.99 \cdot 10^{-6}$	$1.81 \cdot 10^{-6}$	-5.74	9.8	1.82	8.06
b	32.00	$2.99 \cdot 10^{-6}$	$1.80 \cdot 10^{-6}$	-5.74	9.8	1.83	8.07
7a	32.00	$1.00 \cdot 10^{-6}$	$4.08 \cdot 10^{-7}$	-6.39	9.8	2.17	8.04
b	32.00	$1.00 \cdot 10^{-6}$	$4.07 \cdot 10^{-7}$	-6.39	9.8	2.17	8.04
8a	32.00	$3.00 \cdot 10^{-7}$	$8.07 \cdot 10^{-8}$	-7.09	9.8	2.44	8.08
b	32.00	$3.00 \cdot 10^{-7}$	$8.03 \cdot 10^{-8}$	-7.10	9.8	2.44	8.07
9a	32.00	$3.04 \cdot 10^{-8}$	$1.02 \cdot 10^{-9}$	-8.99	9.8	2.91	8.06
b	32.00	$3.04 \cdot 10^{-8}$	$9.73 \cdot 10^{-10}$	-9.01	9.8	2.94	8.05
10a	32.00	$1.45 \cdot 10^{-9}$	$3.91 \cdot 10^{-11}$	-10.41	9.8	3.02	7.96
b	32.00	$1.45 \cdot 10^{-9}$	$3.88 \cdot 10^{-11}$	-10.41	9.8	3.02	8.02

Tab. A-2: Experimental data for Cs on sample BOZ-440 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	32.00	$2.99 \cdot 10$	$2.82 \cdot 10$	-1.55	33.3	0.26	7.90
b	32.00	$2.99 \cdot 10$	$2.84 \cdot 10$	-1.55	33.3	0.20	7.88
2a	32.00	$2.99 \cdot 10^{-3}$	$2.38 \cdot 10^{-3}$	-2.62	33.3	0.89	8.03
b	32.00	$2.99 \cdot 10^{-3}$	$2.39 \cdot 10^{-3}$	-2.62	33.3	0.88	8.05
3a	32.00	$2.99 \cdot 10^{-4}$	$1.94 \cdot 10^{-4}$	-3.71	33.3	1.21	8.03
b	32.00	$2.99 \cdot 10^{-4}$	$1.91 \cdot 10^{-4}$	-3.72	33.3	1.23	8.00
4a	32.00	$2.99 \cdot 10^{-5}$	$1.29 \cdot 10^{-5}$	-4.89	33.3	1.60	8.00
b	32.00	$2.99 \cdot 10^{-5}$	$1.25 \cdot 10^{-5}$	-4.90	33.3	1.62	7.97
5a	32.00	$1.00 \cdot 10^{-5}$	$6.96 \cdot 10^{-6}$	-5.16	10.0	1.65	7.99
b	32.00	$1.00 \cdot 10^{-5}$	$6.99 \cdot 10^{-6}$	-5.16	10.0	1.64	8.05
6a	32.00	$2.99 \cdot 10^{-6}$	$1.61 \cdot 10^{-6}$	-5.79	10.0	1.93	8.02
b	32.00	$2.99 \cdot 10^{-6}$	$1.61 \cdot 10^{-6}$	-5.79	10.0	1.93	7.96
7a	32.00	$1.00 \cdot 10^{-6}$	$3.52 \cdot 10^{-7}$	-6.45	10.0	2.27	8.00
b	32.00	$1.00 \cdot 10^{-6}$	$3.49 \cdot 10^{-7}$	-6.46	10.0	2.27	7.96
8a	32.00	$3.00 \cdot 10^{-7}$	$7.52 \cdot 10^{-8}$	-7.12	10.0	2.47	7.96
b	32.00	$3.00 \cdot 10^{-7}$	$6.59 \cdot 10^{-8}$	-7.18	10.0	2.55	7.96
9a	32.00	$3.04 \cdot 10^{-8}$	$7.93 \cdot 10^{-10}$	-9.10	10.0	3.03	7.98
b	32.00	$3.04 \cdot 10^{-8}$	$8.49 \cdot 10^{-10}$	-9.07	10.0	3.00	8.00
10a	32.00	$1.45 \cdot 10^{-9}$	$2.95 \cdot 10^{-11}$	-10.53	10.0	3.15	8.04
b	32.00	$1.45 \cdot 10^{-9}$	$3.11 \cdot 10^{-11}$	-10.51	10.0	3.12	8.06

Tab. A-3: Experimental data for Cs on sample BOZ-493 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	32.00	$2.99 \cdot 10$	$2.37 \cdot 10$	-1.62	34.8	0.88	7.86
b	32.00	$2.99 \cdot 10$	$2.39 \cdot 10$	-1.62	34.8	0.86	7.86
2a	32.00	$2.99 \cdot 10^{-3}$	$1.56 \cdot 10^{-3}$	-2.81	34.8	1.42	7.92
b	32.00	$2.99 \cdot 10^{-3}$	$1.57 \cdot 10^{-3}$	-2.80	34.8	1.42	7.95
3a	32.00	$2.99 \cdot 10^{-4}$	$1.23 \cdot 10^{-4}$	-3.91	34.8	1.61	7.94
b	32.00	$2.99 \cdot 10^{-4}$	$1.25 \cdot 10^{-4}$	-3.90	34.8	1.60	7.95
4a	32.00	$2.99 \cdot 10^{-5}$	$7.46 \cdot 10^{-6}$	-5.13	34.8	1.94	7.98
b	32.00	$2.99 \cdot 10^{-5}$	$7.40 \cdot 10^{-6}$	-5.13	34.8	1.94	8.01
5a	32.00	$1.00 \cdot 10^{-5}$	$5.22 \cdot 10^{-6}$	-5.28	10.4	1.95	8.04
b	32.00	$1.00 \cdot 10^{-5}$	$5.25 \cdot 10^{-6}$	-5.28	10.4	1.94	8.00
6a	32.00	$2.99 \cdot 10^{-6}$	$1.03 \cdot 10^{-6}$	-5.99	10.4	2.26	7.98
b	32.00	$2.99 \cdot 10^{-6}$	$1.03 \cdot 10^{-6}$	-5.99	10.4	2.26	8.01
7a	32.00	$1.00 \cdot 10^{-6}$	$1.61 \cdot 10^{-7}$	-6.79	10.4	2.70	8.00
b	32.00	$1.00 \cdot 10^{-6}$	$1.60 \cdot 10^{-7}$	-6.79	10.4	2.70	8.04
8a	32.00	$3.00 \cdot 10^{-7}$	$2.62 \cdot 10^{-8}$	-7.58	10.4	3.00	7.95
b	32.00	$3.00 \cdot 10^{-7}$	$2.62 \cdot 10^{-8}$	-7.58	10.4	3.00	8.04
9a	32.00	$3.04 \cdot 10^{-8}$	$3.90 \cdot 10^{-10}$	-9.41	10.4	3.34	7.94
b	32.00	$3.04 \cdot 10^{-8}$	$3.90 \cdot 10^{-10}$	-9.41	10.4	3.34	8.01
10a	32.00	$1.45 \cdot 10^{-9}$	$1.72 \cdot 10^{-11}$	-10.76	10.4	3.37	8.01
b	32.00	$1.45 \cdot 10^{-9}$	$1.55 \cdot 10^{-11}$	-10.81	10.4	3.42	8.00

Tab. A-4: Experimental data for Cs on sample BOZ-521 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	32.00	$2.99 \cdot 10$	$2.44 \cdot 10$	-1.61	27.2	0.92	7.90
b	32.00	$2.99 \cdot 10$	$2.42 \cdot 10$	-1.62	27.2	0.94	7.92
2a	32.00	$2.99 \cdot 10^{-3}$	$1.59 \cdot 10^{-3}$	-2.80	27.2	1.51	7.89
b	32.00	$2.99 \cdot 10^{-3}$	$1.59 \cdot 10^{-3}$	-2.80	27.2	1.51	7.90
3a	32.00	$2.99 \cdot 10^{-4}$	$1.20 \cdot 10^{-4}$	-3.92	27.2	1.74	7.97
b	32.00	$2.99 \cdot 10^{-4}$	$1.20 \cdot 10^{-4}$	-3.92	27.2	1.74	7.96
4a	32.00	$2.99 \cdot 10^{-5}$	$6.71 \cdot 10^{-6}$	-5.17	27.2	2.11	7.93
b	32.00	$2.99 \cdot 10^{-5}$	$6.62 \cdot 10^{-6}$	-5.18	27.2	2.11	7.95
5a	32.00	$1.00 \cdot 10^{-5}$	$4.86 \cdot 10^{-6}$	-5.31	8.1	2.12	7.89
b	32.00	$1.00 \cdot 10^{-5}$	$4.88 \cdot 10^{-6}$	-5.31	8.1	2.11	7.92
6a	32.00	$2.99 \cdot 10^{-6}$	$8.81 \cdot 10^{-7}$	-6.05	8.1	2.47	7.95
b	32.00	$2.99 \cdot 10^{-6}$	$8.73 \cdot 10^{-7}$	-6.06	8.1	2.48	7.92
7a	32.00	$1.00 \cdot 10^{-6}$	$1.15 \cdot 10^{-7}$	-6.94	8.1	2.98	7.98
b	32.00	$1.00 \cdot 10^{-6}$	$1.20 \cdot 10^{-7}$	-6.92	8.1	2.96	7.99
8a	32.00	$3.00 \cdot 10^{-7}$	$1.90 \cdot 10^{-8}$	-7.72	8.1	3.26	7.95
b	32.00	$3.00 \cdot 10^{-7}$	$1.88 \cdot 10^{-8}$	-7.73	8.1	3.26	7.96
9a	32.00	$3.04 \cdot 10^{-8}$	$9.93 \cdot 10^{-10}$	-9.00	8.1	3.56	7.98
b	32.00	$3.04 \cdot 10^{-8}$	$9.90 \cdot 10^{-10}$	-9.00	8.1	3.56	8.00
10a	32.00	$1.45 \cdot 10^{-9}$	$5.32 \cdot 10^{-11}$	-10.27	8.1	3.51	8.01
b	32.00	$1.45 \cdot 10^{-9}$	$4.48 \cdot 10^{-11}$	-10.35	8.1	3.59	8.05

Tab. A-5: Experimental data for Cs on sample BOZ-572 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	32.00	$2.99 \cdot 10$	$2.62 \cdot 10$	-1.58	36.1	0.60	7.84
b	32.00	$2.99 \cdot 10$	$2.65 \cdot 10$	-1.58	36.1	0.56	7.82
2a	32.00	$2.99 \cdot 10^{-3}$	$1.93 \cdot 10^{-3}$	-2.72	36.1	1.19	7.86
b	32.00	$2.99 \cdot 10^{-3}$	$1.93 \cdot 10^{-3}$	-2.72	36.1	1.19	7.88
3a	32.00	$2.99 \cdot 10^{-4}$	$1.46 \cdot 10^{-4}$	-3.83	36.1	1.46	7.87
b	32.00	$2.99 \cdot 10^{-4}$	$1.46 \cdot 10^{-4}$	-3.84	36.1	1.47	7.84
4a	32.00	$2.99 \cdot 10^{-5}$	$8.84 \cdot 10^{-6}$	-5.05	36.1	1.82	7.83
b	32.00	$2.99 \cdot 10^{-5}$	$8.87 \cdot 10^{-6}$	-5.05	36.1	1.82	7.84
5a	32.00	$1.00 \cdot 10^{-5}$	$5.74 \cdot 10^{-6}$	-5.24	10.8	1.84	7.87
b	32.00	$1.00 \cdot 10^{-5}$	$5.74 \cdot 10^{-6}$	-5.24	10.8	1.84	7.89
6a	32.00	$2.99 \cdot 10^{-6}$	$1.21 \cdot 10^{-6}$	-5.92	10.8	2.14	7.91
b	32.00	$2.99 \cdot 10^{-6}$	$1.20 \cdot 10^{-6}$	-5.92	10.8	2.14	7.90
7a	32.00	$1.00 \cdot 10^{-6}$	$2.09 \cdot 10^{-7}$	-6.68	10.8	2.55	7.88
b	32.00	$1.00 \cdot 10^{-6}$	$2.11 \cdot 10^{-7}$	-6.68	10.8	2.54	7.91
8a	32.00	$3.00 \cdot 10^{-7}$	$3.47 \cdot 10^{-8}$	-7.46	10.8	2.85	7.90
b	32.00	$3.00 \cdot 10^{-7}$	$3.55 \cdot 10^{-8}$	-7.45	10.8	2.84	7.88
9a	32.00	$3.04 \cdot 10^{-8}$	$1.45 \cdot 10^{-9}$	-8.84	10.8	3.27	7.90
b	32.00	$3.04 \cdot 10^{-8}$	$1.47 \cdot 10^{-9}$	-8.83	10.8	3.26	7.85
10a	32.00	$1.45 \cdot 10^{-9}$	$6.20 \cdot 10^{-11}$	-10.21	10.8	3.32	7.87
b	32.00	$1.45 \cdot 10^{-9}$	$6.63 \cdot 10^{-11}$	-10.18	10.8	3.29	7.91

Tab. A-6: Experimental data for Cs on sample BOZ-681 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	32.00	$2.99 \cdot 10$	$2.33 \cdot 10$	-1.63	26.3	1.03	7.82
b	32.00	$2.99 \cdot 10$	$2.35 \cdot 10$	-1.63	26.3	1.02	7.85
2a	32.00	$2.99 \cdot 10^{-3}$	$1.42 \cdot 10^{-3}$	-2.85	26.3	1.62	7.84
b	32.00	$2.99 \cdot 10^{-3}$	$1.44 \cdot 10^{-3}$	-2.84	26.3	1.61	7.86
3a	32.00	$2.99 \cdot 10^{-4}$	$8.69 \cdot 10^{-5}$	-4.06	26.3	1.97	7.85
b	32.00	$2.99 \cdot 10^{-4}$	$8.62 \cdot 10^{-5}$	-4.06	26.3	1.97	7.87
4a	32.00	$2.99 \cdot 10^{-5}$	$3.74 \cdot 10^{-6}$	-5.43	26.3	2.43	7.85
b	32.00	$2.99 \cdot 10^{-5}$	$3.70 \cdot 10^{-6}$	-5.43	26.3	2.43	7.86
5a	32.00	$1.00 \cdot 10^{-5}$	$3.33 \cdot 10^{-6}$	-5.48	7.9	2.41	7.95
b	32.00	$1.00 \cdot 10^{-5}$	$3.38 \cdot 10^{-6}$	-5.47	7.9	2.40	7.93
6a	32.00	$2.99 \cdot 10^{-6}$	$4.86 \cdot 10^{-7}$	-6.31	7.9	2.82	7.98
b	32.00	$2.99 \cdot 10^{-6}$	$4.77 \cdot 10^{-7}$	-6.32	7.9	2.83	7.98
7a	32.00	$1.00 \cdot 10^{-6}$	$6.12 \cdot 10^{-8}$	-7.21	7.9	3.29	7.90
b	32.00	$1.00 \cdot 10^{-6}$	$6.15 \cdot 10^{-8}$	-7.21	7.9	3.29	7.89
8a	32.00	$3.00 \cdot 10^{-7}$	$1.21 \cdot 10^{-8}$	-7.92	7.9	3.48	7.88
b	32.00	$3.00 \cdot 10^{-7}$	$1.30 \cdot 10^{-8}$	-7.89	7.9	3.45	7.90
9a	32.00	$3.04 \cdot 10^{-8}$	$6.64 \cdot 10^{-10}$	-9.18	7.9	3.75	7.84
b	32.00	$3.04 \cdot 10^{-8}$	$7.82 \cdot 10^{-10}$	-9.11	7.9	3.68	7.88
10a	32.00	$1.45 \cdot 10^{-9}$	$3.38 \cdot 10^{-11}$	-10.47	7.9	3.73	7.86
b	32.00	$1.45 \cdot 10^{-9}$	$3.64 \cdot 10^{-11}$	-10.44	7.9	3.69	7.85

A.2 Experimental data for Cs on BUL1-1 samples

Tab. A-7: Experimental data for Cs on sample BUL-845 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1	30.00	$3.33 \cdot 10$	$3.32 \cdot 10$	-1.48	172.2	-1.63	7.70
2	30.00	$9.99 \cdot 10^{-3}$	$9.74 \cdot 10^{-3}$	-2.01	170.5	-0.83	7.68
3	30.00	$3.00 \cdot 10^{-3}$	$2.88 \cdot 10^{-3}$	-2.54	167.9	-0.61	7.70
4	30.00	$9.99 \cdot 10^{-4}$	$9.46 \cdot 10^{-4}$	-3.02	168.9	-0.48	7.71
5	30.00	$3.33 \cdot 10^{-4}$	$3.11 \cdot 10^{-4}$	-3.51	168.2	-0.37	7.69
6	30.00	$9.99 \cdot 10^{-5}$	$8.86 \cdot 10^{-5}$	-4.05	170.7	-0.13	7.69
7	30.00	$3.00 \cdot 10^{-5}$	$2.42 \cdot 10^{-5}$	-4.62	172.9	0.14	7.71
8	30.00	$9.99 \cdot 10^{-6}$	$7.29 \cdot 10^{-6}$	-5.14	171.1	0.34	7.70
9	30.00	$3.33 \cdot 10^{-6}$	$1.92 \cdot 10^{-6}$	-5.72	169.6	0.64	7.71
10	30.00	$9.99 \cdot 10^{-7}$	$3.76 \cdot 10^{-7}$	-6.42	169.4	0.99	7.71
11	30.00	$3.00 \cdot 10^{-7}$	$6.73 \cdot 10^{-8}$	-7.17	171.9	1.30	7.68
12	30.00	$1.00 \cdot 10^{-7}$	$1.65 \cdot 10^{-8}$	-7.78	167.6	1.48	7.69
13	30.00	$3.38 \cdot 10^{-8}$	$4.26 \cdot 10^{-9}$	-8.37	172.2	1.60	7.71
14	30.00	$1.04 \cdot 10^{-8}$	$1.24 \cdot 10^{-9}$	-8.91	172.2	1.64	7.69
15	30.00	$3.45 \cdot 10^{-9}$	$4.31 \cdot 10^{-10}$	-9.37	168.8	1.62	7.67
16	30.00	$1.45 \cdot 10^{-9}$	$1.70 \cdot 10^{-10}$	-9.77	179.8	1.62	7.74

Tab. A-8: Experimental data for Cs on sample BUL-861 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37.00	$3.33 \cdot 10$	$3.17 \cdot 10$	-1.50	189.2	0.67	7.69
b	37.00	$3.33 \cdot 10$	$3.21 \cdot 10$	-1.49	189.2	0.53	7.61
2a	37.00	$9.99 \cdot 10^{-3}$	$9.22 \cdot 10^{-3}$	-2.04	189.2	0.88	7.59
b	37.00	$9.99 \cdot 10^{-3}$	$9.15 \cdot 10^{-3}$	-2.04	189.2	0.92	7.55
3a	37.00	$3.00 \cdot 10^{-3}$	$2.82 \cdot 10^{-3}$	-2.55	189.2	0.76	7.60
b	37.00	$3.00 \cdot 10^{-3}$	$2.63 \cdot 10^{-3}$	-2.58	189.2	1.11	7.55
4a	37.00	$9.99 \cdot 10^{-4}$	$8.36 \cdot 10^{-4}$	-3.08	189.2	1.25	7.61
b	37.00	$9.99 \cdot 10^{-4}$	$8.32 \cdot 10^{-4}$	-3.08	189.2	1.26	7.56
5a	37.00	$3.33 \cdot 10^{-4}$	$2.71 \cdot 10^{-4}$	-3.57	189.2	1.33	7.69
b	37.00	$3.33 \cdot 10^{-4}$	$2.67 \cdot 10^{-4}$	-3.57	189.2	1.36	7.64
6a	37.00	$9.99 \cdot 10^{-5}$	$7.63 \cdot 10^{-5}$	-4.12	189.2	1.45	7.62
b	37.00	$9.99 \cdot 10^{-5}$	$7.76 \cdot 10^{-5}$	-4.11	189.2	1.42	7.58
7a	37.00	$3.00 \cdot 10^{-5}$	$2.10 \cdot 10^{-5}$	-4.68	189.2	1.59	7.63
b	37.00	$3.00 \cdot 10^{-5}$	$1.98 \cdot 10^{-5}$	-4.70	189.2	1.68	7.57
8a	37.00	$9.99 \cdot 10^{-6}$	$5.10 \cdot 10^{-6}$	-5.29	189.2	1.95	7.64
b	37.00	$9.99 \cdot 10^{-6}$	$5.11 \cdot 10^{-6}$	-5.29	189.2	1.94	7.57
9a	37.00	$3.33 \cdot 10^{-6}$	$1.03 \cdot 10^{-6}$	-5.99	189.2	2.31	7.63
b	37.00	$3.33 \cdot 10^{-6}$	$9.53 \cdot 10^{-7}$	-6.02	189.2	2.36	7.53
10a	37.00	$9.99 \cdot 10^{-7}$	$1.22 \cdot 10^{-7}$	-6.91	189.2	2.82	7.55
b	37.00	$9.99 \cdot 10^{-7}$	$1.19 \cdot 10^{-7}$	-6.92	189.2	2.83	7.64
11a	37.00	$3.00 \cdot 10^{-7}$	$2.44 \cdot 10^{-8}$	-7.61	189.2	3.02	7.60
b	37.00	$3.00 \cdot 10^{-7}$	$1.91 \cdot 10^{-8}$	-7.72	189.2	3.13	7.54
12a	37.00	$1.00 \cdot 10^{-7}$	$6.60 \cdot 10^{-9}$	-8.18	189.2	3.12	7.57
b	37.00	$1.00 \cdot 10^{-7}$	$5.39 \cdot 10^{-9}$	-8.27	189.2	3.21	7.58
13a	37.00	$3.38 \cdot 10^{-8}$	$1.85 \cdot 10^{-9}$	-8.73	189.2	3.20	7.73
b	37.00	$3.38 \cdot 10^{-8}$	$2.52 \cdot 10^{-9}$	-8.60	189.2	3.06	7.71
14a	37.00	$1.04 \cdot 10^{-8}$	$5.26 \cdot 10^{-10}$	-9.28	189.2	3.24	7.68
b	37.00	$1.04 \cdot 10^{-8}$	$6.53 \cdot 10^{-10}$	-9.19	189.2	3.14	7.71
15a	37.00	$3.45 \cdot 10^{-9}$	$2.66 \cdot 10^{-10}$	-9.57	189.2	3.04	7.73
b	37.00	$3.45 \cdot 10^{-9}$	$2.03 \cdot 10^{-10}$	-9.69	189.2	3.17	7.71
16a	37.00	$1.45 \cdot 10^{-9}$	$9.22 \cdot 10^{-11}$	-10.04	189.2	3.13	7.63
b	37.00	$1.45 \cdot 10^{-9}$	$7.57 \cdot 10^{-11}$	-10.12	189.2	3.22	7.59

Tab. A-9: Experimental data for Cs on sample BUL-921 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37.00	$3.33 \cdot 10$	$3.25 \cdot 10$	-1.49	10.4	0.37	7.49
b	37.00	$3.33 \cdot 10$	$3.23 \cdot 10$	-1.49	10.4	0.47	7.52
2a	37.00	$9.99 \cdot 10^{-3}$	$9.44 \cdot 10^{-3}$	-2.03	10.4	0.75	7.54
b	37.00	$9.99 \cdot 10^{-3}$	$9.51 \cdot 10^{-3}$	-2.02	10.4	0.69	7.56
3a	37.00	$3.00 \cdot 10^{-3}$	$2.79 \cdot 10^{-3}$	-2.55	10.4	0.86	7.50
b	37.00	$3.00 \cdot 10^{-3}$	$2.77 \cdot 10^{-3}$	-2.56	10.4	0.90	7.55
4a	37.00	$9.99 \cdot 10^{-4}$	$9.20 \cdot 10^{-4}$	-3.04	10.4	0.91	7.46
b	37.00	$9.99 \cdot 10^{-4}$	$9.20 \cdot 10^{-4}$	-3.04	10.4	0.91	7.48
5a	37.00	$3.33 \cdot 10^{-4}$	$2.97 \cdot 10^{-4}$	-3.53	10.4	1.07	7.54
b	37.00	$3.33 \cdot 10^{-4}$	$2.93 \cdot 10^{-4}$	-3.53	10.4	1.11	7.55
6a	37.00	$9.99 \cdot 10^{-5}$	$8.18 \cdot 10^{-5}$	-4.09	10.4	1.33	7.47
b	37.00	$9.99 \cdot 10^{-5}$	$8.28 \cdot 10^{-5}$	-4.08	10.4	1.30	7.54
7a	37.00	$3.00 \cdot 10^{-5}$	$2.32 \cdot 10^{-5}$	-4.63	10.4	1.45	7.47
b	37.00	$3.00 \cdot 10^{-5}$	$2.35 \cdot 10^{-5}$	-4.63	10.4	1.42	7.51
8a	37.00	$9.99 \cdot 10^{-6}$	$6.85 \cdot 10^{-6}$	-5.16	10.4	1.64	7.49
b	37.00	$9.99 \cdot 10^{-6}$	$6.87 \cdot 10^{-6}$	-5.16	10.4	1.64	7.41
9a	37.00	$3.33 \cdot 10^{-6}$	$1.73 \cdot 10^{-6}$	-5.76	10.4	1.95	7.48
b	37.00	$3.33 \cdot 10^{-6}$	$1.68 \cdot 10^{-6}$	-5.78	10.4	1.97	7.40
10a	37.00	$9.99 \cdot 10^{-7}$	$3.00 \cdot 10^{-7}$	-6.52	10.4	2.35	7.47
b	37.00	$9.99 \cdot 10^{-7}$	$2.73 \cdot 10^{-7}$	-6.56	10.4	2.41	7.52
11a	37.00	$3.00 \cdot 10^{-7}$	$4.34 \cdot 10^{-8}$	-7.36	189.2	2.75	7.46
b	37.00	$3.00 \cdot 10^{-7}$	$4.37 \cdot 10^{-8}$	-7.36	189.2	2.75	7.36
12a	37.00	$1.00 \cdot 10^{-7}$	$1.04 \cdot 10^{-8}$	-7.98	189.2	2.92	7.37
b	37.00	$1.00 \cdot 10^{-7}$	$1.11 \cdot 10^{-8}$	-7.95	189.2	2.89	7.43
13a	37.00	$3.38 \cdot 10^{-8}$	$3.11 \cdot 10^{-9}$	-8.51	189.2	2.98	7.38
b	37.00	$3.38 \cdot 10^{-8}$	$3.13 \cdot 10^{-9}$	-8.50	189.2	2.97	7.35
14a	37.00	$1.04 \cdot 10^{-8}$	$9.65 \cdot 10^{-10}$	-9.02	189.2	2.97	7.46
b	37.00	$1.04 \cdot 10^{-8}$	$9.56 \cdot 10^{-10}$	-9.02	189.2	2.98	7.37
15a	37.00	$3.45 \cdot 10^{-9}$	$3.12 \cdot 10^{-10}$	-9.51	189.2	2.98	7.38
b	37.00	$3.45 \cdot 10^{-9}$	$3.27 \cdot 10^{-10}$	-9.49	189.2	2.96	7.33
16a	37.00	$1.45 \cdot 10^{-9}$	$1.46 \cdot 10^{-10}$	-9.83	189.2	2.93	7.43
b	37.00	$1.45 \cdot 10^{-9}$	$1.34 \cdot 10^{-10}$	-9.87	189.2	2.98	7.42

Tab. A-10: 10xperimental data for Cs on sample BUL-955 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37.00	$3.33 \cdot 10$	$3.24 \cdot 10$	-1.49	10.4	0.42	7.49
b	37.00	$3.33 \cdot 10$	$3.25 \cdot 10$	-1.49	10.4	0.37	7.52
2a	37.00	$9.99 \cdot 10^{-3}$	$9.41 \cdot 10^{-3}$	-2.03	10.4	0.77	7.54
b	37.00	$9.99 \cdot 10^{-3}$	$9.39 \cdot 10^{-3}$	-2.03	10.4	0.79	7.56
3a	37.00	$3.00 \cdot 10^{-3}$	$2.68 \cdot 10^{-3}$	-2.57	10.4	1.06	7.50
b	37.00	$3.00 \cdot 10^{-3}$	$2.68 \cdot 10^{-3}$	-2.57	10.4	1.05	7.55
4a	37.00	$9.99 \cdot 10^{-4}$	$8.75 \cdot 10^{-4}$	-3.06	10.4	1.13	7.46
b	37.00	$9.99 \cdot 10^{-4}$	$8.76 \cdot 10^{-4}$	-3.06	10.4	1.13	7.48
5a	37.00	$3.33 \cdot 10^{-4}$	$2.77 \cdot 10^{-4}$	-3.56	10.4	1.29	7.54
b	37.00	$3.33 \cdot 10^{-4}$	$2.78 \cdot 10^{-4}$	-3.56	10.4	1.28	7.55
6a	37.00	$9.99 \cdot 10^{-5}$	$7.74 \cdot 10^{-5}$	-4.11	10.4	1.45	7.47
b	37.00	$9.99 \cdot 10^{-5}$	$7.80 \cdot 10^{-5}$	-4.11	10.4	1.43	7.54
7a	37.00	$3.00 \cdot 10^{-5}$	$2.08 \cdot 10^{-5}$	-4.68	10.4	1.63	7.47
b	37.00	$3.00 \cdot 10^{-5}$	$2.08 \cdot 10^{-5}$	-4.68	10.4	1.63	7.51
8a	37.00	$9.99 \cdot 10^{-6}$	$5.84 \cdot 10^{-6}$	-5.23	10.4	1.83	7.49
b	37.00	$9.99 \cdot 10^{-6}$	$5.80 \cdot 10^{-6}$	-5.24	10.4	1.84	7.41
9a	37.00	$3.33 \cdot 10^{-6}$	$1.34 \cdot 10^{-6}$	-5.87	10.4	2.16	7.48
b	37.00	$3.33 \cdot 10^{-6}$	$1.33 \cdot 10^{-6}$	-5.87	10.4	2.16	7.40
10a	37.00	$9.99 \cdot 10^{-7}$	$1.84 \cdot 10^{-7}$	-6.74	10.4	2.63	7.47
b	37.00	$9.99 \cdot 10^{-7}$	$1.80 \cdot 10^{-7}$	-6.74	10.4	2.64	7.52
11a	37.00	$3.00 \cdot 10^{-7}$	$3.06 \cdot 10^{-8}$	-7.51	10.4	2.93	7.46
b	37.00	$3.00 \cdot 10^{-7}$	$2.99 \cdot 10^{-8}$	-7.52	10.4	2.94	7.36
12a	37.00	$1.00 \cdot 10^{-7}$	$7.71 \cdot 10^{-9}$	-8.11	10.4	3.06	7.37
b	37.00	$1.00 \cdot 10^{-7}$	$7.53 \cdot 10^{-9}$	-8.12	10.4	3.07	7.43
13a	37.00	$3.38 \cdot 10^{-8}$	$2.56 \cdot 10^{-9}$	-8.59	10.4	3.07	7.38
b	37.00	$3.38 \cdot 10^{-8}$	$2.39 \cdot 10^{-9}$	-8.62	10.4	3.10	7.35
14a	37.00	$1.04 \cdot 10^{-8}$	$7.35 \cdot 10^{-10}$	-9.13	10.4	3.10	7.46
b	37.00	$1.04 \cdot 10^{-8}$	$7.38 \cdot 10^{-10}$	-9.13	10.4	3.10	7.37
15a	37.00	$3.45 \cdot 10^{-9}$	$2.38 \cdot 10^{-10}$	-9.62	10.4	3.11	7.38
b	37.00	$3.45 \cdot 10^{-9}$	$2.35 \cdot 10^{-10}$	-9.63	10.4	3.12	7.33
16a	37.00	$1.45 \cdot 10^{-9}$	$9.98 \cdot 10^{-11}$	-10.00	10.4	3.11	7.43
b	37.00	$1.45 \cdot 10^{-9}$	$1.04 \cdot 10^{-10}$	-9.98	10.4	3.09	7.42

Tab. A-11: Experimental data for Cs on sample BUL-995 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$2.85 \cdot 10$	$2.77 \cdot 10$	-1.56	6.4	0.68	7.63
b	35.00	$2.85 \cdot 10$	$2.78 \cdot 10$	-1.56	6.4	0.65	7.63
2a	35.00	$8.57 \cdot 10^{-3}$	$8.17 \cdot 10^{-3}$	-2.09	6.4	0.88	7.62
b	35.00	$8.57 \cdot 10^{-3}$	$8.19 \cdot 10^{-3}$	-2.09	6.4	0.87	7.61
3a	35.00	$2.57 \cdot 10^{-3}$	$2.42 \cdot 10^{-3}$	-2.62	6.4	0.98	7.63
b	35.00	$2.57 \cdot 10^{-3}$	$2.41 \cdot 10^{-3}$	-2.62	6.4	1.01	7.63
4a	35.00	$8.57 \cdot 10^{-4}$	$7.80 \cdot 10^{-4}$	-3.11	6.4	1.18	7.63
b	35.00	$8.57 \cdot 10^{-4}$	$7.78 \cdot 10^{-4}$	-3.11	6.4	1.20	7.63
5a	35.00	$2.57 \cdot 10^{-4}$	$2.27 \cdot 10^{-4}$	-3.64	6.4	1.32	7.62
b	35.00	$2.57 \cdot 10^{-4}$	$2.28 \cdot 10^{-4}$	-3.64	6.4	1.30	7.61
6a	35.00	$8.57 \cdot 10^{-5}$	$7.30 \cdot 10^{-5}$	-4.14	6.4	1.43	7.63
b	35.00	$8.57 \cdot 10^{-5}$	$7.26 \cdot 10^{-5}$	-4.14	6.4	1.45	7.62
7a	35.00	$2.57 \cdot 10^{-5}$	$2.07 \cdot 10^{-5}$	-4.68	6.4	1.57	7.62
b	35.00	$2.57 \cdot 10^{-5}$	$2.06 \cdot 10^{-5}$	-4.69	6.4	1.59	7.62
8a	35.00	$8.57 \cdot 10^{-6}$	$5.93 \cdot 10^{-6}$	-5.23	6.4	1.84	7.62
b	35.00	$8.57 \cdot 10^{-6}$	$6.24 \cdot 10^{-6}$	-5.20	6.4	1.76	7.58
9a	35.00	$2.57 \cdot 10^{-6}$	$1.40 \cdot 10^{-6}$	-5.85	6.4	2.11	7.61
b	35.00	$2.57 \cdot 10^{-6}$	$1.34 \cdot 10^{-6}$	-5.87	6.4	2.15	7.61
10a	35.00	$8.58 \cdot 10^{-7}$	$2.85 \cdot 10^{-7}$	-6.55	6.4	2.49	7.62
b	35.00	$8.58 \cdot 10^{-7}$	$2.72 \cdot 10^{-7}$	-6.57	6.4	2.53	7.60
11a	35.00	$2.58 \cdot 10^{-7}$	$4.81 \cdot 10^{-8}$	-7.32	6.4	2.83	7.61
b	35.00	$2.58 \cdot 10^{-7}$	$4.85 \cdot 10^{-8}$	-7.31	6.4	2.83	7.61
12a	35.00	$8.64 \cdot 10^{-8}$	$1.14 \cdot 10^{-8}$	-7.94	6.4	3.01	7.62
b	35.00	$8.64 \cdot 10^{-8}$	$1.13 \cdot 10^{-8}$	-7.95	6.4	3.01	7.62
13a	35.00	$2.64 \cdot 10^{-8}$	$3.21 \cdot 10^{-9}$	-8.49	6.4	3.05	7.61
b	35.00	$2.64 \cdot 10^{-8}$	$3.04 \cdot 10^{-9}$	-8.52	6.4	3.08	7.62
14a	35.00	$9.29 \cdot 10^{-9}$	$1.05 \cdot 10^{-9}$	-8.98	6.4	3.09	7.60
b	35.00	$9.29 \cdot 10^{-9}$	$1.02 \cdot 10^{-9}$	-8.99	6.4	3.10	7.62
15a	35.00	$3.29 \cdot 10^{-9}$	$3.45 \cdot 10^{-10}$	-9.46	6.4	3.12	7.60
b	35.00	$3.29 \cdot 10^{-9}$	$3.27 \cdot 10^{-10}$	-9.49	6.4	3.15	7.61
16a	35.00	$1.57 \cdot 10^{-9}$	$1.52 \cdot 10^{-10}$	-9.82	6.4	3.16	7.59
b	35.00	$1.57 \cdot 10^{-9}$	$1.50 \cdot 10^{-10}$	-9.82	6.4	3.17	7.59

Tab. A-12: Experimental data for Cs on sample BUL-1002 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37.00	$3.33 \cdot 10$	$3.29 \cdot 10$	-1.48	9.2	0.12	7.49
b	37.00	$3.33 \cdot 10$	$3.30 \cdot 10$	-1.48	9.2	-0.04	7.52
2a	37.00	$9.99 \cdot 10^{-3}$	$9.81 \cdot 10^{-3}$	-2.01	9.2	0.29	7.54
b	37.00	$9.99 \cdot 10^{-3}$	$9.78 \cdot 10^{-3}$	-2.01	9.2	0.36	7.56
3a	37.00	$3.00 \cdot 10^{-3}$	$2.88 \cdot 10^{-3}$	-2.54	9.2	0.66	7.5
b	37.00	$3.00 \cdot 10^{-3}$	$2.85 \cdot 10^{-3}$	-2.55	9.2	0.76	7.55
4a	37.00	$9.99 \cdot 10^{-4}$	$9.30 \cdot 10^{-4}$	-3.03	9.2	0.91	7.46
b	37.00	$9.99 \cdot 10^{-4}$	$9.33 \cdot 10^{-4}$	-3.03	9.2	0.88	7.48
5a	37.00	$3.33 \cdot 10^{-4}$	$2.97 \cdot 10^{-4}$	-3.53	9.2	1.11	7.54
b	37.00	$3.33 \cdot 10^{-4}$	$2.98 \cdot 10^{-4}$	-3.53	9.2	1.10	7.55
6a	37.00	$9.99 \cdot 10^{-5}$	$8.52 \cdot 10^{-5}$	-4.07	9.2	1.27	7.47
b	37.00	$9.99 \cdot 10^{-5}$	$7.71 \cdot 10^{-5}$	-4.11	9.2	1.51	7.54
7a	37.00	$3.00 \cdot 10^{-5}$	$2.38 \cdot 10^{-5}$	-4.62	9.2	1.45	7.47
b	37.00	$3.00 \cdot 10^{-5}$	$2.39 \cdot 10^{-5}$	-4.62	9.2	1.44	7.51
8a	37.00	$9.99 \cdot 10^{-6}$	$7.14 \cdot 10^{-6}$	-5.15	9.2	1.64	7.49
b	37.00	$9.99 \cdot 10^{-6}$	$6.97 \cdot 10^{-6}$	-5.16	9.2	1.67	7.41
9a	37.00	$3.33 \cdot 10^{-6}$	$1.91 \cdot 10^{-6}$	-5.72	9.2	1.90	7.48
b	37.00	$3.33 \cdot 10^{-6}$	$1.95 \cdot 10^{-6}$	-5.71	9.2	1.89	7.40
10a	37.00	$9.99 \cdot 10^{-7}$	$3.72 \cdot 10^{-7}$	-6.43	9.2	2.26	7.47
b	37.00	$9.99 \cdot 10^{-7}$	$3.50 \cdot 10^{-7}$	-6.46	9.2	2.30	7.52
11a	37.00	$3.00 \cdot 10^{-7}$	$5.77 \cdot 10^{-8}$	-7.24	9.2	2.66	7.46
b	37.00	$3.00 \cdot 10^{-7}$	$6.14 \cdot 10^{-8}$	-7.21	9.2	2.62	7.36
12a	37.00	$1.00 \cdot 10^{-7}$	$1.40 \cdot 10^{-8}$	-7.85	9.2	2.82	7.37
b	37.00	$1.00 \cdot 10^{-7}$	$1.45 \cdot 10^{-8}$	-7.84	9.2	2.81	7.43
13a	37.00	$3.38 \cdot 10^{-8}$	$4.11 \cdot 10^{-9}$	-8.39	9.2	2.89	7.38
b	37.00	$3.38 \cdot 10^{-8}$	$3.94 \cdot 10^{-9}$	-8.40	9.2	2.91	7.35
14a	37.00	$1.04 \cdot 10^{-8}$	$1.24 \cdot 10^{-9}$	-8.91	9.2	2.91	7.46
b	37.00	$1.04 \cdot 10^{-8}$	$1.23 \cdot 10^{-9}$	-8.91	9.2	2.91	7.37
15a	37.00	$3.45 \cdot 10^{-9}$	$4.12 \cdot 10^{-10}$	-9.38	9.2	2.90	7.38
b	37.00	$3.45 \cdot 10^{-9}$	$4.86 \cdot 10^{-10}$	-9.31	9.2	2.82	7.33
16a	37.00	$1.45 \cdot 10^{-9}$	$1.90 \cdot 10^{-10}$	-9.72	9.2	2.86	7.43
b	37.00	$1.45 \cdot 10^{-9}$	$1.86 \cdot 10^{-10}$	-9.73	9.2	2.87	7.42

Tab. A-13: Experimental data for Cs on sample BUL-1017 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37.00	$3.33 \cdot 10$	$3.31 \cdot 10$	-1.48	6.4	-0.07	7.49
b	37.00	$3.33 \cdot 10$	$3.24 \cdot 10$	-1.49	6.4	0.62	7.52
2a	37.00	$9.99 \cdot 10^{-3}$	$9.55 \cdot 10^{-3}$	-2.02	6.4	0.85	7.54
b	37.00	$9.99 \cdot 10^{-3}$	$9.70 \cdot 10^{-3}$	-2.01	6.4	0.68	7.56
3a	37.00	$3.00 \cdot 10^{-3}$	$2.83 \cdot 10^{-3}$	-2.55	6.4	0.97	7.50
b	37.00	$3.00 \cdot 10^{-3}$	$2.84 \cdot 10^{-3}$	-2.55	6.4	0.95	7.55
4a	37.00	$9.99 \cdot 10^{-4}$	$9.43 \cdot 10^{-4}$	-3.03	6.4	0.97	7.46
b	37.00	$9.99 \cdot 10^{-4}$	$9.21 \cdot 10^{-4}$	-3.04	6.4	1.12	7.48
5a	37.00	$3.33 \cdot 10^{-4}$	$3.04 \cdot 10^{-4}$	-3.52	6.4	1.18	7.54
b	37.00	$3.33 \cdot 10^{-4}$	$3.08 \cdot 10^{-4}$	-3.51	6.4	1.11	7.55
6a	37.00	$9.99 \cdot 10^{-5}$	$9.06 \cdot 10^{-5}$	-4.04	6.4	1.21	7.47
b	37.00	$9.99 \cdot 10^{-5}$	$8.81 \cdot 10^{-5}$	-4.06	6.4	1.32	7.54
7a	37.00	$3.00 \cdot 10^{-5}$	$2.52 \cdot 10^{-5}$	-4.60	6.4	1.47	7.47
b	37.00	$3.00 \cdot 10^{-5}$	$2.53 \cdot 10^{-5}$	-4.60	6.4	1.46	7.51
8a	37.00	$9.99 \cdot 10^{-6}$	$7.60 \cdot 10^{-6}$	-5.12	6.4	1.69	7.49
b	37.00	$9.99 \cdot 10^{-6}$	$7.25 \cdot 10^{-6}$	-5.14	6.4	1.77	7.41
9a	37.00	$3.33 \cdot 10^{-6}$	$1.94 \cdot 10^{-6}$	-5.71	6.4	2.05	7.48
b	37.00	$3.33 \cdot 10^{-6}$	$1.94 \cdot 10^{-6}$	-5.71	6.4	2.05	7.40
10a	37.00	$9.99 \cdot 10^{-7}$	$3.41 \cdot 10^{-7}$	-6.47	6.4	2.48	7.47
b	37.00	$9.99 \cdot 10^{-7}$	$3.20 \cdot 10^{-7}$	-6.49	6.4	2.52	7.52
11a	37.00	$3.00 \cdot 10^{-7}$	$8.18 \cdot 10^{-8}$	-7.09	6.4	2.62	7.46
b	37.00	$3.00 \cdot 10^{-7}$	$7.31 \cdot 10^{-8}$	-7.14	6.4	2.69	7.36
12a	37.00	$1.00 \cdot 10^{-7}$	$1.81 \cdot 10^{-8}$	-7.74	6.4	2.85	7.37
b	37.00	$1.00 \cdot 10^{-7}$	$2.46 \cdot 10^{-8}$	-7.61	6.4	2.68	7.43
13a	37.00	$3.37 \cdot 10^{-8}$	$5.47 \cdot 10^{-9}$	-8.26	6.4	2.91	7.38
b	37.00	$3.37 \cdot 10^{-8}$	$5.40 \cdot 10^{-9}$	-8.27	6.4	2.91	7.35
14a	37.00	$1.04 \cdot 10^{-8}$	$1.59 \cdot 10^{-9}$	-8.80	6.4	2.94	7.46
b	37.00	$1.04 \cdot 10^{-8}$	$1.66 \cdot 10^{-9}$	-8.78	6.4	2.91	7.37
15a	37.00	$3.36 \cdot 10^{-9}$	$5.23 \cdot 10^{-10}$	-9.28	6.4	2.93	7.38
b	37.00	$3.36 \cdot 10^{-9}$	$4.71 \cdot 10^{-10}$	-9.33	6.4	2.98	7.33
16a	37.00	$1.37 \cdot 10^{-9}$	$2.00 \cdot 10^{-10}$	-9.70	6.4	2.96	7.43
b	37.00	$1.37 \cdot 10^{-9}$	$1.68 \cdot 10^{-10}$	-9.77	6.4	3.05	7.42

A.3 Experimental data for Cs on TRU1-1 samples

Tab. A-14: Experimental data for Cs on sample TRU-748 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37.00	$3.33 \cdot 10$	$3.07 \cdot 10$	-1.51	18.1	0.66	7.60
b	37.00	$3.33 \cdot 10$	$3.09 \cdot 10$	-1.51	18.1	0.64	7.58
2a	37.00	$3.33 \cdot 10^{-3}$	$2.74 \cdot 10^{-3}$	-2.56	18.1	1.08	7.59
b	37.00	$3.33 \cdot 10^{-3}$	$2.73 \cdot 10^{-3}$	-2.56	18.1	1.08	7.63
3a	37.00	$3.33 \cdot 10^{-4}$	$2.35 \cdot 10^{-4}$	-3.63	18.1	1.37	7.60
b	37.00	$3.33 \cdot 10^{-4}$	$2.33 \cdot 10^{-4}$	-3.63	18.1	1.37	7.59
4a	37.00	$3.33 \cdot 10^{-5}$	$1.76 \cdot 10^{-5}$	-4.75	18.1	1.69	7.53
b	37.00	$3.33 \cdot 10^{-5}$	$1.89 \cdot 10^{-5}$	-4.72	18.1	1.63	7.56
5a	37.00	$1.12 \cdot 10^{-5}$	$6.00 \cdot 10^{-6}$	-5.22	12.0	1.85	7.63
b	37.00	$1.12 \cdot 10^{-5}$	$5.99 \cdot 10^{-6}$	-5.22	12.0	1.85	7.58
6a	37.00	$3.33 \cdot 10^{-6}$	$1.14 \cdot 10^{-6}$	-5.94	12.0	2.20	7.61
b	37.00	$3.33 \cdot 10^{-6}$	$1.19 \cdot 10^{-6}$	-5.92	12.0	2.17	7.55
7a	37.00	$1.12 \cdot 10^{-6}$	$2.12 \cdot 10^{-7}$	-6.67	12.0	2.55	7.56
b	37.00	$1.12 \cdot 10^{-6}$	$2.03 \cdot 10^{-7}$	-6.69	12.0	2.57	7.64
8a	37.00	$3.33 \cdot 10^{-7}$	$3.63 \cdot 10^{-8}$	-7.44	12.0	2.83	7.51
b	37.00	$3.33 \cdot 10^{-7}$	$3.56 \cdot 10^{-8}$	-7.45	12.0	2.84	7.61
9a	37.00	$3.38 \cdot 10^{-8}$	$2.88 \cdot 10^{-9}$	-8.54	12.0	2.95	7.62
b	37.00	$3.38 \cdot 10^{-8}$	$3.09 \cdot 10^{-9}$	-8.51	12.0	2.92	7.68
10a	37.00	$1.59 \cdot 10^{-9}$	$1.47 \cdot 10^{-10}$	-9.83	12.0	2.91	7.66
b	37.00	$1.59 \cdot 10^{-9}$	$1.31 \cdot 10^{-10}$	-9.88	12.0	2.97	7.65

Tab. A-15: Experimental data for Cs on sample TRU-794 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37.00	$3.33 \cdot 10$	$3.06 \cdot 10$	-1.51	17.9	0.69	7.64
b	37.00	$3.33 \cdot 10$	$3.02 \cdot 10$	-1.52	17.9	0.76	7.65
2a	37.00	$3.33 \cdot 10^{-3}$	$2.68 \cdot 10^{-3}$	-2.57	17.9	1.13	7.56
b	37.00	$3.33 \cdot 10^{-3}$	$2.68 \cdot 10^{-3}$	-2.57	17.9	1.14	7.60
3a	37.00	$3.33 \cdot 10^{-4}$	$2.29 \cdot 10^{-4}$	-3.64	17.9	1.40	7.60
b	37.00	$3.33 \cdot 10^{-4}$	$2.29 \cdot 10^{-4}$	-3.64	17.9	1.40	7.60
4a	37.00	$3.33 \cdot 10^{-5}$	$1.69 \cdot 10^{-5}$	-4.77	17.9	1.74	7.63
b	37.00	$3.33 \cdot 10^{-5}$	$1.70 \cdot 10^{-5}$	-4.77	17.9	1.73	7.66
5a	37.00	$1.12 \cdot 10^{-5}$	$5.73 \cdot 10^{-6}$	-5.24	11.9	1.90	7.60
b	37.00	$1.12 \cdot 10^{-5}$	$5.75 \cdot 10^{-6}$	-5.24	11.9	1.90	7.62
6a	37.00	$3.33 \cdot 10^{-6}$	$1.00 \cdot 10^{-6}$	-6.00	11.9	2.29	7.63
b	37.00	$3.33 \cdot 10^{-6}$	$1.00 \cdot 10^{-6}$	-6.00	11.9	2.29	7.64
7a	37.00	$1.12 \cdot 10^{-6}$	$1.52 \cdot 10^{-7}$	-6.82	11.9	2.73	7.55
b	37.00	$1.12 \cdot 10^{-6}$	$1.57 \cdot 10^{-7}$	-6.80	11.9	2.71	7.60
8a	37.00	$3.33 \cdot 10^{-7}$	$2.66 \cdot 10^{-8}$	-7.58	11.9	2.99	7.60
b	37.00	$3.33 \cdot 10^{-7}$	$2.62 \cdot 10^{-8}$	-7.58	11.9	2.99	7.58
9a	37.00	$3.38 \cdot 10^{-8}$	$2.09 \cdot 10^{-9}$	-8.68	11.9	3.10	7.67
b	37.00	$3.38 \cdot 10^{-8}$	$2.26 \cdot 10^{-9}$	-8.65	11.9	3.07	7.70
10a	37.00	$1.59 \cdot 10^{-9}$	$9.93 \cdot 10^{-11}$	-10.00	11.9	3.10	7.70
b	37.00	$1.59 \cdot 10^{-9}$	$1.00 \cdot 10^{-10}$	-10.00	11.9	3.09	7.73

Tab. A-16: Experimental data for Cs on sample TRU-815 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37.00	$3.33 \cdot 10$	$3.26 \cdot 10$	-1.49	12.5	0.25	7.63
b	37.00	$3.33 \cdot 10$	$3.23 \cdot 10$	-1.49	12.5	0.37	7.64
2a	37.00	$3.33 \cdot 10^{-3}$	$3.08 \cdot 10^{-3}$	-2.51	12.5	0.81	7.66
b	37.00	$3.33 \cdot 10^{-3}$	$3.06 \cdot 10^{-3}$	-2.51	12.5	0.85	7.63
3a	37.00	$3.33 \cdot 10^{-4}$	$2.82 \cdot 10^{-4}$	-3.55	12.5	1.16	7.64
b	37.00	$3.33 \cdot 10^{-4}$	$2.81 \cdot 10^{-4}$	-3.55	12.5	1.17	7.64
4a	37.00	$3.33 \cdot 10^{-5}$	$2.42 \cdot 10^{-5}$	-4.62	12.5	1.48	7.63
b	37.00	$3.33 \cdot 10^{-5}$	$2.40 \cdot 10^{-5}$	-4.62	12.5	1.49	7.64
5a	37.00	$1.12 \cdot 10^{-5}$	$8.82 \cdot 10^{-6}$	-5.05	8.3	1.50	7.65
b	37.00	$1.12 \cdot 10^{-5}$	$8.76 \cdot 10^{-6}$	-5.06	8.3	1.52	7.64
6a	37.00	$3.33 \cdot 10^{-6}$	$1.99 \cdot 10^{-6}$	-5.70	8.3	1.91	7.69
b	37.00	$3.33 \cdot 10^{-6}$	$1.97 \cdot 10^{-6}$	-5.71	8.3	1.92	7.65
7a	37.00	$1.12 \cdot 10^{-6}$	$4.28 \cdot 10^{-7}$	-6.37	8.3	2.28	7.67
b	37.00	$1.12 \cdot 10^{-6}$	$4.26 \cdot 10^{-7}$	-6.37	8.3	2.29	7.65
8a	37.00	$3.33 \cdot 10^{-7}$	$6.86 \cdot 10^{-8}$	-7.16	8.3	2.67	7.63
b	37.00	$3.33 \cdot 10^{-7}$	$6.80 \cdot 10^{-8}$	-7.17	8.3	2.67	7.68
9a	37.00	$3.38 \cdot 10^{-8}$	$4.13 \cdot 10^{-9}$	-8.38	8.3	2.93	7.63
b	37.00	$3.38 \cdot 10^{-8}$	$3.99 \cdot 10^{-9}$	-8.40	8.3	2.95	7.65
10a	37.00	$1.59 \cdot 10^{-9}$	$1.87 \cdot 10^{-10}$	-9.73	8.3	2.95	7.61
b	37.00	$1.59 \cdot 10^{-9}$	$1.63 \cdot 10^{-10}$	-9.79	8.3	3.02	7.66

Tab. A-17: Experimental data for Cs on sample TRU-831 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37.00	$3.33 \cdot 10$	$3.04 \cdot 10$	-1.52	17.5	0.74	7.51
b	37.00	$3.33 \cdot 10$	$3.03 \cdot 10$	-1.52	17.5	0.75	7.51
2a	37.00	$3.33 \cdot 10^{-3}$	$2.59 \cdot 10^{-3}$	-2.59	17.5	1.21	7.40
b	37.00	$3.33 \cdot 10^{-3}$	$2.54 \cdot 10^{-3}$	-2.60	17.5	1.25	7.53
3a	37.00	$3.33 \cdot 10^{-4}$	$2.11 \cdot 10^{-4}$	-3.68	17.5	1.52	7.55
b	37.00	$3.33 \cdot 10^{-4}$	$2.14 \cdot 10^{-4}$	-3.67	17.5	1.50	7.48
4a	37.00	$3.33 \cdot 10^{-5}$	$1.48 \cdot 10^{-5}$	-4.83	17.5	1.85	7.56
b	37.00	$3.33 \cdot 10^{-5}$	$1.47 \cdot 10^{-5}$	-4.83	17.5	1.86	7.50
5a	37.00	$1.12 \cdot 10^{-5}$	$5.99 \cdot 10^{-6}$	-5.22	11.7	1.87	7.56
b	37.00	$1.12 \cdot 10^{-5}$	$5.98 \cdot 10^{-6}$	-5.22	11.7	1.87	7.53
6a	37.00	$3.33 \cdot 10^{-6}$	$8.03 \cdot 10^{-7}$	-6.10	11.7	2.43	7.57
b	37.00	$3.33 \cdot 10^{-6}$	$7.78 \cdot 10^{-7}$	-6.11	11.7	2.45	7.53
7a	37.00	$1.12 \cdot 10^{-6}$	$1.11 \cdot 10^{-7}$	-6.95	11.7	2.89	7.58
b	37.00	$1.12 \cdot 10^{-6}$	$1.15 \cdot 10^{-7}$	-6.94	11.7	2.87	7.57
8a	37.00	$3.33 \cdot 10^{-7}$	$1.96 \cdot 10^{-8}$	-7.71	11.7	3.14	7.54
b	37.00	$3.33 \cdot 10^{-7}$	$1.86 \cdot 10^{-8}$	-7.73	11.7	3.16	7.56
9a	37.00	$3.38 \cdot 10^{-8}$	$1.45 \cdot 10^{-9}$	-8.84	11.7	3.28	7.56
b	37.00	$3.38 \cdot 10^{-8}$	$1.45 \cdot 10^{-9}$	-8.84	11.7	3.28	7.55
10a	37.00	$1.59 \cdot 10^{-9}$	$6.35 \cdot 10^{-11}$	-10.20	11.7	3.31	7.54
b	37.00	$1.59 \cdot 10^{-9}$	$6.57 \cdot 10^{-11}$	-10.18	11.7	3.30	7.50

Tab. A-18: Experimental data for Cs on sample TRU-882 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	32.00	3.00E	2.61E	-1.58	25.7	0.76	7.53
b	32.00	3.00E	2.63E	-1.58	25.7	0.74	7.53
2a	32.00	$3.00E^{-3}$	$2.22E^{-3}$	-2.65	25.7	1.14	7.57
b	32.00	$3.00E^{-3}$	$2.20E^{-3}$	-2.66	25.7	1.15	7.55
3a	32.00	$3.00E^{-4}$	$1.88E^{-4}$	-3.73	25.7	1.37	7.60
b	32.00	$3.00E^{-4}$	$1.76E^{-4}$	-3.75	25.7	1.44	7.59
4a	32.00	$3.00E^{-5}$	$1.17E^{-5}$	-4.93	25.7	1.78	7.55
b	32.00	$3.00E^{-5}$	$1.18E^{-5}$	-4.93	25.7	1.78	7.53
5a	32.00	$1.01E^{-5}$	$5.01E^{-6}$	-5.30	12.8	1.89	7.61
b	32.00	$1.01E^{-5}$	$5.59E^{-6}$	-5.25	12.8	1.79	7.61
6a	32.00	$3.00E^{-6}$	$1.09E^{-6}$	-5.96	12.8	2.14	7.63
b	32.00	$3.00E^{-6}$	$1.12E^{-6}$	-5.95	12.8	2.12	7.63
7a	32.00	$1.01E^{-6}$	$1.24E^{-7}$	-6.91	12.8	2.75	7.63
b	32.00	$1.01E^{-6}$	$1.19E^{-7}$	-6.92	12.8	2.76	7.62
8a	32.00	$3.00E^{-7}$	$2.43E^{-8}$	-7.61	12.8	2.95	7.47
b	32.00	$3.00E^{-7}$	$2.53E^{-8}$	-7.60	12.8	2.93	7.48
9a	32.00	$3.05E^{-8}$	$1.43E^{-9}$	-8.84	12.8	3.20	7.55
b	32.00	$3.05E^{-8}$	$1.47E^{-9}$	-8.83	12.8	3.19	7.49
10a	32.00	$1.48E^{-9}$	$5.78E^{-11}$	-10.24	12.8	3.28	7.61
b	32.00	$1.48E^{-9}$	$6.15E^{-11}$	-10.21	12.8	3.25	7.62

Tab. A-19: Experimental data for Cs on sample TRU-923 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	32.00	$3.00 \cdot 10$	$2.61 \cdot 10$	-1.58	22.1	0.83	7.57
b	32.00	$3.00 \cdot 10$	$2.58 \cdot 10$	-1.59	22.1	0.86	7.58
2a	32.00	$3.00 \cdot 10^{-3}$	$2.12 \cdot 10^{-3}$	-2.67	22.1	1.28	7.59
b	32.00	$3.00 \cdot 10^{-3}$	$2.09 \cdot 10^{-3}$	-2.68	22.1	1.29	7.59
3a	32.00	$3.00 \cdot 10^{-4}$	$1.83 \cdot 10^{-4}$	-3.74	22.1	1.46	7.60
b	32.00	$3.00 \cdot 10^{-4}$	$1.74 \cdot 10^{-4}$	-3.76	22.1	1.51	7.56
4a	32.00	$3.00 \cdot 10^{-5}$	$1.05 \cdot 10^{-5}$	-4.98	22.1	1.92	7.62
b	32.00	$3.00 \cdot 10^{-5}$	$1.05 \cdot 10^{-5}$	-4.98	22.1	1.92	7.62
5a	32.00	$1.01 \cdot 10^{-5}$	$5.31 \cdot 10^{-6}$	-5.27	11.1	1.91	7.64
b	32.00	$1.01 \cdot 10^{-5}$	$4.93 \cdot 10^{-6}$	-5.31	11.1	1.97	7.64
6a	32.00	$3.00 \cdot 10^{-6}$	$1.11 \cdot 10^{-6}$	-5.96	11.1	2.19	7.66
b	32.00	$3.00 \cdot 10^{-6}$	$1.01 \cdot 10^{-6}$	-6.00	11.1	2.25	7.59
7a	32.00	$1.01 \cdot 10^{-6}$	$1.17 \cdot 10^{-7}$	-6.93	11.1	2.83	7.64
b	32.00	$1.01 \cdot 10^{-6}$	$1.15 \cdot 10^{-7}$	-6.94	11.1	2.84	7.61
8a	32.00	$3.00 \cdot 10^{-7}$	$2.19 \cdot 10^{-8}$	-7.66	11.1	3.06	7.63
b	32.00	$3.00 \cdot 10^{-7}$	$2.06 \cdot 10^{-8}$	-7.69	11.1	3.09	7.63
9a	32.00	$3.05 \cdot 10^{-8}$	$1.38 \cdot 10^{-9}$	-8.86	11.1	3.28	7.62
b	32.00	$3.05 \cdot 10^{-8}$	$1.61 \cdot 10^{-9}$	-8.79	11.1	3.21	7.60
10a	32.00	$1.48 \cdot 10^{-9}$	$6.36 \cdot 10^{-11}$	-10.20	11.1	3.30	7.62
b	32.00	$1.48 \cdot 10^{-9}$	$6.40 \cdot 10^{-11}$	-10.19	11.1	3.30	7.62

Tab. A-20: Experimental data for Cs on sample TRU-938 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Cs_{in}** (M)	**Cs_{aq}** (M)	**Log Cs_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	32.00	$3.00 \cdot 10$	$2.72 \cdot 10$	-1.57	24.6	0.62	7.69
b	32.00	$3.00 \cdot 10$	$2.76 \cdot 10$	-1.56	24.6	0.55	7.67
2a	32.00	$3.00 \cdot 10^{-3}$	$2.40 \cdot 10^{-3}$	-2.62	24.6	1.01	7.72
b	32.00	$3.00 \cdot 10^{-3}$	$2.49 \cdot 10^{-3}$	-2.60	24.6	0.92	7.74
3a	32.00	$3.00 \cdot 10^{-4}$	$2.18 \cdot 10^{-4}$	-3.66	24.6	1.18	7.73
b	32.00	$3.00 \cdot 10^{-4}$	$2.07 \cdot 10^{-4}$	-3.68	24.6	1.26	7.72
4a	32.00	$3.00 \cdot 10^{-5}$	$1.60 \cdot 10^{-5}$	-4.80	24.6	1.55	7.71
b	32.00	$3.00 \cdot 10^{-5}$	$1.22 \cdot 10^{-5}$	-4.91	24.6	1.77	7.72
5a	32.00	$1.01 \cdot 10^{-5}$	$6.53 \cdot 10^{-6}$	-5.18	12.3	1.64	7.70
b	32.00	$1.01 \cdot 10^{-5}$	$6.34 \cdot 10^{-6}$	-5.20	12.3	1.68	7.71
6a	32.00	$3.00 \cdot 10^{-6}$	$1.75 \cdot 10^{-6}$	-5.76	12.3	1.77	7.69
b	32.00	$3.00 \cdot 10^{-6}$	$1.21 \cdot 10^{-6}$	-5.92	12.3	2.08	7.70
7a	32.00	$1.01 \cdot 10^{-6}$	$1.20 \cdot 10^{-7}$	-6.92	12.3	2.78	7.70
b	32.00	$1.01 \cdot 10^{-6}$	$2.19 \cdot 10^{-7}$	-6.66	12.3	2.46	7.68
8a	32.00	$3.00 \cdot 10^{-7}$	$3.58 \cdot 10^{-8}$	-7.45	12.3	2.78	7.69
b	32.00	$3.00 \cdot 10^{-7}$	$3.59 \cdot 10^{-8}$	-7.45	12.3	2.78	7.69
9a	32.00	$3.05 \cdot 10^{-8}$	$2.51 \cdot 10^{-9}$	-8.60	12.3	2.96	7.70
b	32.00	$3.05 \cdot 10^{-8}$	$3.24 \cdot 10^{-9}$	-8.49	12.3	2.84	7.69
10a	32.00	$1.48 \cdot 10^{-9}$	$1.40 \cdot 10^{-10}$	-9.85	12.3	2.89	7.63
b	32.00	$1.48 \cdot 10^{-9}$	$1.48 \cdot 10^{-10}$	-9.83	12.3	2.86	7.67

App. B Experimental data for nickel

B.1 Experimental data for Ni on BOZ1-1 samples

Tab. B-1: Experimental data for Ni on sample BOZ-323 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$5.20E^{-5}$	$2.68E^{-6}$	-5.57	13.9	3.12	8.09
b	30.00	$5.20E^{-5}$	$2.88E^{-6}$	-5.54	13.9	3.09	8.10
2a	30.00	$2.60E^{-5}$	$2.77E^{-6}$	-5.56	13.9	2.78	8.08
b	30.00	$2.60E^{-5}$	$2.80E^{-6}$	-5.55	13.9	2.77	8.10
3a	30.00	$8.67E^{-6}$	$8.11E^{-7}$	-6.09	13.9	2.84	8.04
b	30.00	$8.67E^{-6}$	$1.36E^{-6}$	-5.87	13.9	2.59	8.08
4a	30.00	$2.61E^{-6}$	$5.60E^{-7}$	-6.25	13.9	2.42	8.04
b	30.00	$2.61E^{-6}$	$5.45E^{-7}$	-6.26	13.9	2.43	8.11
5a	30.00	$8.73E^{-7}$	$1.57E^{-7}$	-6.80	13.9	2.52	8.07
b	30.00	$8.73E^{-7}$	$1.48E^{-7}$	-6.83	13.9	2.55	8.11
6a	30.00	$2.66E^{-7}$	$3.79E^{-8}$	-7.42	13.9	2.64	8.10
b	30.00	$2.66E^{-7}$	$5.16E^{-8}$	-7.29	13.9	2.47	8.11
7a	30.00	$9.25E^{-8}$	$5.42E^{-9}$	-8.27	13.9	3.06	8.11
b	30.00	$9.25E^{-8}$	$9.67E^{-9}$	-8.01	13.9	2.79	8.10
8a	30.00	$3.18E^{-8}$	$3.32E^{-9}$	-8.48	13.9	2.79	8.05
b	30.00	$3.18E^{-8}$	$4.46E^{-9}$	-8.35	13.9	2.64	8.13

Tab. B-2: Experimental data for Ni on sample BOZ-440 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$5.20E^{-5}$	$6.36E^{-7}$	-6.20	14.2	3.75	8.05
b	30.00	$5.20E^{-5}$	$9.04E^{-7}$	-6.04	14.2	3.60	8.04
2a	30.00	$2.60E^{-5}$	$4.38E^{-7}$	-6.36	14.2	3.61	8.13
b	30.00	$2.60E^{-5}$	$4.86E^{-7}$	-6.31	14.2	3.57	8.13
3a	30.00	$8.67E^{-6}$	$1.50E^{-7}$	-6.82	14.2	3.60	8.14
b	30.00	$8.67E^{-6}$	$1.61E^{-7}$	-6.79	14.2	3.57	8.15
4a	30.00	$2.61E^{-6}$	$2.00E^{-8}$	-7.70	14.2	3.96	8.13
b	30.00	$2.61E^{-6}$	$3.54E^{-8}$	-7.45	14.2	3.71	8.12
5a	30.00	$8.73E^{-7}$	$8.13E^{-9}$	-8.09	14.2	3.87	8.12
b	30.00	$8.73E^{-7}$	$1.37E^{-8}$	-7.86	14.2	3.64	8.09
6a	30.00	$2.66E^{-7}$	$7.00E^{-9}$	-8.15	14.2	3.41	8.05
b	30.00	$2.66E^{-7}$	$1.41E^{-9}$	-8.85	14.2	4.12	8.00
7a	30.00	$9.25E^{-8}$	$5.16E^{-10}$	-9.29	14.2	4.10	8.00
b	30.00	$9.25E^{-8}$	$3.36E^{-10}$	-9.47	14.2	4.29	8.00
8a	30.00	$3.18E^{-8}$	$4.35E^{-10}$	-9.36	14.2	3.70	8.00
b	30.00	$3.18E^{-8}$	$3.16E^{-10}$	-9.50	14.2	3.85	8.00

Tab. B-3: Experimental data for Ni on sample BOZ-493 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$5.20 \cdot 10^{-5}$	$3.68 \cdot 10^{-6}$	-5.43	14.9	2.95	8.08
b	30.00	$5.20 \cdot 10^{-5}$	$3.95 \cdot 10^{-6}$	-5.40	14.9	2.91	8.05
2a	30.00	$2.60 \cdot 10^{-5}$	$3.48 \cdot 10^{-6}$	-5.46	14.9	2.64	8.10
b	30.00	$2.60 \cdot 10^{-5}$	$3.23 \cdot 10^{-6}$	-5.49	14.9	2.68	8.11
3a	30.00	$8.67 \cdot 10^{-6}$	$1.66 \cdot 10^{-6}$	-5.78	14.9	2.45	8.10
b	30.00	$8.67 \cdot 10^{-6}$	$1.62 \cdot 10^{-6}$	-5.79	14.9	2.47	8.09
4a	30.00	$2.61 \cdot 10^{-6}$	$4.36 \cdot 10^{-7}$	-6.36	14.9	2.52	8.06
b	30.00	$2.61 \cdot 10^{-6}$	$4.38 \cdot 10^{-7}$	-6.36	14.9	2.52	8.10
5a	30.00	$8.73 \cdot 10^{-7}$	$4.08 \cdot 10^{-8}$	-7.39	14.9	3.14	8.07
b	30.00	$8.73 \cdot 10^{-7}$	$9.90 \cdot 10^{-8}$	-7.00	14.9	2.72	8.05
6a	30.00	$2.66 \cdot 10^{-7}$	$9.52 \cdot 10^{-9}$	-8.02	14.9	3.26	8.05
b	30.00	$2.66 \cdot 10^{-7}$	$1.41 \cdot 10^{-8}$	-7.85	14.9	3.08	8.06
7a	30.00	$9.25 \cdot 10^{-8}$	$2.49 \cdot 10^{-9}$	-8.60	14.9	3.39	8.04
b	30.00	$9.25 \cdot 10^{-8}$	$8.73 \cdot 10^{-10}$	-9.06	14.9	3.85	8.07
8a	30.00	$3.18 \cdot 10^{-8}$	$4.22 \cdot 10^{-10}$	-9.37	14.9	3.70	8.07
b	30.00	$3.18 \cdot 10^{-8}$	$4.93 \cdot 10^{-10}$	-9.31	14.9	3.63	8.07

Tab. B-4: Experimental data for Ni on sample BOZ-521 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$5.20\cdot10^{-5}$	$7.79\cdot10^{-6}$	-5.11	11.6	2.69	8.02
b	30.00	$5.20\cdot10^{-5}$	$7.32\cdot10^{-6}$	-5.14	11.6	2.72	7.96
2a	30.00	$2.60\cdot10^{-5}$	$5.33\cdot10^{-6}$	-5.27	11.6	2.52	7.98
b	30.00	$2.60\cdot10^{-5}$	$5.27\cdot10^{-6}$	-5.28	11.6	2.53	8.00
3a	30.00	$8.67\cdot10^{-6}$	$1.32\cdot10^{-6}$	-5.88	11.6	2.68	8.12
b	30.00	$8.67\cdot10^{-6}$	$1.86\cdot10^{-6}$	-5.73	11.6	2.50	8.11
4a	30.00	$2.61\cdot10^{-6}$	$7.29\cdot10^{-7}$	-6.14	11.6	2.34	8.08
b	30.00	$2.61\cdot10^{-6}$	$6.95\cdot10^{-7}$	-6.16	11.6	2.37	8.12
5a	30.00	$8.72\cdot10^{-7}$	$2.16\cdot10^{-7}$	-6.66	11.6	2.42	8.09
b	30.00	$8.72\cdot10^{-7}$	$1.87\cdot10^{-7}$	-6.73	11.6	2.50	8.09
6a	30.00	$2.66\cdot10^{-7}$	$6.24\cdot10^{-9}$	-8.20	11.6	3.55	8..09
b	30.00	$2.66\cdot10^{-7}$	$5.68\cdot10^{-8}$	-7.25	11.6	2.50	8.07
7a	30.00	$9.24\cdot10^{-8}$	$2.05\cdot10^{-8}$	-7.69	11.6	2.48	8.09
b	30.00	$9.24\cdot10^{-8}$	$1.81\cdot10^{-8}$	-7.74	11.6	2.55	8.08
8a	30.00	$3.18\cdot10^{-8}$	$6.28\cdot10^{-9}$	-8.20	11.6	2.54	8.00
b	30.00	$3.18\cdot10^{-8}$	$6.16\cdot10^{-9}$	-8.21	11.6	2.55	8.11

Tab. B-5: Experimental data for Ni on sample BOZ-572 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$5.20 \cdot 10^{-5}$	$4.76 \cdot 10^{-6}$	-5.32	15.4	2.81	7.91
b	30.00	$5.20 \cdot 10^{-5}$	$5.43 \cdot 10^{-6}$	-5.27	15.4	2.75	7.90
2a	30.00	$2.60 \cdot 10^{-5}$	$3.40 \cdot 10^{-6}$	-5.47	15.4	2.63	7.95
b	30.00	$2.60 \cdot 10^{-5}$	$2.96 \cdot 10^{-6}$	-5.53	15.4	2.70	7.96
3a	30.00	$8.67 \cdot 10^{-6}$	$1.25 \cdot 10^{-6}$	-5.90	15.4	2.59	8.03
b	30.00	$8.67 \cdot 10^{-6}$	$9.24 \cdot 10^{-7}$	-6.03	15.4	2.74	7.95
4a	30.00	$2.61 \cdot 10^{-6}$	$2.10 \cdot 10^{-7}$	-6.68	15.4	2.87	7.96
b	30.00	$2.61 \cdot 10^{-6}$	$2.53 \cdot 10^{-7}$	-6.60	15.4	2.78	7.99
5a	30.00	$8.72 \cdot 10^{-7}$	$7.30 \cdot 10^{-8}$	-7.14	15.4	2.85	7.86
b	30.00	$8.72 \cdot 10^{-7}$	$7.11 \cdot 10^{-8}$	-7.15	15.4	2.86	7.93
6a	30.00	$2.66 \cdot 10^{-7}$	$9.28 \cdot 10^{-9}$	-8.03	15.4	3.25	7.97
b	30.00	$2.66 \cdot 10^{-7}$	$6.40 \cdot 10^{-9}$	-8.19	15.4	3.42	7.95
7a	30.00	$9.24 \cdot 10^{-8}$	$5.65 \cdot 10^{-9}$	-8.25	15.4	3.00	7.99
8a	30.00	$3.18 \cdot 10^{-8}$	$4.45 \cdot 10^{-10}$	-9.35	15.4	3.66	7.98
b	30.00	$3.18 \cdot 10^{-8}$	$2.57 \cdot 10^{-9}$	-8.59	15.4	2.87	8.01

Tab. B-6: Experimental data for Ni on sample BOZ-681 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$5.20 \cdot 10^{-5}$	$4.78 \cdot 10^{-6}$	-5.32	11.3	2.94	8.03
b	30.00	$5.20 \cdot 10^{-5}$	$3.90 \cdot 10^{-6}$	-5.41	11.3	3.04	8.00
2a	30.00	$2.60 \cdot 10^{-5}$	$3.00 \cdot 10^{-6}$	-5.52	11.3	2.83	8.00
b	30.00	$2.60 \cdot 10^{-5}$	$2.11 \cdot 10^{-6}$	-5.68	11.3	3.00	8.02
3a	30.00	$8.67 \cdot 10^{-6}$	$9.89 \cdot 10^{-7}$	-6.00	11.3	2.84	8.04
b	30.00	$8.67 \cdot 10^{-6}$	$9.51 \cdot 10^{-7}$	-6.02	11.3	2.86	8.06
4a	30.00	$2.61 \cdot 10^{-6}$	$2.35 \cdot 10^{-7}$	-6.63	11.3	2.95	8.05
b	30.00	$2.61 \cdot 10^{-6}$	$9.59 \cdot 10^{-7}$	-6.02	11.3	2.18	8.08
5a	30.00	$8.72 \cdot 10^{-7}$	$7.50 \cdot 10^{-9}$	-8.13	11.3	4.01	8.06
b	30.00	$8.72 \cdot 10^{-7}$	$7.52 \cdot 10^{-8}$	-7.12	11.3	2.97	8.08
6a	30.00	$2.66 \cdot 10^{-7}$	$2.63 \cdot 10^{-8}$	-7.58	11.3	2.91	8.10
b	30.00	$2.66 \cdot 10^{-7}$	$5.24 \cdot 10^{-9}$	-8.28	11.3	3.64	8.09
7a	30.00	$9.24 \cdot 10^{-8}$	$7.10 \cdot 10^{-9}$	-8.15	11.3	3.03	8.05
b	30.00	$9.24 \cdot 10^{-8}$	$1.70 \cdot 10^{-8}$	-7.77	11.3	2.59	8.08
8a	30.00	$3.18 \cdot 10^{-8}$	$1.99 \cdot 10^{-9}$	-8.70	11.3	3.12	7.98
b	30.00	$3.18 \cdot 10^{-8}$	$2.54 \cdot 10^{-9}$	-8.60	11.3	3.01	8.06

B.2 Experimental data for Ni on BUL1-1 samples

Tab. B-7: Experimental data for Ni on sample BUL-845 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$6.00 \cdot 10^{-5}$	$7.88 \cdot 10^{-6}$	-5.10	167.433	1.60	7.74
b	30.00	$6.00 \cdot 10^{-5}$	$8.07 \cdot 10^{-6}$	-5.09	168.500	1.58	7.76
2a	30.00	$3.00 \cdot 10^{-5}$	$5.72 \cdot 10^{-6}$	-5.24	168.867	1.40	7.75
b	30.00	$3.00 \cdot 10^{-5}$	$5.54 \cdot 10^{-6}$	-5.26	166.000	1.43	7.77
3a	30.00	$1.00 \cdot 10^{-5}$	$1.68 \cdot 10^{-6}$	-5.78	165.433	1.48	7.76
b	30.00	$1.00 \cdot 10^{-5}$	$1.83 \cdot 10^{-6}$	-5.74	167.133	1.43	7.79
4a	30.00	$3.01 \cdot 10^{-6}$	$4.89 \cdot 10^{-7}$	-6.31	167.333	1.49	7.75
b	30.00	$3.01 \cdot 10^{-6}$	$4.39 \cdot 10^{-7}$	-6.36	170.667	1.54	7.74
5a	30.00	$1.01 \cdot 10^{-6}$	$1.44 \cdot 10^{-7}$	-6.84	167.067	1.56	7.71
b	30.00	$1.01 \cdot 10^{-6}$	$1.42 \cdot 10^{-7}$	-6.85	167.367	1.57	7.72
6a	30.00	$3.13 \cdot 10^{-7}$	$3.14 \cdot 10^{-8}$	-7.50	167.267	1.73	7.60
b	30.00	$3.13 \cdot 10^{-7}$	$5.13 \cdot 10^{-8}$	-7.29	168.333	1.48	7.69
7a	30.00	$1.13 \cdot 10^{-7}$	$1.57 \cdot 10^{-8}$	-7.80	166.967	1.57	7.70
b	30.00	$1.13 \cdot 10^{-7}$	$1.56 \cdot 10^{-8}$	-7.81	171.333	1.57	7.65
8a	30.00	$4.33 \cdot 10^{-8}$	$6.19 \cdot 10^{-9}$	-8.21	167.667	1.55	8.28
b	30.00	$4.33 \cdot 10^{-8}$	$1.67 \cdot 10^{-9}$	-8.78	166.333	2.18	7.74

Tab. B-8: Experimental data for Ni on sample BUL-861 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$5.14 \cdot 10^{-5}$	$3.68 \cdot 10^{-5}$	-4.43	8.2	1.68	7.53
b	35.00	$5.14 \cdot 10^{-5}$	$3.67 \cdot 10^{-5}$	-4.44	8.2	1.69	7.55
2a	35.00	$2.57 \cdot 10^{-5}$	$1.96 \cdot 10^{-5}$	-4.71	8.2	1.58	7.59
b	35.00	$2.57 \cdot 10^{-5}$	$1.83 \cdot 10^{-5}$	-4.74	8.2	1.69	7.55
3a	35.00	$8.58 \cdot 10^{-6}$	$6.16 \cdot 10^{-6}$	-5.21	8.2	1.68	7.58
b	35.00	$8.58 \cdot 10^{-6}$	$5.85 \cdot 10^{-6}$	-5.23	8.2	1.76	7.63
4a	35.00	$2.58 \cdot 10^{-6}$	$1.61 \cdot 10^{-6}$	-5.79	8.2	1.86	7.60
b	35.00	$2.58 \cdot 10^{-6}$	$1.57 \cdot 10^{-6}$	-5.81	8.2	1.90	7.56
5a	35.00	$8.70 \cdot 10^{-7}$	$5.33 \cdot 10^{-7}$	-6.27	8.2	1.89	7.57
b	35.00	$8.70 \cdot 10^{-7}$	$5.31 \cdot 10^{-8}$	-7.27	8.2	3.27	7.58
6a	35.00	$2.70 \cdot 10^{-7}$	$1.13 \cdot 10^{-7}$	-6.95	8.2	2.23	7.52
b	35.00	$2.70 \cdot 10^{-7}$	$1.53 \cdot 10^{-7}$	-6.82	8.2	1.97	7.53
7a	35.00	$9.90 \cdot 10^{-8}$	$3.33 \cdot 10^{-8}$	-7.48	8.2	2.38	7.57
b	35.00	$9.90 \cdot 10^{-8}$	$5.23 \cdot 10^{-8}$	-7.28	8.2	2.04	7.52
8a	35.00	$3.90 \cdot 10^{-8}$	$1.09 \cdot 10^{-8}$	-7.96	8.2	2.50	7.50
b	35.00	$3.90 \cdot 10^{-8}$	$4.73 \cdot 10^{-9}$	-8.33	8.2	2.95	7.53

Tab. B-9: Experimental data for Ni on sample BUL-921 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$7.00 \cdot 10^{-5}$	$5.04 \cdot 10^{-5}$	-4.30	7.9	1.69	7.54
b	35.00	$7.00 \cdot 10^{-5}$	$5.01 \cdot 10^{-5}$	-4.30	7.9	1.70	7.50
2a	35.00	$3.50 \cdot 10^{-5}$	$2.68 \cdot 10^{-5}$	-4.57	7.9	1.59	7.55
b	35.00	$3.50 \cdot 10^{-5}$	$2.54 \cdot 10^{-5}$	-4.60	7.9	1.68	7.54
3a	35.00	$1.17 \cdot 10^{-5}$	$8.45 \cdot 10^{-6}$	-5.07	7.9	1.69	7.56
b	35.00	$1.17 \cdot 10^{-5}$	$8.04 \cdot 10^{-6}$	-5.09	7.9	1.76	7.50
4a	35.00	$3.51 \cdot 10^{-6}$	$2.22 \cdot 10^{-6}$	-5.65	7.9	1.87	7.52
b	35.00	$3.51 \cdot 10^{-6}$	$2.15 \cdot 10^{-6}$	-5.67	7.9	1.91	7.58
5a	35.00	$1.18 \cdot 10^{-6}$	$7.25 \cdot 10^{-7}$	-6.14	7.9	1.90	7.59
b	35.00	$1.18 \cdot 10^{-6}$	$7.33 \cdot 10^{-7}$	-6.14	7.9	1.89	7.55
6a	35.00	$3.63 \cdot 10^{-7}$	$1.53 \cdot 10^{-7}$	-6.81	7.9	2.24	7.45
b	35.00	$3.63 \cdot 10^{-7}$	$2.08 \cdot 10^{-7}$	-6.68	7.9	1.98	7.50
7a	35.00	$1.30 \cdot 10^{-7}$	$4.41 \cdot 10^{-8}$	-7.36	7.9	2.39	7.54
b	35.00	$1.30 \cdot 10^{-7}$	$6.95 \cdot 10^{-8}$	-7.16	7.9	2.04	7.45
8a	35.00	$4.83 \cdot 10^{-8}$	$1.36 \cdot 10^{-8}$	-7.87	7.9	2.51	7.58
b	35.00	$4.83 \cdot 10^{-8}$	$5.93 \cdot 10^{-9}$	-8.23	7.9	2.96	7.57

Tab. B-10: Experimental data for Ni on sample BUL-955 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$7.00 \cdot 10^{-5}$	$3.02 \cdot 10^{-5}$	-4.52	7.9	2.22	7.51
b	35.00	$7.00 \cdot 10^{-5}$	$3.12 \cdot 10^{-5}$	-4.51	7.9	2.20	7.75
2a	35.00	$3.50 \cdot 10^{-5}$	$1.76 \cdot 10^{-5}$	-4.75	7.9	2.10	7.54
b	35.00	$3.50 \cdot 10^{-5}$	$1.77 \cdot 10^{-5}$	-4.75	7.9	2.10	7.53
3a	35.00	$1.17 \cdot 10^{-5}$	$4.97 \cdot 10^{-6}$	-5.30	7.9	2.23	7.52
b	35.00	$1.17 \cdot 10^{-5}$	$4.86 \cdot 10^{-6}$	-5.31	7.9	2.25	7.50
4a	35.00	$3.51 \cdot 10^{-6}$	$1.17 \cdot 10^{-6}$	-5.93	7.9	2.40	7.51
b	35.00	$3.51 \cdot 10^{-6}$	$8.40 \cdot 10^{-7}$	-6.08	7.9	2.61	7.54
5a	35.00	$1.18 \cdot 10^{-6}$	$2.53 \cdot 10^{-7}$	-6.60	7.9	2.67	7.52
b	35.00	$1.18 \cdot 10^{-6}$	$8.95 \cdot 10^{-8}$	-7.05	7.9	3.19	7.54
6a	35.00	$3.63 \cdot 10^{-7}$	$1.00 \cdot 10^{-8}$	-8.00	7.9	3.65	7.53
b	35.00	$3.63 \cdot 10^{-7}$	$1.11 \cdot 10^{-7}$	-6.95	7.9	2.46	7.54
7a	35.00	$1.30 \cdot 10^{-7}$	$2.93 \cdot 10^{-8}$	-7.53	7.9	2.64	7.51
b	35.00	$1.30 \cdot 10^{-7}$	$2.67 \cdot 10^{-8}$	-7.57	7.9	2.69	7.49
8a	35.00	$4.83 \cdot 10^{-8}$	$7.24 \cdot 10^{-9}$	-8.14	7.9	2.86	7.46
b	35.00	$4.83 \cdot 10^{-8}$	$1.36 \cdot 10^{-8}$	-7.87	7.9	2.51	7.51

Tab. B-11: Experimental data for Ni on sample BUL-995 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$2.33 \cdot 10^{-4}$	$7.19 \cdot 10^{-5}$	-4.14	6.4	2.54	7.46
b	35.00	$2.33 \cdot 10^{-4}$	$7.18 \cdot 10^{-5}$	-4.14	6.4	2.54	7.46
2a	35.00	$1.17 \cdot 10^{-4}$	$4.22 \cdot 10^{-5}$	-4.37	6.4	2.44	7.53
b	35.00	$1.17 \cdot 10^{-4}$	$4.08 \cdot 10^{-5}$	-4.39	6.4	2.46	7.50
3a	35.00	$7.00 \cdot 10^{-5}$	$2.82 \cdot 10^{-5}$	-4.55	6.4	2.36	7.56
b	35.00	$7.00 \cdot 10^{-5}$	$2.83 \cdot 10^{-5}$	-4.55	6.4	2.36	7.56
4a	35.00	$3.50 \cdot 10^{-5}$	$1.42 \cdot 10^{-5}$	-4.85	6.4	2.36	7.58
b	35.00	$3.50 \cdot 10^{-5}$	$1.35 \cdot 10^{-5}$	-4.87	6.4	2.39	7.58
5a	35.00	$1.17 \cdot 10^{-5}$	$4.16 \cdot 10^{-6}$	-5.38	6.4	2.45	7.58
b	35.00	$1.17 \cdot 10^{-5}$	$3.93 \cdot 10^{-6}$	-5.41	6.4	2.49	7.58
6a	35.00	$3.51 \cdot 10^{-6}$	$9.44 \cdot 10^{-7}$	-6.03	6.4	2.63	7.58
b	35.00	$3.51 \cdot 10^{-6}$	$8.83 \cdot 10^{-7}$	-6.05	6.4	2.67	7.58
7a	35.00	$1.18 \cdot 10^{-6}$	$2.48 \cdot 10^{-7}$	-6.61	6.4	2.77	7.59
b	35.00	$1.18 \cdot 10^{-6}$	$2.73 \cdot 10^{-7}$	-6.56	6.4	2.71	7.58
8a	35.00	$3.63 \cdot 10^{-7}$	$7.30 \cdot 10^{-8}$	-7.14	6.4	2.79	7.59
b	35.00	$3.63 \cdot 10^{-7}$	$7.46 \cdot 10^{-8}$	-7.13	6.4	2.78	7.59
9a	35.00	$1.29 \cdot 10^{-7}$	$2.64 \cdot 10^{-8}$	-7.58	6.4	2.78	7.59
b	35.00	$1.29 \cdot 10^{-7}$	$2.47 \cdot 10^{-8}$	-7.61	6.4	2.82	7.58
10a	35.00	$4.78 \cdot 10^{-8}$	$9.29 \cdot 10^{-9}$	-8.03	6.4	2.81	7.59
b	35.00	$4.78 \cdot 10^{-8}$	$9.11 \cdot 10^{-9}$	-8.04	6.4	2.82	7.58
11a	35.00	$2.31 \cdot 10^{-8}$	$4.90 \cdot 10^{-9}$	-8.31	6.4	2.76	7.60
b	35.00	$2.31 \cdot 10^{-8}$	$4.52 \cdot 10^{-9}$	-8.35	6.4	2.80	7.59
12a	35.00	$1.49 \cdot 10^{-8}$	$2.83 \cdot 10^{-9}$	-8.55	6.4	2.82	7.59
b	35.00	$1.49 \cdot 10^{-8}$	$2.83 \cdot 10^{-9}$	-8.55	6.4	2.82	7.60

Tab. B-12: Experimental data for Ni on sample BUL-1002 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$7.00 \cdot 10^{-5}$	$5.22 \cdot 10^{-5}$	-4.28	7.0	1.69	7.51
b	35.00	$7.00 \cdot 10^{-5}$	$5.27 \cdot 10^{-5}$	-4.28	7.0	1.67	7.75
2a	35.00	$3.50 \cdot 10^{-5}$	$2.77 \cdot 10^{-5}$	-4.56	7.0	1.58	7.54
b	35.00	$3.50 \cdot 10^{-5}$	$2.73 \cdot 10^{-5}$	-4.56	7.0	1.61	7.53
3a	35.00	$1.17 \cdot 10^{-5}$	$8.23 \cdot 10^{-6}$	-5.08	7.0	1.78	7.52
b	35.00	$1.17 \cdot 10^{-5}$	$8.63 \cdot 10^{-6}$	-5.06	7.0	1.71	7.50
4a	35.00	$3.51 \cdot 10^{-6}$	$2.43 \cdot 10^{-6}$	-5.61	7.0	1.81	7.51
b	35.00	$3.51 \cdot 10^{-6}$	$2.39 \cdot 10^{-6}$	-5.62	7.0	1.83	7.54
5a	35.00	$1.18 \cdot 10^{-6}$	$7.61 \cdot 10^{-7}$	-6.12	7.0	1.90	7.52
b	35.00	$1.18 \cdot 10^{-6}$	$7.03 \cdot 10^{-7}$	-6.15	7.0	1.99	7.54
6a	35.00	$3.63 \cdot 10^{-7}$	$2.31 \cdot 10^{-7}$	-6.64	7.0	1.91	7.53
b	35.00	$3.63 \cdot 10^{-7}$	$2.10 \cdot 10^{-7}$	-6.68	7.0	2.02	7.54
7a	35.00	$1.30 \cdot 10^{-7}$	$7.59 \cdot 10^{-8}$	-7.12	7.0	2.01	7.51
b	35.00	$1.30 \cdot 10^{-7}$	$8.01 \cdot 10^{-8}$	-7.10	7.0	1.95	7.49
8a	35.00	$4.83 \cdot 10^{-8}$	$2.83 \cdot 10^{-8}$	-7.55	7.0	2.01	7.46
b	35.00	$4.83 \cdot 10^{-8}$	$2.94 \cdot 10^{-8}$	-7.53	7.0	1.97	7.51

Tab. B-13: Experimental data for Ni on sample BUL-1017 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$7.00 \cdot 10^{-5}$	$5.08 \cdot 10^{-5}$	-4.29	4.8	1.89	7.58
b	35.00	$7.00 \cdot 10^{-5}$	$5.10 \cdot 10^{-5}$	-4.29	4.8	1.89	7.58
2a	35.00	$3.50 \cdot 10^{-5}$	$2.49 \cdot 10^{-5}$	-4.60	4.8	1.93	7.60
b	35.00	$3.50 \cdot 10^{-5}$	$2.47 \cdot 10^{-5}$	-4.61	4.8	1.94	7.58
3a	35.00	$1.17 \cdot 10^{-5}$	$7.60 \cdot 10^{-6}$	-5.12	4.8	2.05	7.55
b	35.00	$1.17 \cdot 10^{-5}$	$7.60 \cdot 10^{-6}$	-5.12	4.8	2.05	7.58
4a	35.00	$3.51 \cdot 10^{-6}$	$1.99 \cdot 10^{-6}$	-5.70	4.8	2.20	7.56
b	35.00	$3.51 \cdot 10^{-6}$	$1.94 \cdot 10^{-6}$	-5.71	4.8	2.23	7.57
5a	35.00	$1.18 \cdot 10^{-6}$	$5.81 \cdot 10^{-7}$	-6.24	4.8	2.33	7.55
b	35.00	$1.18 \cdot 10^{-6}$	$6.18 \cdot 10^{-7}$	-6.21	4.8	2.28	7.57
6a	35.00	$3.63 \cdot 10^{-7}$	$1.91 \cdot 10^{-7}$	-6.72	4.8	2.27	7.58
b	35.00	$3.63 \cdot 10^{-7}$	$1.65 \cdot 10^{-7}$	-6.78	4.8	2.40	7.56
7a	35.00	$1.30 \cdot 10^{-7}$	$6.35 \cdot 10^{-8}$	-7.20	4.8	2.34	7.55
b	35.00	$1.30 \cdot 10^{-7}$	$6.35 \cdot 10^{-8}$	-7.20	4.8	2.34	7.57
8a	35.00	$4.83 \cdot 10^{-8}$	$2.36 \cdot 10^{-8}$	-7.63	4.8	2.34	7.48
b	35.00	$4.83 \cdot 10^{-8}$	$2.21 \cdot 10^{-8}$	-7.66	4.8	2.39	7.56

B.3 Experimental data for Ni on TRU1-1 samples

Tab. B-14: Experimental data for Ni on sample TRU-748 in its corresponding SPW (cf. Tab. 2-4).

Sample	Vol (10^{-3} L)	Ni_{in} (M)	Ni_{aq} (M)	Log Ni_{aq} (M)	S/L ratio (10^{-3} kg/L)	log R_d (L/kg)	pH
1a	35.00	$7.00 \cdot 10^{-5}$	$3.74 \cdot 10^{-5}$	-4.43	6.4	2.14	7.69
b	35.00	$7.00 \cdot 10^{-5}$	$3.77 \cdot 10^{-5}$	-4.42	6.4	2.13	7.65
2a	35.00	$3.50 \cdot 10^{-5}$	$2.02 \cdot 10^{-5}$	-4.69	6.4	2.06	7.61
b	35.00	$3.50 \cdot 10^{-5}$	$2.01 \cdot 10^{-5}$	-4.70	6.4	2.06	7.32
3a	35.00	$1.17 \cdot 10^{-5}$	$7.42 \cdot 10^{-6}$	-5.13	6.4	1.95	7.67
b	35.00	$1.17 \cdot 10^{-5}$	$7.41 \cdot 10^{-6}$	-5.13	6.4	1.96	7.70
4a	35.00	$3.51 \cdot 10^{-6}$	$1.41 \cdot 10^{-6}$	-5.85	6.4	2.37	7.63
b	35.00	$3.51 \cdot 10^{-6}$	$1.74 \cdot 10^{-6}$	-5.76	6.4	2.20	7.62
5a	35.00	$1.17 \cdot 10^{-6}$	$5.48 \cdot 10^{-7}$	-6.26	6.4	2.25	7.65
b	35.00	$1.17 \cdot 10^{-6}$	$5.65 \cdot 10^{-7}$	-6.25	6.4	2.23	7.67
6a	35.00	$3.56 \cdot 10^{-7}$	$1.26 \cdot 10^{-7}$	-6.90	6.4	2.46	7.63
b	35.00	$3.56 \cdot 10^{-7}$	$1.34 \cdot 10^{-7}$	-6.87	6.4	2.42	7.61
7a	35.00	$1.22 \cdot 10^{-7}$	$4.73 \cdot 10^{-8}$	-7.33	6.4	2.40	7.64
b	35.00	$1.22 \cdot 10^{-7}$	$1.06 \cdot 10^{-8}$	-7.97	6.4	3.22	7.68
8a	35.00	$4.07 \cdot 10^{-8}$	$9.87 \cdot 10^{-9}$	-8.01	6.4	2.69	7.66
b	35.00	$4.07 \cdot 10^{-8}$	$1.45 \cdot 10^{-8}$	-7.84	6.4	2.45	7.59

Tab. B-15: Experimental data for Ni on sample TRU-794 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$7.00 \cdot 10^{-5}$	$4.21 \cdot 10^{-5}$	-4.38	6.3	2.02	7.62
b	35.00	$7.00 \cdot 10^{-5}$	$4.32 \cdot 10^{-5}$	-4.36	6.3	1.99	7.60
2a	35.00	$3.50 \cdot 10^{-5}$	$2.20 \cdot 10^{-5}$	-4.66	6.3	1.97	7.60
b	35.00	$3.50 \cdot 10^{-5}$	$2.21 \cdot 10^{-5}$	-4.66	6.3	1.97	7.61
3a	35.00	$1.17 \cdot 10^{-5}$	$7.63 \cdot 10^{-6}$	-5.12	6.3	1.92	7.59
b	35.00	$1.17 \cdot 10^{-5}$	$7.64 \cdot 10^{-6}$	-5.12	6.3	1.92	7.72
4a	35.00	$3.51 \cdot 10^{-6}$	$2.08 \cdot 10^{-6}$	-5.68	6.3	2.04	7.72
b	35.00	$3.51 \cdot 10^{-6}$	$2.12 \cdot 10^{-6}$	-5.67	6.3	2.01	7.70
5a	35.00	$1.17 \cdot 10^{-6}$	$6.02 \cdot 10^{-7}$	-6.22	6.3	2.18	7.62
b	35.00	$1.17 \cdot 10^{-6}$	$5.36 \cdot 10^{-7}$	-6.27	6.3	2.28	7.66
6a	35.00	$3.56 \cdot 10^{-7}$	$1.54 \cdot 10^{-7}$	-6.81	6.3	2.32	7.63
b	35.00	$3.56 \cdot 10^{-7}$	$1.43 \cdot 10^{-7}$	-6.84	6.3	2.37	7.73
7a	35.00	$1.22 \cdot 10^{-7}$	$4.71 \cdot 10^{-8}$	-7.33	6.3	2.40	7.60
b	35.00	$1.22 \cdot 10^{-7}$	$5.28 \cdot 10^{-8}$	-7.28	6.3	2.32	7.65
8a	35.00	$4.07 \cdot 10^{-8}$	$1.76 \cdot 10^{-8}$	-7.75	6.3	2.32	7.57
b	35.00	$4.07 \cdot 10^{-8}$	$1.68 \cdot 10^{-9}$	-8.77	6.3	3.57	7.65

Tab. B-16: Experimental data for Ni on sample TRU-815 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$7.00 \cdot 10^{-5}$	$4.87 \cdot 10^{-5}$	-4.31	5.1	1.93	7.62
b	30.00	$7.00 \cdot 10^{-5}$	$4.57 \cdot 10^{-5}$	-4.34	5.1	2.02	7.62
2a	30.00	$3.50 \cdot 10^{-5}$	$2.50 \cdot 10^{-5}$	-4.60	5.1	1.89	7.64
b	30.00	$3.50 \cdot 10^{-5}$	$2.54 \cdot 10^{-5}$	-4.59	5.1	1.86	7.63
3a	30.00	$1.17 \cdot 10^{-5}$	$8.43 \cdot 10^{-6}$	-5.07	5.1	1.87	7.63
b	30.00	$1.17 \cdot 10^{-5}$	$8.35 \cdot 10^{-6}$	-5.08	5.1	1.89	7.66
4a	30.00	$3.51 \cdot 10^{-6}$	$2.59 \cdot 10^{-6}$	-5.59	5.1	1.84	7.65
5a	30.00	$1.17 \cdot 10^{-6}$	$8.16 \cdot 10^{-7}$	-6.09	5.1	1.93	7.61
b	30.00	$1.17 \cdot 10^{-6}$	$7.55 \cdot 10^{-7}$	-6.12	5.1	2.03	7.67
6a	30.00	$3.56 \cdot 10^{-7}$	$2.23 \cdot 10^{-7}$	-6.65	5.1	2.06	7.66
b	30.00	$3.56 \cdot 10^{-7}$	$1.90 \cdot 10^{-7}$	-6.72	5.1	2.23	7.66
7a	30.00	$1.22 \cdot 10^{-7}$	$7.00 \cdot 10^{-8}$	-7.16	5.1	2.16	7.61
b	30.00	$1.22 \cdot 10^{-7}$	$7.21 \cdot 10^{-8}$	-7.14	5.1	2.13	7.65
8a	30.00	$4.07 \cdot 10^{-8}$	$1.54 \cdot 10^{-8}$	-7.81	5.1	2.51	7.61

Tab. B-17: Experimental data for Ni on sample TRU-831 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$7.00 \cdot 10^{-5}$	$2.98 \cdot 10^{-5}$	-4.53	7.2	2.27	7.53
b	30.00	$7.00 \cdot 10^{-5}$	$3.04 \cdot 10^{-5}$	-4.52	7.2	2.26	7.54
2a	30.00	$3.50 \cdot 10^{-5}$	$1.44 \cdot 10^{-5}$	-4.84	7.2	2.30	7.55
b	30.00	$3.50 \cdot 10^{-5}$	$1.56 \cdot 10^{-5}$	-4.81	7.2	2.24	7.56
3a	30.00	$1.17 \cdot 10^{-5}$	$5.00 \cdot 10^{-6}$	-5.30	7.2	2.27	7.58
b	30.00	$1.17 \cdot 10^{-5}$	$4.94 \cdot 10^{-6}$	-5.31	7.2	2.28	7.58
4a	30.00	$3.51 \cdot 10^{-6}$	$1.16 \cdot 10^{-6}$	-5.94	7.2	2.45	7.56
5a	30.00	$1.17 \cdot 10^{-6}$	$2.82 \cdot 10^{-7}$	-6.55	7.2	2.64	7.58
b	30.00	$1.17 \cdot 10^{-6}$	$3.30 \cdot 10^{-7}$	-6.48	7.2	2.55	7.36
6a	30.00	$3.56 \cdot 10^{-7}$	$6.49 \cdot 10^{-8}$	-7.19	7.2	2.79	7.60
b	30.00	$3.56 \cdot 10^{-7}$	$6.48 \cdot 10^{-8}$	-7.19	7.2	2.79	7.59
7a	30.00	$1.22 \cdot 10^{-7}$	$1.26 \cdot 10^{-8}$	-7.90	7.2	3.08	7.57
8a	30.00	$4.07 \cdot 10^{-8}$	$4.80 \cdot 10^{-9}$	-8.32	7.2	3.02	7.56
b	30.00	$4.07 \cdot 10^{-8}$	$4.59 \cdot 10^{-9}$	-8.34	7.2	3.04	7.58

Tab. B-18: Experimental data for Ni on sample TRU-882 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	29.00	$7.00 \cdot 10^{-5}$	$2.66 \cdot 10^{-5}$	-4.58	11.4	2.16	7.72
b	29.00	$7.00 \cdot 10^{-5}$	$2.64 \cdot 10^{-5}$	-4.58	11.4	2.16	7.69
2a	29.00	$3.50 \cdot 10^{-5}$	$1.43 \cdot 10^{-5}$	-4.84	11.4	2.10	7.71
b	29.00	$3.50 \cdot 10^{-5}$	$1.41 \cdot 10^{-5}$	-4.85	11.4	2.11	7.70
3a	29.00	$1.17 \cdot 10^{-5}$	$4.49 \cdot 10^{-6}$	-5.35	11.4	2.15	7.74
b	29.00	$1.17 \cdot 10^{-5}$	$4.04 \cdot 10^{-6}$	-5.39	11.4	2.22	7.74
4a	29.00	$3.51 \cdot 10^{-6}$	$1.12 \cdot 10^{-6}$	-5.95	11.4	2.27	7.74
b	29.00	$3.51 \cdot 10^{-6}$	$1.06 \cdot 10^{-6}$	-5.97	11.4	2.31	7.74
5a	29.00	$1.17 \cdot 10^{-6}$	$2.99 \cdot 10^{-7}$	-6.52	11.4	2.41	7.74
b	29.00	$1.17 \cdot 10^{-6}$	$2.80 \cdot 10^{-7}$	-6.55	11.4	2.45	7.77
6a	29.00	$3.56 \cdot 10^{-7}$	$7.38 \cdot 10^{-8}$	-7.13	11.4	2.53	7.75
b	29.00	$3.56 \cdot 10^{-7}$	$7.64 \cdot 10^{-8}$	-7.12	11.4	2.51	7.73
7a	29.00	$1.22 \cdot 10^{-7}$	$2.67 \cdot 10^{-8}$	-7.57	11.4	2.50	7.72
b	29.00	$1.22 \cdot 10^{-7}$	$2.59 \cdot 10^{-8}$	-7.59	11.4	2.52	7.75
8a	29.00	$4.07 \cdot 10^{-8}$	$8.00 \cdot 10^{-9}$	-8.10	11.4	2.56	7.68
b	29.00	$4.07 \cdot 10^{-8}$	$7.48 \cdot 10^{-9}$	-8.13	11.4	2.59	7.72

Tab. B-19: Experimental data for Ni on sample TRU-923 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	29.00	$7.00 \cdot 10^{-5}$	$2.43 \cdot 10^{-5}$	-4.61	9.8	2.28	7.77
b	29.00	$7.00 \cdot 10^{-5}$	$2.07 \cdot 10^{-5}$	-4.68	9.8	2.39	7.79
2a	29.00	$3.50 \cdot 10^{-5}$	$1.22 \cdot 10^{-5}$	-4.91	9.8	2.28	7.74
b	29.00	$3.50 \cdot 10^{-5}$	$1.23 \cdot 10^{-5}$	-4.91	9.8	2.27	7.77
3a	29.00	$1.17 \cdot 10^{-5}$	$3.63 \cdot 10^{-6}$	-5.44	9.8	2.36	7.82
b	29.00	$1.17 \cdot 10^{-5}$	$3.37 \cdot 10^{-6}$	-5.47	9.8	2.40	7.80
4a	29.00	$3.51 \cdot 10^{-6}$	$7.61 \cdot 10^{-7}$	-6.12	9.8	2.57	7.82
b	29.00	$3.51 \cdot 10^{-6}$	$7.54 \cdot 10^{-7}$	-6.12	9.8	2.57	7.82
5a	29.00	$1.17 \cdot 10^{-6}$	$2.29 \cdot 10^{-7}$	-6.64	9.8	2.62	7.83
b	29.00	$1.17 \cdot 10^{-6}$	$2.24 \cdot 10^{-7}$	-6.65	9.8	2.64	7.82
6a	29.00	$3.56 \cdot 10^{-7}$	$6.64 \cdot 10^{-8}$	-7.18	9.8	2.65	7.82
b	29.00	$3.56 \cdot 10^{-7}$	$6.56 \cdot 10^{-8}$	-7.18	9.8	2.65	7.82
7a	29.00	$1.22 \cdot 10^{-7}$	$2.16 \cdot 10^{-8}$	-7.67	9.8	2.68	7.80
b	29.00	$1.22 \cdot 10^{-7}$	$2.15 \cdot 10^{-8}$	-7.67	9.8	2.68	7.85
8a	29.00	$4.07 \cdot 10^{-8}$	$6.48 \cdot 10^{-9}$	-8.19	9.8	2.73	7.73
b	29.00	$4.07 \cdot 10^{-8}$	$6.41 \cdot 10^{-9}$	-8.19	9.8	2.74	7.79

Tab. B-20: Experimental data for Ni on sample TRU-938 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Ni_{in}** (M)	**Ni_{aq}** (M)	**Log Ni_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	29.00	$7.00 \cdot 10^{-5}$	$4.47 \cdot 10^{-5}$	-4.35	10.9	1.72	7.80
b	29.00	$7.00 \cdot 10^{-5}$	$4.35 \cdot 10^{-5}$	-4.36	10.9	1.75	7.82
2a	29.00	$3.50 \cdot 10^{-5}$	$2.35 \cdot 10^{-5}$	-4.63	10.9	1.65	7.83
b	29.00	$3.50 \cdot 10^{-5}$	$2.36 \cdot 10^{-5}$	-4.63	10.9	1.65	7.80
3a	29.00	$1.17 \cdot 10^{-5}$	$7.97 \cdot 10^{-6}$	-5.10	10.9	1.63	7.80
b	29.00	$1.17 \cdot 10^{-5}$	$7.86 \cdot 10^{-6}$	-5.10	10.9	1.65	7.83
4a	29.00	$3.51 \cdot 10^{-6}$	$2.19 \cdot 10^{-6}$	-5.66	10.9	1.75	7.81
b	29.00	$3.51 \cdot 10^{-6}$	$2.16 \cdot 10^{-6}$	-5.67	10.9	1.76	7.80
5a	29.00	$1.17 \cdot 10^{-6}$	$7.17 \cdot 10^{-7}$	-6.14	10.9	1.77	7.79
b	29.00	$1.17 \cdot 10^{-6}$	$7.14 \cdot 10^{-7}$	-6.15	10.9	1.77	7.80
6a	29.00	$3.56 \cdot 10^{-7}$	$2.08 \cdot 10^{-7}$	-6.68	10.9	1.81	7.82
b	29.00	$3.56 \cdot 10^{-7}$	$2.08 \cdot 10^{-7}$	-6.68	10.9	1.81	7.80
7a	29.00	$1.22 \cdot 10^{-7}$	$6.21 \cdot 10^{-8}$	-7.21	10.9	1.95	7.81
b	29.00	$1.22 \cdot 10^{-7}$	$7.48 \cdot 10^{-8}$	-7.13	10.9	1.77	7.81
8a	29.00	$4.07 \cdot 10^{-8}$	$2.28 \cdot 10^{-8}$	-7.64	10.9	1.86	7.80
b	35.00	$4.07 \cdot 10^{-8}$	$2.22 \cdot 10^{-8}$	-7.65	10.9	1.88	7.80

App. C Experimental data for europium

C.1 Experimental data for Eu on BOZ1-1 samples

Tab. C-1: Experimental data for Eu on sample BOZ-323 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.77 \cdot 10^{-6}$	$8.75 \cdot 10^{-9}$	-8.06	6.0	4.86	8.04
b	35.00	$3.77 \cdot 10^{-6}$	$8.98 \cdot 10^{-9}$	-8.05	6.0	4.85	8.02
2a	35.00	$1.89 \cdot 10^{-6}$	$5.80 \cdot 10^{-9}$	-8.24	6.0	4.73	7.98
b	35.00	$1.89 \cdot 10^{-6}$	$4.08 \cdot 10^{-9}$	-8.39	6.0	4.89	8.01
3a	35.00	$7.57 \cdot 10^{-7}$	$1.41 \cdot 10^{-9}$	-8.85	6.0	4.95	8.08
b	35.00	$7.57 \cdot 10^{-7}$	$1.46 \cdot 10^{-9}$	-8.83	6.0	4.94	8.04
4a	35.00	$1.91 \cdot 10^{-7}$	$3.64 \cdot 10^{-10}$	-9.44	6.0	4.94	8.00
b	35.00	$1.91 \cdot 10^{-7}$	$4.06 \cdot 10^{-10}$	-9.39	6.0	4.89	8.06
5a	35.00	$7.79 \cdot 10^{-8}$	$1.51 \cdot 10^{-10}$	-9.82	6.0	4.93	8.16
b	35.00	$7.79 \cdot 10^{-8}$	$1.49 \cdot 10^{-10}$	-9.83	6.0	4.94	8.12
6a	35.00	$2.13 \cdot 10^{-8}$	$4.43 \cdot 10^{-11}$	-10.35	6.0	4.90	8.02
b	35.00	$2.13 \cdot 10^{-8}$	$3.90 \cdot 10^{-11}$	-10.41	6.0	4.96	8.07
7a	35.00	$1.00 \cdot 10^{-8}$	$1.98 \cdot 10^{-11}$	-10.70	6.0	4.93	8.06
b	35.00	$1.00 \cdot 10^{-8}$	$1.78 \cdot 10^{-11}$	-10.75	6.0	4.97	8.05
8a	35.00	$3.40 \cdot 10^{-9}$	$7.13 \cdot 10^{-12}$	-11.15	6.0	4.90	7.99
b	35.00	$3.40 \cdot 10^{-9}$	$6.87 \cdot 10^{-12}$	-11.16	6.0	4.92	8.03

Tab. C-2: Experimental data for Eu on sample BOZ-440 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.77 \cdot 10^{-6}$	$1.03 \cdot 10^{-8}$	-7.99	6.1	4.78	8.01
b	35.00	$3.77 \cdot 10^{-6}$	$1.27 \cdot 10^{-8}$	-7.90	6.1	4.69	8.07
2a	35.00	$1.89 \cdot 10^{-6}$	$4.55 \cdot 10^{-9}$	-8.34	6.1	4.83	8.06
b	35.00	$1.89 \cdot 10^{-6}$	$3.96 \cdot 10^{-9}$	-8.40	6.1	4.89	8.05
3a	35.00	$7.57 \cdot 10^{-7}$	$2.22 \cdot 10^{-9}$	-8.65	6.1	4.75	7.97
b	35.00	$7.57 \cdot 10^{-7}$	$1.38 \cdot 10^{-9}$	-8.86	6.1	4.95	8.01
4a	35.00	$1.91 \cdot 10^{-7}$	$4.45 \cdot 10^{-10}$	-9.35	6.1	4.85	8.08
b	35.00	$1.91 \cdot 10^{-7}$	$4.14 \cdot 10^{-10}$	-9.38	6.1	4.88	7.98
5a	35.00	$7.80 \cdot 10^{-8}$	$1.65 \cdot 10^{-10}$	-9.78	6.1	4.89	8.02
b	35.00	$7.80 \cdot 10^{-8}$	$1.61 \cdot 10^{-10}$	-9.79	6.1	4.90	8.07
6a	35.00	$2.14 \cdot 10^{-8}$	$6.39 \cdot 10^{-11}$	-10.19	6.1	4.74	8.06
b	35.00	$2.14 \cdot 10^{-8}$	$3.87 \cdot 10^{-11}$	-10.41	6.1	4.96	8.07
7a	35.00	$1.01 \cdot 10^{-8}$	$1.86 \cdot 10^{-11}$	-10.73	6.1	4.95	7.99
b	35.00	$1.01 \cdot 10^{-8}$	$2.46 \cdot 10^{-11}$	-10.61	6.1	4.83	8.03
8a	35.00	$3.49 \cdot 10^{-9}$	$7.60 \cdot 10^{-12}$	-11.12	6.1	4.88	7.98
b	35.00	$3.49 \cdot 10^{-9}$	$7.69 \cdot 10^{-12}$	-11.11	6.1	4.87	7.99

Tab. C-3: Experimental data for Eu on sample BOZ-493 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.77 \cdot 10^{-6}$	$3.56 \cdot 10^{-8}$	-7.45	6.4	4.22	8.00
b	35.00	$3.77 \cdot 10^{-6}$	$3.84 \cdot 10^{-8}$	-7.42	6.4	4.18	8.05
2a	35.00	$1.89 \cdot 10^{-6}$	$1.41 \cdot 10^{-8}$	-7.85	6.4	4.32	8.07
b	35.00	$1.89 \cdot 10^{-6}$	$1.46 \cdot 10^{-8}$	-7.83	6.4	4.30	8.06
3a	35.00	$7.57 \cdot 10^{-7}$	$4.78 \cdot 10^{-9}$	-8.32	6.4	4.39	8.06
b	35.00	$7.57 \cdot 10^{-7}$	$4.64 \cdot 10^{-9}$	-8.33	6.4	4.41	8.05
4a	35.00	$1.91 \cdot 10^{-7}$	$1.02 \cdot 10^{-9}$	-8.99	6.4	4.47	8.00
b	35.00	$1.91 \cdot 10^{-7}$	$1.30 \cdot 10^{-9}$	-8.89	6.4	4.36	8.05
5a	35.00	$7.79 \cdot 10^{-8}$	$4.47 \cdot 10^{-10}$	-9.35	6.4	4.44	8.03
b	35.00	$7.79 \cdot 10^{-8}$	$4.18 \cdot 10^{-10}$	-9.38	6.4	4.46	8.06
6a	35.00	$2.13 \cdot 10^{-8}$	$1.10 \cdot 10^{-10}$	-9.96	6.4	4.48	8.03
b	35.00	$2.13 \cdot 10^{-8}$	$1.12 \cdot 10^{-10}$	-9.95	6.4	4.47	8.10
7a	35.00	$1.00 \cdot 10^{-8}$	$5.33 \cdot 10^{-11}$	-10.27	6.4	4.47	7.96
b	35.00	$1.00 \cdot 10^{-8}$	$5.37 \cdot 10^{-11}$	-10.27	6.4	4.46	7.98
8a	35.00	$3.40 \cdot 10^{-9}$	$1.92 \cdot 10^{-11}$	-10.72	6.4	4.44	8.00
b	35.00	$3.40 \cdot 10^{-9}$	$2.06 \cdot 10^{-11}$	-10.69	6.4	4.41	7.96

Tab. C-4: Experimental data for Eu on sample BOZ-521 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.77 \cdot 10^{-6}$	$6.88 \cdot 10^{-8}$	-7.16	5.0	4.04	8.06
b	35.00	$3.77 \cdot 10^{-6}$	$6.27 \cdot 10^{-8}$	-7.20	5.0	4.08	8.12
2a	35.00	$1.89 \cdot 10^{-6}$	$1.96 \cdot 10^{-8}$	-7.71	5.0	4.28	8.10
b	35.00	$1.89 \cdot 10^{-6}$	$1.84 \cdot 10^{-8}$	-7.73	5.0	4.31	8.08
3a	35.00	$7.57 \cdot 10^{-7}$	$5.52 \cdot 10^{-9}$	-8.26	5.0	4.44	8.05
b	35.00	$7.57 \cdot 10^{-7}$	$5.95 \cdot 10^{-9}$	-8.23	5.0	4.40	8.05
4a	35.00	$1.91 \cdot 10^{-7}$	$1.35 \cdot 10^{-9}$	-8.87	5.0	4.45	8.07
b	35.00	$1.91 \cdot 10^{-7}$	$1.37 \cdot 10^{-9}$	-8.86	5.0	4.45	8.06
5a	35.00	$7.79 \cdot 10^{-8}$	$4.90 \cdot 10^{-10}$	-9.31	5.0	4.50	8.00
b	35.00	$7.79 \cdot 10^{-8}$	$5.12 \cdot 10^{-10}$	-9.29	5.0	4.48	8.02
6a	35.00	$2.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-10}$	-9.95	5.0	4.58	8.02
b	35.00	$2.13 \cdot 10^{-8}$	$1.12 \cdot 10^{-10}$	-9.95	5.0	4.58	8.01
7a	35.00	$1.00 \cdot 10^{-8}$	$5.58 \cdot 10^{-11}$	-10.25	5.0	4.56	8.05
b	35.00	$1.00 \cdot 10^{-8}$	$5.45 \cdot 10^{-11}$	-10.26	5.0	4.57	8.05
8a	35.00	$3.40 \cdot 10^{-9}$	$1.74 \cdot 10^{-11}$	-10.76	5.0	4.59	7.98
b	35.00	$3.40 \cdot 10^{-9}$	$1.86 \cdot 10^{-11}$	-10.73	5.0	4.56	8.02

Tab. C-5: Experimental data for Eu on sample BOZ-572 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.77 \cdot 10^{-6}$	$1.82 \cdot 10^{-8}$	-7.74	6.6	4.50	7.90
b	35.00	$3.77 \cdot 10^{-6}$	$2.76 \cdot 10^{-8}$	-7.56	6.6	4.31	7.90
2a	35.00	$1.89 \cdot 10^{-6}$	$6.25 \cdot 10^{-9}$	-8.20	6.6	4.66	7.91
b	35.00	$1.89 \cdot 10^{-6}$	$5.33 \cdot 10^{-9}$	-8.27	6.6	4.73	7.90
3a	35.00	$7.57 \cdot 10^{-7}$	$1.66 \cdot 10^{-9}$	-8.78	6.6	4.84	7.90
b	35.00	$7.57 \cdot 10^{-7}$	$1.55 \cdot 10^{-9}$	-8.81	6.6	4.87	7.93
4a	35.00	$1.91 \cdot 10^{-7}$	$2.91 \cdot 10^{-10}$	-9.54	6.6	5.00	7.88
b	35.00	$1.91 \cdot 10^{-7}$	$2.75 \cdot 10^{-10}$	-9.56	6.6	5.02	7.89
5a	35.00	$7.80 \cdot 10^{-8}$	$1.54 \cdot 10^{-10}$	-9.81	6.6	4.88	7.88
b	35.00	$7.80 \cdot 10^{-8}$	$1.18 \cdot 10^{-10}$	-9.93	6.6	5.00	7.89
6a	35.00	$2.14 \cdot 10^{-8}$	$3.47 \cdot 10^{-11}$	-10.46	6.6	4.97	7.90
b	35.00	$2.14 \cdot 10^{-8}$	$2.45 \cdot 10^{-11}$	-10.61	6.6	5.12	7.87
7a	35.00	$1.01 \cdot 10^{-8}$	$2.37 \cdot 10^{-11}$	-10.62	6.6	4.81	7.88
b	35.00	$1.01 \cdot 10^{-8}$	$1.82 \cdot 10^{-11}$	-10.74	6.6	4.92	7.87
8a	35.00	$3.49 \cdot 10^{-9}$	$5.56 \cdot 10^{-12}$	-11.25	6.6	4.98	7.97
b	35.00	$3.49 \cdot 10^{-9}$	$5.43 \cdot 10^{-12}$	-11.26	6.6	4.99	7.95

Tab. C-6: Experimental data for Eu on sample BOZ-681 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.77 \cdot 10^{-6}$	$3.72 \cdot 10^{-8}$	-7.43	4.8	4.32	8.14
b	35.00	$3.77 \cdot 10^{-6}$	$3.54 \cdot 10^{-8}$	-7.45	4.8	4.34	8.10
2a	35.00	$1.89 \cdot 10^{-6}$	$1.27 \cdot 10^{-8}$	-7.90	4.8	4.49	8.14
b	35.00	$1.89 \cdot 10^{-6}$	$1.40 \cdot 10^{-8}$	-7.85	4.8	4.44	8.12
3a	35.00	$7.57 \cdot 10^{-7}$	$3.62 \cdot 10^{-9}$	-8.44	4.8	4.64	8.08
b	35.00	$7.57 \cdot 10^{-7}$	$5.10 \cdot 10^{-9}$	-8.29	4.8	4.49	8.10
4a	35.00	$1.91 \cdot 10^{-7}$	$7.45 \cdot 10^{-10}$	-9.13	4.8	4.73	8.05
b	35.00	$1.91 \cdot 10^{-7}$	$6.65 \cdot 10^{-10}$	-9.18	4.8	4.77	8.08
5a	35.00	$7.79 \cdot 10^{-8}$	$2.86 \cdot 10^{-10}$	-9.54	4.8	4.75	8.02
b	35.00	$7.79 \cdot 10^{-8}$	$2.42 \cdot 10^{-10}$	-9.62	4.8	4.82	8.01
6a	35.00	$2.13 \cdot 10^{-8}$	$6.69 \cdot 10^{-11}$	-10.17	4.8	4.82	7.96
b	35.00	$2.13 \cdot 10^{-8}$	$7.45 \cdot 10^{-11}$	-10.13	4.8	4.77	7.99
7a	35.00	$1.00 \cdot 10^{-8}$	$3.48 \cdot 10^{-11}$	-10.46	4.8	4.77	8.02
b	35.00	$1.00 \cdot 10^{-8}$	$3.97 \cdot 10^{-11}$	-10.40	4.8	4.72	8.01
8a	35.00	$3.40 \cdot 10^{-9}$	$1.01 \cdot 10^{-11}$	-11.00	4.8	4.84	8.04
b	35.00	$3.40 \cdot 10^{-9}$	$9.90 \cdot 10^{-12}$	-11.00	4.8	4.85	8.02

C.2 Experimental data for Eu on BUL1-1 samples

Tab. C-7: Experimental data for Eu on sample BUL-845 in its corresponding SPW (cf. Tab. 2-4).

Sample	Vol (10^{-3} L)	Eu_{in} (M)	Eu_{aq} (M)	Log Eu_{aq} (M)	S/L ratio (10^{-3} kg/L)	log R_d (L/kg)	pH
1a	30.00	$4.80 \cdot 10^{-6}$	$3.47 \cdot 10^{-9}$	-8.46	33.5	4.62	7.68
b	30.00	$4.80 \cdot 10^{-6}$	$2.42 \cdot 10^{-9}$	-8.62	33.3	4.77	7.61
2a	30.00	$2.00 \cdot 10^{-6}$	$1.34 \cdot 10^{-9}$	-8.87	35.3	4.63	7.71
b	30.00	$2.00 \cdot 10^{-6}$	$1.31 \cdot 10^{-9}$	-8.88	34.3	4.65	7.70
3a	30.00	$8.03 \cdot 10^{-7}$	$1.37 \cdot 10^{-9}$	-8.86	33.5	4.24	7.67
b	30.00	$8.03 \cdot 10^{-7}$	$6.54 \cdot 10^{-10}$	-9.18	33.5	4.56	7.69
4a	30.00	$2.03 \cdot 10^{-7}$	$7.57 \cdot 10^{-11}$	-10.12	66.2	4.61	7.63
b	30.00	$2.03 \cdot 10^{-7}$	$9.13 \cdot 10^{-11}$	-10.04	65.9	4.53	7.60
5a	30.00	$8.26 \cdot 10^{-8}$	$5.80 \cdot 10^{-11}$	-10.24	66.5	4.33	7.56
b	30.00	$8.26 \cdot 10^{-8}$	$3.55 \cdot 10^{-11}$	-10.45	66.5	4.54	7.65
6a	30.00	$2.26 \cdot 10^{-8}$	$7.83 \cdot 10^{-12}$	-11.11	166.3	4.24	7.14
b	30.00	$2.26 \cdot 10^{-8}$	$5.14 \cdot 10^{-12}$	-11.29	166.2	4.42	7.52
7a	30.00	$1.06 \cdot 10^{-8}$	$1.44 \cdot 10^{-12}$	-11.84	166.3	4.65	7.52
b	30.00	$1.06 \cdot 10^{-8}$	$2.68 \cdot 10^{-12}$	-11.57	168.9	4.37	7.55
8a	30.00	$3.60 \cdot 10^{-9}$	$7.54 \cdot 10^{-13}$	-12.12	166.8	4.46	7.61
b	30.00	$3.60 \cdot 10^{-9}$	$5.99 \cdot 10^{-13}$	-12.22	167.0	4.56	7.60

Tab. C-8: Experimental data for Eu on sample BUL-861 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$4.12 \cdot 10^{-6}$	$1.55 \cdot 10^{-7}$	-6.81	8.2	3.49	7.56
b	35.00	$4.12 \cdot 10^{-6}$	$1.20 \cdot 10^{-7}$	-6.92	8.2	3.61	7.53
2a	35.00	$1.72 \cdot 10^{-6}$	$3.49 \cdot 10^{-8}$	-7.46	8.2	3.77	7.56
b	35.00	$1.72 \cdot 10^{-6}$	$3.34 \cdot 10^{-8}$	-7.48	8.2	3.79	7.52
3a	35.00	$6.88 \cdot 10^{-7}$	$6.94 \cdot 10^{-9}$	-8.16	8.2	4.08	7.58
b	35.00	$6.88 \cdot 10^{-7}$	$6.87 \cdot 10^{-9}$	-8.16	8.2	4.08	7.64
4a	35.00	$1.74 \cdot 10^{-7}$	$1.40 \cdot 10^{-9}$	-8.85	8.2	4.18	7.62
b	35.00	$1.74 \cdot 10^{-7}$	$1.65 \cdot 10^{-9}$	-8.78	8.2	4.10	7.62
5a	35.00	$7.08 \cdot 10^{-8}$	$4.66 \cdot 10^{-10}$	-9.33	8.2	4.26	7.61
b	35.00	$7.08 \cdot 10^{-8}$	$5.67 \cdot 10^{-10}$	-9.25	8.2	4.18	7.57
6a	35.00	$1.94 \cdot 10^{-8}$	$1.17 \cdot 10^{-10}$	-9.93	8.2	4.30	7.59
b	35.00	$1.94 \cdot 10^{-8}$	$1.11 \cdot 10^{-10}$	-9.95	8.2	4.32	7.58
7a	35.00	$9.09 \cdot 10^{-9}$	$5.21 \cdot 10^{-11}$	-10.28	8.2	4.32	7.57
b	35.00	$9.09 \cdot 10^{-9}$	$4.89 \cdot 10^{-11}$	-10.31	8.2	4.35	7.56
8a	35.00	$3.09 \cdot 10^{-9}$	$1.77 \cdot 10^{-11}$	-10.75	8.2	4.32	7.49
b	35.00	$3.09 \cdot 10^{-9}$	$1.29 \cdot 10^{-11}$	-10.89	8.2	4.46	7.54

Tab. C-9: Experimental data for Eu on sample BUL-921 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$4.12 \cdot 10^{-6}$	$1.11 \cdot 10^{-7}$	-6.96	7.9	3.66	7.55
b	35.00	$4.12 \cdot 10^{-6}$	$1.03 \cdot 10^{-7}$	-6.99	7.9	3.69	7.59
2a	35.00	$1.72 \cdot 10^{-6}$	$1.48 \cdot 10^{-8}$	-7.83	7.9	4.16	7.43
b	35.00	$1.72 \cdot 10^{-6}$	$2.85 \cdot 10^{-8}$	-7.55	7.9	3.88	7.54
3a	35.00	$6.88 \cdot 10^{-7}$	$2.62 \cdot 10^{-9}$	-8.58	7.9	4.52	7.46
b	35.00	$6.88 \cdot 10^{-7}$	$2.39 \cdot 10^{-9}$	-8.62	7.9	4.56	7.45
4a	35.00	$1.74 \cdot 10^{-7}$	$5.70 \cdot 10^{-10}$	-9.24	7.9	4.59	7.43
b	35.00	$1.74 \cdot 10^{-7}$	$5.46 \cdot 10^{-10}$	-9.26	7.9	4.60	7.49
5a	35.00	$7.08 \cdot 10^{-8}$	$1.87 \cdot 10^{-10}$	-9.73	7.9	4.68	7.49
b	35.00	$7.08 \cdot 10^{-8}$	$2.05 \cdot 10^{-10}$	-9.69	7.9	4.64	7.42
6a	35.00	$1.94 \cdot 10^{-8}$	$3.80 \cdot 10^{-11}$	-10.42	7.9	4.81	7.42
b	35.00	$1.94 \cdot 10^{-8}$	$3.90 \cdot 10^{-11}$	-10.41	7.9	4.80	7.40
7a	35.00	$9.09 \cdot 10^{-9}$	$2.42 \cdot 10^{-11}$	-10.62	7.9	4.68	7.37
b	35.00	$9.09 \cdot 10^{-9}$	$3.50 \cdot 10^{-11}$	-10.46	7.9	4.52	7.38
8a	35.00	$3.09 \cdot 10^{-9}$	$8.26 \cdot 10^{-12}$	-11.08	7.9	4.68	7.39
b	35.00	$3.09 \cdot 10^{-9}$	$1.33 \cdot 10^{-11}$	-10.88	7.9	4.47	7.39

Tab. C-10: Experimental data for Eu on sample BUL-955 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$4.12 \cdot 10^{-6}$	$9.88 \cdot 10^{-8}$	-7.01	7.9	3.71	7.55
b	35.00	$4.12 \cdot 10^{-6}$	$5.30 \cdot 10^{-8}$	-7.28	7.9	3.99	7.49
2a	35.00	$1.72 \cdot 10^{-6}$	$2.58 \cdot 10^{-8}$	-7.59	7.9	3.92	7.40
b	35.00	$1.72 \cdot 10^{-6}$	$2.45 \cdot 10^{-8}$	-7.61	7.9	3.94	7.48
3a	35.00	$6.88 \cdot 10^{-7}$	$2.43 \cdot 10^{-9}$	-8.61	7.9	4.56	7.48
b	35.00	$6.88 \cdot 10^{-7}$	$1.79 \cdot 10^{-9}$	-8.75	7.9	4.69	7.49
4a	35.00	$1.74 \cdot 10^{-7}$	$4.32 \cdot 10^{-10}$	-9.36	7.9	4.71	7.48
b	35.00	$1.74 \cdot 10^{-7}$	$4.88 \cdot 10^{-10}$	-9.31	7.9	4.65	7.51
5a	35.00	$7.08 \cdot 10^{-8}$	$1.75 \cdot 10^{-10}$	-9.76	7.9	4.71	7.38
b	35.00	$7.08 \cdot 10^{-8}$	$1.65 \cdot 10^{-10}$	-9.78	7.9	4.74	7.48
6a	35.00	$1.94 \cdot 10^{-8}$	$3.64 \cdot 10^{-11}$	-10.44	7.9	4.83	7.43
b	35.00	$1.94 \cdot 10^{-8}$	$4.06 \cdot 10^{-11}$	-10.39	7.9	4.78	7.47
7a	35.00	$9.09 \cdot 10^{-9}$	$2.62 \cdot 10^{-11}$	-10.58	7.9	4.64	7.35
b	35.00	$9.09 \cdot 10^{-9}$	$2.85 \cdot 10^{-11}$	-10.54	7.9	4.61	7.34
8a	35.00	$3.09 \cdot 10^{-9}$	$8.97 \cdot 10^{-12}$	-11.05	7.9	4.64	7.38
b	35.00	$3.09 \cdot 10^{-9}$	$8.78 \cdot 10^{-12}$	-11.06	7.9	4.65	7.38

Tab. C-11: Experimental data for Eu on sample BUL-995 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$1.72 \cdot 10^{-6}$	$1.54 \cdot 10^{-8}$	-7.81	6.4	4.24	7.52
b	35.00	$1.72 \cdot 10^{-6}$	$1.35 \cdot 10^{-8}$	-7.87	6.4	4.29	7.53
2a	35.00	$8.60 \cdot 10^{-7}$	$5.67 \cdot 10^{-9}$	-8.25	6.4	4.37	7.52
b	35.00	$8.60 \cdot 10^{-7}$	$5.04 \cdot 10^{-9}$	-8.30	6.4	4.42	7.51
3a	35.00	$5.17 \cdot 10^{-7}$	$2.93 \cdot 10^{-9}$	-8.53	6.4	4.43	7.42
b	35.00	$5.17 \cdot 10^{-7}$	$2.72 \cdot 10^{-9}$	-8.57	6.4	4.47	7.49
4a	35.00	$2.60 \cdot 10^{-7}$	$1.66 \cdot 10^{-9}$	-8.78	6.4	4.38	7.48
b	35.00	$2.60 \cdot 10^{-7}$	$1.15 \cdot 10^{-9}$	-8.94	6.4	4.54	7.52
5a	35.00	$8.84 \cdot 10^{-8}$	$4.37 \cdot 10^{-10}$	-9.36	6.4	4.50	7.51
b	35.00	$8.84 \cdot 10^{-8}$	$4.92 \cdot 10^{-10}$	-9.31	6.4	4.44	7.48
6a	35.00	$5.41 \cdot 10^{-8}$	$2.27 \cdot 10^{-10}$	-9.64	6.4	4.57	7.50
b	35.00	$5.41 \cdot 10^{-8}$	$2.05 \cdot 10^{-10}$	-9.69	6.4	4.61	7.51
7a	35.00	$2.83 \cdot 10^{-8}$	$1.28 \cdot 10^{-10}$	-9.89	6.4	4.53	7.43
b	35.00	$2.83 \cdot 10^{-8}$	$1.11 \cdot 10^{-10}$	-9.95	6.4	4.60	7.48
8a	35.00	$1.11 \cdot 10^{-8}$	$4.92 \cdot 10^{-11}$	-10.31	6.4	4.54	7.51
b	35.00	$1.11 \cdot 10^{-8}$	$3.91 \cdot 10^{-11}$	-10.41	6.4	4.64	7.51
9a	35.00	$7.47 \cdot 10^{-9}$	$3.36 \cdot 10^{-11}$	-10.47	6.4	4.54	7.51
b	35.00	$7.47 \cdot 10^{-9}$	$3.46 \cdot 10^{-11}$	-10.46	6.4	4.52	7.50
10a	35.00	$4.84 \cdot 10^{-9}$	$1.77 \cdot 10^{-11}$	-10.75	6.4	4.63	7.50
b	35.00	$4.84 \cdot 10^{-9}$	$1.49 \cdot 10^{-11}$	-10.83	6.4	4.70	7.49
11a	35.00	$3.23 \cdot 10^{-9}$	$1.30 \cdot 10^{-11}$	-10.89	6.4	4.59	7.50
b	35.00	$3.23 \cdot 10^{-9}$	$1.16 \cdot 10^{-11}$	-10.94	6.4	4.63	7.51
12a	35.00	$2.74 \cdot 10^{-9}$	$9.22 \cdot 10^{-12}$	-11.04	6.4	4.66	7.54
b	35.00	$2.74 \cdot 10^{-9}$	$7.64 \cdot 10^{-12}$	-11.12	6.4	4.75	7.54

Tab. C-12: Experimental data for Eu on sample BUL-1002 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$4.12 \cdot 10^{-6}$	$2.27 \cdot 10^{-8}$	-7.64	7.0	4.41	7.56
b	35.00	$4.12 \cdot 10^{-6}$	$2.21 \cdot 10^{-8}$	-7.65	7.0	4.42	7.60
2a	35.00	$1.72 \cdot 10^{-6}$	$8.01 \cdot 10^{-9}$	-8.10	7.0	4.49	7.54
b	35.00	$1.72 \cdot 10^{-6}$	$6.98 \cdot 10^{-9}$	-8.16	7.0	4.55	7.54
3a	35.00	$6.88 \cdot 10^{-7}$	$2.80 \cdot 10^{-9}$	-8.55	7.0	4.55	7.61
b	35.00	$6.88 \cdot 10^{-7}$	$2.48 \cdot 10^{-9}$	-8.61	7.0	4.60	7.61
4a	35.00	$1.74 \cdot 10^{-7}$	$6.95 \cdot 10^{-10}$	-9.16	7.0	4.55	7.59
b	35.00	$1.74 \cdot 10^{-7}$	$6.71 \cdot 10^{-10}$	-9.17	7.0	4.57	7.63
5a	35.00	$7.08 \cdot 10^{-8}$	$2.93 \cdot 10^{-10}$	-9.53	7.0	4.54	7.40
b	35.00	$7.08 \cdot 10^{-8}$	$2.85 \cdot 10^{-10}$	-9.55	7.0	4.55	7.55
6a	35.00	$1.94 \cdot 10^{-8}$	$6.71 \cdot 10^{-11}$	-10.17	7.0	4.62	7.61
b	35.00	$1.94 \cdot 10^{-8}$	$6.98 \cdot 10^{-11}$	-10.16	7.0	4.60	7.66
7a	35.00	$9.09 \cdot 10^{-9}$	$5.60 \cdot 10^{-11}$	-10.25	7.0	4.36	7.59
b	35.00	$9.09 \cdot 10^{-9}$	$4.31 \cdot 10^{-11}$	-10.37	7.0	4.48	7.54
8a	35.00	$3.09 \cdot 10^{-9}$	$1.06 \cdot 10^{-11}$	-10.98	7.0	4.62	7.59
b	35.00	$3.09 \cdot 10^{-9}$	$9.16 \cdot 10^{-12}$	-11.04	7.0	4.68	7.50

Tab. C-13: Experimental data for Eu on sample BUL-1017 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$4.12 \cdot 10^{-6}$	$2.15 \cdot 10^{-7}$	-6.67	4.8	3.58	7.54
b	35.00	$4.12 \cdot 10^{-6}$	$2.03 \cdot 10^{-7}$	-6.69	4.8	3.60	7.55
2a	35.00	$1.72 \cdot 10^{-6}$	$5.73 \cdot 10^{-8}$	-7.24	4.8	3.78	7.54
b	35.00	$1.72 \cdot 10^{-6}$	$2.12 \cdot 10^{-8}$	-7.67	4.8	4.22	7.47
3a	35.00	$6.88 \cdot 10^{-7}$	$5.33 \cdot 10^{-9}$	-8.27	4.8	4.43	7.56
b	35.00	$6.88 \cdot 10^{-7}$	$5.15 \cdot 10^{-9}$	-8.29	4.8	4.44	7.57
4a	35.00	$1.74 \cdot 10^{-7}$	$1.14 \cdot 10^{-9}$	-8.94	4.8	4.50	7.54
b	35.00	$1.74 \cdot 10^{-7}$	$1.09 \cdot 10^{-9}$	-8.96	4.8	4.52	7.56
5a	35.00	$7.08 \cdot 10^{-8}$	$3.41 \cdot 10^{-10}$	-9.47	4.8	4.63	7.51
b	35.00	$7.08 \cdot 10^{-8}$	$4.37 \cdot 10^{-10}$	-9.36	4.8	4.52	7.51
6a	35.00	$1.94 \cdot 10^{-8}$	$8.72 \cdot 10^{-11}$	-10.06	4.8	4.66	7.54
b	35.00	$1.94 \cdot 10^{-8}$	$9.69 \cdot 10^{-11}$	-10.01	4.8	4.62	7.59
7a	35.00	$9.09 \cdot 10^{-9}$	$5.76 \cdot 10^{-11}$	-10.24	4.8	4.51	7.51
b	35.00	$9.09 \cdot 10^{-9}$	$5.94 \cdot 10^{-11}$	-10.23	4.8	4.50	7.50c
8a	35.00	$3.09 \cdot 10^{-9}$	$2.21 \cdot 10^{-11}$	-10.66	4.8	4.46	7.48
b	35.00	$3.09 \cdot 10^{-9}$	$2.10 \cdot 10^{-11}$	-10.68	4.8	4.48	7.48

C.3 Experimental data for Eu on TRU1-1 samples

Tab. C-14: Experimental data for Eu on sample TRU-748 in its corresponding SPW (cf. Tab. 2-4).

Sample	Vol (10^{-3} L)	Eu_{in} (M)	Eu_{aq} (M)	Log Eu_{aq} (M)	S/L ratio (10^{-3} kg/L)	log R_d (L/kg)	pH
1a	35.00	$3.43 \cdot 10^{-6}$	$7.19 \cdot 10^{-8}$	-7.14	6.4	3.87	7.64
b	35.00	$3.43 \cdot 10^{-6}$	$7.32 \cdot 10^{-8}$	-7.14	6.4	3.86	7.61
2a	35.00	$1.72 \cdot 10^{-6}$	$1.46 \cdot 10^{-8}$	-7.84	6.4	4.26	7.65
b	35.00	$1.72 \cdot 10^{-6}$	$1.22 \cdot 10^{-8}$	-7.91	6.4	4.34	7.66
3a	35.00	$6.88 \cdot 10^{-7}$	$5.88 \cdot 10^{-9}$	-8.23	6.4	4.26	7.69
b	35.00	$6.88 \cdot 10^{-7}$	$5.64 \cdot 10^{-9}$	-8.25	6.4	4.28	7.67
4a	35.00	$1.74 \cdot 10^{-7}$	$1.27 \cdot 10^{-9}$	-8.90	6.4	4.33	7.70
b	35.00	$1.74 \cdot 10^{-7}$	$1.24 \cdot 10^{-9}$	-8.91	6.4	4.34	7.71
5a	35.00	$7.07 \cdot 10^{-8}$	$2.29 \cdot 10^{-10}$	-9.64	6.4	4.69	7.65
b	35.00	$7.07 \cdot 10^{-8}$	$4.75 \cdot 10^{-10}$	-9.32	6.4	4.37	7.65
6a	35.00	$1.93 \cdot 10^{-8}$	$6.27 \cdot 10^{-11}$	-10.20	6.4	4.68	7.64
b	35.00	$1.93 \cdot 10^{-8}$	$1.24 \cdot 10^{-10}$	-9.91	6.4	4.38	7.71
7a	35.00	$9.01 \cdot 10^{-9}$	$3.35 \cdot 10^{-11}$	-10.47	6.4	4.62	7.64
b	35.00	$9.01 \cdot 10^{-9}$	$5.05 \cdot 10^{-11}$	-10.30	6.4	4.44	7.65
8a	35.00	$3.01 \cdot 10^{-9}$	$1.84 \cdot 10^{-11}$	-10.73	6.4	4.41	7.65
b	35.00	$3.01 \cdot 10^{-9}$	$1.97 \cdot 10^{-11}$	-10.71	6.4	4.38	7.67

Tab. C-15: Experimental data for Eu on sample TRU-794 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.43 \cdot 10^{-6}$	$1.85 \cdot 10^{-7}$	-6.73	6.3	3.45	7.58
b	35.00	$3.43 \cdot 10^{-6}$	$1.81 \cdot 10^{-7}$	-6.74	6.3	3.46	7.62
2a	35.00	$1.72 \cdot 10^{-6}$	$5.30 \cdot 10^{-8}$	-7.28	6.3	3.70	7.57
b	35.00	$1.72 \cdot 10^{-6}$	$4.60 \cdot 10^{-8}$	-7.34	6.3	3.76	7.53
3a	35.00	$6.88 \cdot 10^{-7}$	$1.20 \cdot 10^{-8}$	-7.92	6.3	3.95	7.55
b	35.00	$6.88 \cdot 10^{-7}$	$9.36 \cdot 10^{-9}$	-8.03	6.3	4.06	7.62
4a	35.00	$1.74 \cdot 10^{-7}$	$2.39 \cdot 10^{-9}$	-8.62	6.3	4.06	7.61
b	35.00	$1.74 \cdot 10^{-7}$	$2.38 \cdot 10^{-9}$	-8.62	6.3	4.06	7.60
5a	35.00	$7.08 \cdot 10^{-8}$	$8.60 \cdot 10^{-10}$	-9.07	6.3	4.11	7.54
b	35.00	$7.08 \cdot 10^{-8}$	$6.40 \cdot 10^{-10}$	-9.19	6.3	4.24	7.62
6a	35.00	$1.94 \cdot 10^{-8}$	$1.93 \cdot 10^{-10}$	-9.72	6.3	4.20	7.68
b	35.00	$1.94 \cdot 10^{-8}$	$1.81 \cdot 10^{-10}$	-9.74	6.3	4.23	7.58
7a	35.00	$9.09 \cdot 10^{-9}$	$7.86 \cdot 10^{-11}$	-10.10	6.3	4.26	7.68
b	35.00	$9.09 \cdot 10^{-9}$	$8.85 \cdot 10^{-11}$	-10.05	6.3	4.21	7.72
8a	35.00	$3.09 \cdot 10^{-9}$	$3.21 \cdot 10^{-11}$	-10.49	6.3	4.18	7.56
b	35.00	$3.09 \cdot 10^{-9}$	$2.84 \cdot 10^{-11}$	-10.55	6.3	4.23	7.68

Tab. C-16: Experimental data for Eu on sample TRU-815 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.43 \cdot 10^{-6}$	$1.85 \cdot 10^{-7}$	-6.73	4.4	3.60	7.63
b	35.00	$3.43 \cdot 10^{-6}$	$1.86 \cdot 10^{-7}$	-6.73	4.4	3.60	7.60
2a	35.00	$1.72 \cdot 10^{-6}$	$3.52 \cdot 10^{-8}$	-7.45	4.4	4.03	7.61
b	35.00	$1.72 \cdot 10^{-6}$	$4.89 \cdot 10^{-8}$	-7.31	4.4	3.89	7.62
3a	35.00	$6.88 \cdot 10^{-7}$	$1.39 \cdot 10^{-8}$	-7.86	4.4	4.04	7.64
b	35.00	$6.88 \cdot 10^{-7}$	$1.23 \cdot 10^{-8}$	-7.91	4.4	4.09	7.64
4a	35.00	$1.74 \cdot 10^{-7}$	$2.82 \cdot 10^{-9}$	-8.55	4.4	4.14	7.64
b	35.00	$1.74 \cdot 10^{-7}$	$2.89 \cdot 10^{-9}$	-8.54	4.4	4.13	7.64
5a	35.00	$7.07 \cdot 10^{-8}$	$8.00 \cdot 10^{-10}$	-9.10	4.4	4.30	7.64
b	35.00	$7.07 \cdot 10^{-8}$	$8.66 \cdot 10^{-10}$	-9.06	4.4	4.26	7.62
6a	35.00	$1.93 \cdot 10^{-8}$	$2.57 \cdot 10^{-10}$	-9.59	4.4	4.22	7.63
b	35.00	$1.93 \cdot 10^{-8}$	$2.06 \cdot 10^{-10}$	-9.69	4.4	4.32	7.66
7a	35.00	$9.01 \cdot 10^{-9}$	$1.18 \cdot 10^{-10}$	-9.93	4.4	4.23	7.64
b	35.00	$9.01 \cdot 10^{-9}$	$1.19 \cdot 10^{-10}$	-9.92	4.4	4.23	7.65
8a	35.00	$3.01 \cdot 10^{-9}$	$3.57 \cdot 10^{-11}$	-10.45	4.4	4.28	7.58
b	35.00	$3.01 \cdot 10^{-9}$	$3.53 \cdot 10^{-11}$	-10.45	4.4	4.28	7.63

Tab. C-17: Experimental data for Eu on sample TRU-831 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.43 \cdot 10^{-6}$	$9.16 \cdot 10^{-8}$	-7.04	6.2	3.77	7.52
b	35.00	$3.43 \cdot 10^{-6}$	$5.69 \cdot 10^{-8}$	-7.25	6.2	3.98	7.54
2a	35.00	$1.72 \cdot 10^{-6}$	$2.69 \cdot 10^{-8}$	-7.57	6.2	4.01	7.55
b	35.00	$1.72 \cdot 10^{-6}$	$2.57 \cdot 10^{-8}$	-7.59	6.2	4.03	7.54
3a	35.00	$6.88 \cdot 10^{-7}$	$2.43 \cdot 10^{-9}$	-8.61	6.2	4.66	7.49
b	35.00	$6.88 \cdot 10^{-7}$	$4.15 \cdot 10^{-9}$	-8.38	6.2	4.43	7.50
4a	35.00	$1.74 \cdot 10^{-7}$	$1.26 \cdot 10^{-9}$	-8.90	6.2	4.34	7.59
b	35.00	$1.74 \cdot 10^{-7}$	$1.24 \cdot 10^{-9}$	-8.91	6.2	4.35	7.58
5a	35.00	$7.08 \cdot 10^{-8}$	$4.64 \cdot 10^{-10}$	-9.33	6.2	4.39	7.58
b	35.00	$7.08 \cdot 10^{-8}$	$2.18 \cdot 10^{-10}$	-9.66	6.2	4.72	7.57
6a	35.00	$1.94 \cdot 10^{-8}$	$1.16 \cdot 10^{-10}$	-9.93	6.2	4.43	7.58
b	35.00	$1.94 \cdot 10^{-8}$	$6.63 \cdot 10^{-11}$	-10.18	6.2	4.67	7.51
7a	35.00	$9.09 \cdot 10^{-9}$	$3.70 \cdot 10^{-11}$	-10.43	6.2	4.60	7.53
b	35.00	$9.09 \cdot 10^{-9}$	$2.36 \cdot 10^{-11}$	-10.63	6.2	4.79	7.51
8a	35.00	$3.09 \cdot 10^{-9}$	$1.39 \cdot 10^{-11}$	-10.86	6.2	4.55	7.50
b	35.00	$3.09 \cdot 10^{-9}$	$1.28 \cdot 10^{-11}$	-10.89	6.2	4.59	7.49

Tab. C-18: Experimental data for Eu on sample TRU-882 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.66 \cdot 10^{-6}$	$1.70 \cdot 10^{-8}$	-7.77	7.0	4.48	7.63
b	35.00	$3.66 \cdot 10^{-6}$	$2.03 \cdot 10^{-8}$	-7.69	7.0	4.41	7.60
2a	35.00	$1.83 \cdot 10^{-6}$	$5.66 \cdot 10^{-9}$	-8.25	7.0	4.66	7.61
b	35.00	$1.83 \cdot 10^{-6}$	$7.55 \cdot 10^{-9}$	-8.12	7.0	4.54	7.62
3a	35.00	$7.34 \cdot 10^{-7}$	$1.83 \cdot 10^{-9}$	-8.74	7.0	4.76	7.64
b	35.00	$7.34 \cdot 10^{-7}$	$1.77 \cdot 10^{-9}$	-8.75	7.0	4.77	7.64
4a	35.00	$1.85 \cdot 10^{-7}$	$5.52 \cdot 10^{-10}$	-9.26	7.0	4.68	7.64
b	35.00	$1.85 \cdot 10^{-7}$	$4.92 \cdot 10^{-10}$	-9.31	7.0	4.73	7.64
5a	35.00	$7.54 \cdot 10^{-8}$	$1.56 \cdot 10^{-10}$	-9.81	7.0	4.84	7.64
b	35.00	$7.54 \cdot 10^{-8}$	$1.11 \cdot 10^{-10}$	-9.95	7.0	4.98	7.62
6a	35.00	$2.06 \cdot 10^{-8}$	$3.81 \cdot 10^{-11}$	-10.42	7.0	4.88	7.63
b	35.00	$2.06 \cdot 10^{-8}$	$2.45 \cdot 10^{-11}$	-10.61	7.0	5.08	7.66
7a	35.00	$9.61 \cdot 10^{-9}$	$1.88 \cdot 10^{-11}$	-10.73	7.0	4.86	7.64
b	35.00	$9.61 \cdot 10^{-9}$	$1.80 \cdot 10^{-11}$	-10.74	7.0	4.88	7.65
8a	35.00	$3.21 \cdot 10^{-9}$	$4.79 \cdot 10^{-12}$	-10.32	7.0	4.98	7.58
b	35.00	$3.21 \cdot 10^{-9}$	$5.98 \cdot 10^{-12}$	-10.22	7.0	4.88	7.63

Tab. C-19: Experimental data for Eu on sample TRU-923 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.66 \cdot 10^{-6}$	$2.65 \cdot 10^{-8}$	-7.58	6.1	4.35	7.52
b	35.00	$3.66 \cdot 10^{-6}$	$2.54 \cdot 10^{-8}$	-7.60	6.1	4.37	7.54
2a	35.00	$1.83 \cdot 10^{-6}$	$8.26 \cdot 10^{-9}$	-8.08	6.1	4.56	7.55
b	35.00	$1.83 \cdot 10^{-6}$	$9.18 \cdot 10^{-9}$	-8.04	6.1	4.51	7.54
3a	35.00	$7.34 \cdot 10^{-7}$	$2.58 \cdot 10^{-9}$	-8.59	6.1	4.67	7.49
b	35.00	$7.34 \cdot 10^{-7}$	$2.46 \cdot 10^{-9}$	-8.61	6.1	4.69	7.50
4a	35.00	$1.85 \cdot 10^{-7}$	$6.69 \cdot 10^{-10}$	-9.17	6.1	4.66	7.59
b	35.00	$1.85 \cdot 10^{-7}$	$7.06 \cdot 10^{-10}$	-9.15	6.1	4.63	7.58
5a	35.00	$7.55 \cdot 10^{-8}$	$1.92 \cdot 10^{-10}$	-9.72	6.1	4.81	7.58
b	35.00	$7.55 \cdot 10^{-8}$	$1.90 \cdot 10^{-10}$	-9.72	6.1	4.82	7.57
6a	35.00	$2.07 \cdot 10^{-8}$	$5.65 \cdot 10^{-11}$	-10.25	6.1	4.78	7.58
b	35.00	$2.07 \cdot 10^{-8}$	$4.99 \cdot 10^{-11}$	-10.30	6.1	4.83	7.51
7a	35.00	$9.69 \cdot 10^{-9}$	$2.54 \cdot 10^{-11}$	-10.59	6.1	4.80	7.53
b	35.00	$9.69 \cdot 10^{-9}$	$2.48 \cdot 10^{-11}$	-10.61	6.1	4.81	7.51
8a	35.00	$3.29 \cdot 10^{-9}$	$8.66 \cdot 10^{-12}$	-10.06	6.1	4.80	7.50
b	35.00	$3.29 \cdot 10^{-9}$	$7.92 \cdot 10^{-12}$	-10.10	6.1	4.83	7.49

Tab. C-20: Experimental data for Eu on sample TRU-938 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Eu_{in}** (M)	**Eu_{aq}** (M)	**Log Eu_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$3.66 \cdot 10^{-6}$	$3.16 \cdot 10^{-8}$	-7.50	6.7	4.23	7.63
b	35.00	$3.66 \cdot 10^{-6}$	$2.72 \cdot 10^{-8}$	-7.57	6.7	4.30	7.60
2a	35.00	$1.83 \cdot 10^{-6}$	$1.47 \cdot 10^{-8}$	-7.83	6.7	4.26	7.61
b	35.00	$1.83 \cdot 10^{-6}$	$1.23 \cdot 10^{-8}$	-7.91	6.7	4.34	7.62
3a	35.00	$7.34 \cdot 10^{-7}$	$5.77 \cdot 10^{-9}$	-8.24	6.7	4.27	7.64
b	35.00	$7.34 \cdot 10^{-7}$	$3.53 \cdot 10^{-9}$	-8.45	6.7	4.49	7.64
4a	35.00	$1.85 \cdot 10^{-7}$	$1.85 \cdot 10^{-9}$	-8.73	6.7	4.17	7.64
b	35.00	$1.85 \cdot 10^{-7}$	$1.73 \cdot 10^{-9}$	-8.76	6.7	4.20	7.64
5a	35.00	$7.54 \cdot 10^{-8}$	$3.60 \cdot 10^{-10}$	-9.44	6.7	4.49	7.64
b	35.00	$7.54 \cdot 10^{-8}$	$4.13 \cdot 10^{-10}$	-9.38	6.7	4.43	7.62
6a	35.00	$2.06 \cdot 10^{-8}$	$1.85 \cdot 10^{-10}$	-9.73	6.7	4.21	7.63
b	35.00	$2.06 \cdot 10^{-8}$	$1.31 \cdot 10^{-10}$	-9.88	6.7	4.37	7.66
7a	35.00	$9.61 \cdot 10^{-9}$	$6.30 \cdot 10^{-11}$	-10.20	6.7	4.35	7.64
b	35.00	$9.61 \cdot 10^{-9}$	$6.74 \cdot 10^{-11}$	-10.17	6.7	4.32	7.65
8a	35.00	$3.21 \cdot 10^{-9}$	$2.11 \cdot 10^{-11}$	-10.68	6.7	4.35	7.58
b	35.00	$3.21 \cdot 10^{-9}$	$1.90 \cdot 10^{-11}$	-10.72	6.7	4.40	7.63

App. D Experimental data for thorium

D.1 Experimental data for Th on BOZ1-1 samples

Tab. D-1: Experimental data for Th on sample BOZ-323 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.95\cdot10^{-7}$	$4.95\cdot10^{-10}$	-9.31	2.8	5.14	7.56
b	37	$1.95\cdot10^{-7}$	$4.72\cdot10^{-10}$	-9.33	2.8	5.16	7.44
2a	37	$5.85\cdot10^{-8}$	$1.43\cdot10^{-10}$	-9.84	2.8	5.16	7.58
b	37	$5.85\cdot10^{-8}$	$1.48\cdot10^{-10}$	-9.83	2.8	5.14	7.54
3a	37	$1.96\cdot10^{-8}$	$4.60\cdot10^{-11}$	-10.34	2.8	5.17	7.51
b	37	$1.96\cdot10^{-8}$	$4.88\cdot10^{-11}$	-10.31	2.8	5.15	7.51
4a	37	$5.91\cdot10^{-9}$	$1.19\cdot10^{-11}$	-10.92	2.8	5.24	7.54
b	37	$5.91\cdot10^{-9}$	$1.14\cdot10^{-11}$	-10.94	2.8	5.26	7.54
5a	37	$2.01\cdot10^{-9}$	$3.96\cdot10^{-12}$	-11.40	2.8	5.25	7.52
b	37	$2.01\cdot10^{-9}$	$4.21\cdot10^{-12}$	-11.38	2.8	5.23	7.51
6a	37	$6.46\cdot10^{-10}$	$1.34\cdot10^{-12}$	-11.87	2.8	5.23	7.44
b	37	$6.46\cdot10^{-10}$	$1.39\cdot10^{-12}$	-11.86	2.8	5.21	7.58
7a	37	$2.56\cdot10^{-10}$	$5.15\cdot10^{-13}$	-12.29	2.8	5.24	7.51
b	37	$2.56\cdot10^{-10}$	$6.00\cdot10^{-13}$	-12.22	2.8	5.18	7.51
8a	37	$6.07\cdot10^{-11}$	$1.38\cdot10^{-13}$	-12.86	2.8	5.19	7.44
b	37	$6.07\cdot10^{-11}$	$1.34\cdot10^{-13}$	-12.87	2.8	5.20	7.62

Tab. D-2: Experimental data for Th on sample BOZ-440 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.95 \cdot 10^{-7}$	$4.28 \cdot 10^{-10}$	-9.37	2.9	5.20	7.62
b	37	$1.95 \cdot 10^{-7}$	$4.71 \cdot 10^{-10}$	-9.33	2.9	5.16	7.60
2a	37	$5.85 \cdot 10^{-8}$	$1.52 \cdot 10^{-10}$	-9.82	2.9	5.13	7.56
b	37	$5.85 \cdot 10^{-8}$	$1.33 \cdot 10^{-10}$	-9.88	2.9	5.18	7.57
3a	37	$1.96 \cdot 10^{-8}$	$4.63 \cdot 10^{-11}$	-10.33	2.9	5.16	7.57
b	37	$1.96 \cdot 10^{-8}$	$4.67 \cdot 10^{-11}$	-10.33	2.9	5.16	7.59
4a	37	$5.91 \cdot 10^{-9}$	$1.22 \cdot 10^{-11}$	-10.91	2.9	5.23	7.57
b	37	$5.91 \cdot 10^{-9}$	$1.17 \cdot 10^{-11}$	-10.93	2.9	5.24	7.62
5a	37	$2.01 \cdot 10^{-9}$	$3.57 \cdot 10^{-12}$	-11.45	2.9	5.29	7.57
b	37	$2.01 \cdot 10^{-9}$	$4.16 \cdot 10^{-12}$	-11.38	2.9	5.22	7.60
6a	37	$6.46 \cdot 10^{-10}$	$1.72 \cdot 10^{-12}$	-11.76	2.9	5.11	7.56
b	37	$6.46 \cdot 10^{-10}$	$1.50 \cdot 10^{-12}$	-11.82	2.9	5.17	7.62
7a	37	$2.56 \cdot 10^{-10}$	$7.18 \cdot 10^{-13}$	-12.14	2.9	5.09	7.55
b	37	$2.56 \cdot 10^{-10}$	$5.41 \cdot 10^{-13}$	-12.27	2.9	5.21	7.57
8a	37	$6.07 \cdot 10^{-11}$	$1.26 \cdot 10^{-13}$	-12.90	2.9	5.22	7.50
b	37	$6.07 \cdot 10^{-11}$	$1.37 \cdot 10^{-13}$	-12.86	2.9	5.19	7.59

Tab. D-3: Experimental data for Th on sample BOZ-493 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.95 \cdot 10^{-7}$	$4.36 \cdot 10^{-10}$	-9.36	3.0	5.17	7.66
b	37	$1.95 \cdot 10^{-7}$	$6.76 \cdot 10^{-10}$	-9.17	3.0	4.98	7.67
2a	37	$5.85 \cdot 10^{-8}$	$1.73 \cdot 10^{-10}$	-9.76	3.0	5.05	7.67
b	37	$5.85 \cdot 10^{-8}$	$1.31 \cdot 10^{-10}$	-9.88	3.0	5.17	7.68
3a	37	$1.96 \cdot 10^{-8}$	$4.32 \cdot 10^{-11}$	-10.36	3.0	5.18	7.65
b	37	$1.96 \cdot 10^{-8}$	$5.41 \cdot 10^{-11}$	-10.27	3.0	5.08	7.69
4a	37	$5.91 \cdot 10^{-9}$	$1.21 \cdot 10^{-11}$	-10.92	3.0	5.21	7.71
b	37	$5.91 \cdot 10^{-9}$	$1.13 \cdot 10^{-11}$	-10.95	3.0	5.24	7.73
5a	37	$2.01 \cdot 10^{-9}$	$3.83 \cdot 10^{-12}$	-11.42	3.0	5.24	7.68
b	37	$2.01 \cdot 10^{-9}$	$3.98 \cdot 10^{-12}$	-11.40	3.0	5.22	7.68
6a	37	$6.46 \cdot 10^{-10}$	$1.23 \cdot 10^{-12}$	-11.91	3.0	5.24	7.66
b	37	$6.46 \cdot 10^{-10}$	$1.27 \cdot 10^{-12}$	-11.90	3.0	5.23	7.67
7a	37	$2.56 \cdot 10^{-10}$	$5.08 \cdot 10^{-13}$	-12.29	3.0	5.22	7.67
b	37	$2.56 \cdot 10^{-10}$	$4.71 \cdot 10^{-13}$	-12.33	3.0	5.25	7.66
8a	37	$6.07 \cdot 10^{-11}$	$1.13 \cdot 10^{-13}$	-12.95	3.0	5.25	7.69
b	37	$6.07 \cdot 10^{-11}$	$1.12 \cdot 10^{-13}$	-12.95	3.0	5.26	7.70

Tab. D-4: Experimental data for Th on sample BOZ-521 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.95 \cdot 10^{-7}$	$2.44 \cdot 10^{-10}$	-9.61	2.3	5.53	7.78
b	37	$1.95 \cdot 10^{-7}$	$2.28 \cdot 10^{-10}$	-9.64	2.3	5.56	7.75
2a	37	$5.85 \cdot 10^{-8}$	$5.30 \cdot 10^{-11}$	-10.28	2.3	5.67	7.75
b	37	$5.85 \cdot 10^{-8}$	$1.74 \cdot 10^{-10}$	-9.76	2.3	5.15	7.82
3a	37	$1.96 \cdot 10^{-8}$	$1.54 \cdot 10^{-11}$	-10.81	2.3	5.73	7.80
b	37	$1.96 \cdot 10^{-8}$	$2.21 \cdot 10^{-11}$	-10.65	2.3	5.57	7.81
4a	37	$5.91 \cdot 10^{-9}$	$7.01 \cdot 10^{-12}$	-11.15	2.3	5.55	7.75
b	37	$5.91 \cdot 10^{-9}$	$6.51 \cdot 10^{-12}$	-11.19	2.3	5.59	7.77
5a	37	$2.01 \cdot 10^{-9}$	$2.29 \cdot 10^{-12}$	-11.64	2.3	5.57	7.76
b	37	$2.01 \cdot 10^{-9}$	$2.28 \cdot 10^{-12}$	-11.64	2.3	5.57	7.85
6a	37	$6.46 \cdot 10^{-10}$	$2.16 \cdot 10^{-12}$	-11.67	2.3	5.10	7.82
b	37	$6.46 \cdot 10^{-10}$	$8.41 \cdot 10^{-13}$	-12.07	2.3	5.51	7.83
7a	37	$2.56 \cdot 10^{-10}$	$2.36 \cdot 10^{-13}$	-12.63	2.3	5.66	7.76
b	37	$2.56 \cdot 10^{-10}$	$2.97 \cdot 10^{-13}$	-12.53	2.3	5.56	7.77
8a	37	$6.07 \cdot 10^{-11}$	$6.53 \cdot 10^{-14}$	-13.19	2.3	5.60	7.70
b	37	$6.07 \cdot 10^{-11}$	$5.67 \cdot 10^{-14}$	-13.25	2.3	5.66	7.75

Tab. D-5: Experimental data for Th on sample BOZ-572 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.95 \cdot 10^{-7}$	$1.89 \cdot 10^{-10}$	-9.72	3.1	5.52	7.83
b	37	$1.95 \cdot 10^{-7}$	$3.71 \cdot 10^{-10}$	-9.43	3.1	5.23	7.82
2a	37	$5.85 \cdot 10^{-8}$	$1.58 \cdot 10^{-10}$	-9.80	3.1	5.08	7.81
b	37	$5.85 \cdot 10^{-8}$	$3.01 \cdot 10^{-11}$	-10.52	3.1	5.79	7.82
3a	37	$1.96 \cdot 10^{-8}$	$2.71 \cdot 10^{-11}$	-10.57	3.1	5.36	7.81
b	37	$1.96 \cdot 10^{-8}$	$2.69 \cdot 10^{-11}$	-10.57	3.1	5.37	7.75
4a	37	$5.91 \cdot 10^{-9}$	$8.82 \cdot 10^{-12}$	-11.05	3.1	5.33	7.75
b	37	$5.91 \cdot 10^{-9}$	$6.76 \cdot 10^{-12}$	-11.17	3.1	5.45	7.77
5a	37	$2.01 \cdot 10^{-9}$	$2.68 \cdot 10^{-12}$	-11.57	3.1	5.38	7.70
b	37	$2.01 \cdot 10^{-9}$	$2.76 \cdot 10^{-12}$	-11.56	3.1	5.37	7.74
6a	37	$6.46 \cdot 10^{-10}$	$1.06 \cdot 10^{-12}$	-11.98	3.1	5.29	7.85
b	37	$6.46 \cdot 10^{-10}$	$1.31 \cdot 10^{-12}$	-11.88	3.1	5.20	7.77
7a	37	$2.56 \cdot 10^{-10}$	$2.13 \cdot 10^{-13}$	-12.67	3.1	5.58	7.79
b	37	$2.56 \cdot 10^{-10}$	$2.66 \cdot 10^{-13}$	-12.57	3.1	5.49	7.78
8a	37	$6.07 \cdot 10^{-11}$	$7.35 \cdot 10^{-14}$	-13.13	3.1	5.42	7.76
b	37	$6.07 \cdot 10^{-11}$	$6.17 \cdot 10^{-14}$	-13.21	3.1	5.50	7.81

Tab. D-6: Experimental data for Th on sample BOZ-681 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.95 \cdot 10^{-7}$	$1.73 \cdot 10^{-10}$	-9.76	2.3	5.70	8.00
b	37	$1.95 \cdot 10^{-7}$	$2.87 \cdot 10^{-10}$	-9.54	2.3	5.47	8.05
2a	37	$5.85 \cdot 10^{-8}$	$5.38 \cdot 10^{-11}$	-10.27	2.3	5.68	8.03
b	37	$5.85 \cdot 10^{-8}$	$4.40 \cdot 10^{-11}$	-10.36	2.3	5.77	8.02
3a	37	$1.96 \cdot 10^{-8}$	$1.23 \cdot 10^{-11}$	-10.91	2.3	5.84	8.00
b	37	$1.96 \cdot 10^{-8}$	$2.05 \cdot 10^{-11}$	-10.69	2.3	5.62	8.02
4a	37	$5.91 \cdot 10^{-9}$	$7.00 \cdot 10^{-12}$	-11.15	2.3	5.57	7.89
b	37	$5.91 \cdot 10^{-9}$	$4.53 \cdot 10^{-12}$	-11.34	2.3	5.76	7.93
5a	37	$2.01 \cdot 10^{-9}$	$1.75 \cdot 10^{-12}$	-11.76	2.3	5.70	7.90
b	37	$2.01 \cdot 10^{-9}$	$1.65 \cdot 10^{-12}$	-11.78	2.3	5.73	7.88
6a	37	$6.46 \cdot 10^{-10}$	$8.22 \cdot 10^{-13}$	-12.09	2.3	5.54	7.98
b	37	$6.46 \cdot 10^{-10}$	$5.86 \cdot 10^{-13}$	-12.23	2.3	5.68	7.85
7a	37	$2.56 \cdot 10^{-10}$	$2.69 \cdot 10^{-13}$	-12.57	2.3	5.62	7.91
b	37	$2.56 \cdot 10^{-10}$	$4.22 \cdot 10^{-13}$	-12.37	2.3	5.42	7.93
8a	37	$6.07 \cdot 10^{-11}$	$6.11 \cdot 10^{-14}$	-13.21	2.3	5.64	7.85
b	37	$6.07 \cdot 10^{-11}$	$5.39 \cdot 10^{-14}$	-13.27	2.3	5.69	7.87

D.2 Experimental data for Th on BUL1-1 samples

Tab. D-7: Experimental data for Th on sample BUL-845 in its corresponding SPW (cf. Tab. 2-4).

Sample	Vol (10^{-3} L)	Th_{in} (M)	Th_{aq} (M)	Log Th_{aq} (M)	S/L ratio (10^{-3} kg/L)	log R_d (L/kg)	pH
1a	35.00	$1.86 \cdot 10^{-7}$	$5.65 \cdot 10^{-10}$	-9.25	29.1	4.05	7.38
b	35.00	$1.86 \cdot 10^{-7}$	$5.94 \cdot 10^{-10}$	-9.23	28.7	4.04	7.40
2a	35.00	$5.58 \cdot 10^{-8}$	$1.77 \cdot 10^{-10}$	-9.75	28.9	4.04	7.41
b	35.00	$5.58 \cdot 10^{-8}$	$1.69 \cdot 10^{-10}$	-9.77	28.7	4.06	7.41
3a	35.00	$1.86 \cdot 10^{-8}$	$6.64 \cdot 10^{-11}$	-10.18	28.7	3.99	7.41
b	35.00	$1.86 \cdot 10^{-8}$	$6.10 \cdot 10^{-11}$	-10.21	29.2	4.02	7.41
4a	35.00	$5.63 \cdot 10^{-9}$	$1.81 \cdot 10^{-11}$	-10.74	30.9	4.00	7.43
b	35.00	$5.63 \cdot 10^{-9}$	$2.20 \cdot 10^{-11}$	-10.66	28.5	3.95	7.40
5a	35.00	$1.91 \cdot 10^{-9}$	$6.22 \cdot 10^{-12}$	-11.21	29.5	4.02	7.43
b	35.00	$1.91 \cdot 10^{-9}$	$6.17 \cdot 10^{-12}$	-11.21	28.9	4.03	7.43
6a	35.00	$6.02 \cdot 10^{-10}$	$2.22 \cdot 10^{-12}$	-11.65	28.3	3.98	7.41
b	35.00	$6.02 \cdot 10^{-10}$	$2.30 \cdot 10^{-12}$	-11.64	28.6	3.96	7.41
7a	35.00	$2.55 \cdot 10^{-10}$	$1.39 \cdot 10^{-12}$	-11.86	28.7	3.80	7.42
b	35.00	$2.55 \cdot 10^{-10}$	$1.23 \cdot 10^{-12}$	-11.91	28.8	3.85	7.41
8a	35.00	$4.16 \cdot 10^{-11}$	$6.63 \cdot 10^{-13}$	-12.18	29.2	3.33	7.45
b	35.00	$4.16 \cdot 10^{-11}$	$6.71 \cdot 10^{-13}$	-12.17	29.5	3.32	7.44

Tab. D-8: Experimental data for Th on sample BUL-861 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.76 \cdot 10^{-7}$	$1.91 \cdot 10^{-10}$	-9.72	3.1	5.47	7.65
b	37	$1.76 \cdot 10^{-7}$	$1.98 \cdot 10^{-10}$	-9.70	3.1	5.46	7.67
2a	37	$5.28 \cdot 10^{-8}$	$7.80 \cdot 10^{-11}$	-10.11	3.1	5.34	7.65
b	37	$5.28 \cdot 10^{-8}$	$6.53 \cdot 10^{-11}$	-10.18	3.1	5.41	7.64
3a	37	$1.76 \cdot 10^{-8}$	$2.77 \cdot 10^{-11}$	-10.56	3.1	5.31	7.65
b	37	$1.76 \cdot 10^{-8}$	$2.52 \cdot 10^{-11}$	-10.60	3.1	5.35	7.67
4a	37	$5.31 \cdot 10^{-9}$	$9.95 \cdot 10^{-12}$	-11.00	3.1	5.23	7.67
b	37	$5.31 \cdot 10^{-9}$	$1.03 \cdot 10^{-11}$	-10.99	3.1	5.22	7.69
5a	37	$1.80 \cdot 10^{-9}$	$3.58 \cdot 10^{-12}$	-11.45	3.1	5.21	7.67
b	37	$1.80 \cdot 10^{-9}$	$3.41 \cdot 10^{-12}$	-11.47	3.1	5.23	7.64
6a	37	$5.67 \cdot 10^{-10}$	$1.76 \cdot 10^{-12}$	-11.75	3.1	5.01	7.66
b	37	$5.67 \cdot 10^{-10}$	$1.44 \cdot 10^{-12}$	-11.84	3.1	5.10	7.66
7a	37	$2.15 \cdot 10^{-10}$	$8.12 \cdot 10^{-13}$	-12.09	3.1	4.93	7.71
b	37	$2.15 \cdot 10^{-10}$	$7.91 \cdot 10^{-13}$	-12.10	3.1	4.94	7.70
8a	37	$3.94 \cdot 10^{-11}$	$5.06 \cdot 10^{-13}$	-12.30	3.1	4.39	7.67
b	37	$3.94 \cdot 10^{-11}$	$6.07 \cdot 10^{-13}$	-12.22	3.1	4.31	7.65

Tab. D-9: Experimental data for Th on sample BUL-921 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.76 \cdot 10^{-7}$	$4.84 \cdot 10^{-10}$	-9.32	3.0	5.09	7.49
b	37	$1.76 \cdot 10^{-7}$	$4.80 \cdot 10^{-10}$	-9.32	3.0	5.09	7.48
2a	37	$5.28 \cdot 10^{-8}$	$1.61 \cdot 10^{-10}$	-9.79	3.0	5.04	7.46
b	37	$5.28 \cdot 10^{-8}$	$1.65 \cdot 10^{-10}$	-9.78	3.0	5.03	7.47
3a	37	$1.76 \cdot 10^{-8}$	$5.68 \cdot 10^{-11}$	-10.25	3.0	5.02	7.48
b	37	$1.76 \cdot 10^{-8}$	$6.00 \cdot 10^{-11}$	-10.22	3.0	4.99	7.47
4a	37	$5.31 \cdot 10^{-9}$	$1.93 \cdot 10^{-11}$	-10.72	3.0	4.97	7.50
b	37	$5.31 \cdot 10^{-9}$	$1.93 \cdot 10^{-11}$	-10.71	3.0	4.96	7.44
5a	37	$1.80 \cdot 10^{-9}$	$6.84 \cdot 10^{-12}$	-11.16	3.0	4.94	7.51
b	37	$1.80 \cdot 10^{-9}$	$5.83 \cdot 10^{-12}$	-11.23	3.0	5.01	7.48
6a	37	$5.67 \cdot 10^{-10}$	$2.17 \cdot 10^{-12}$	-11.66	3.0	4.94	7.47
b	37	$5.67 \cdot 10^{-10}$	$2.06 \cdot 10^{-12}$	-11.69	3.0	4.96	7.49
7a	37	$2.15 \cdot 10^{-10}$	$1.10 \cdot 10^{-12}$	-11.96	3.0	4.82	7.52
b	37	$2.15 \cdot 10^{-10}$	$1.09 \cdot 10^{-12}$	-11.96	3.0	4.82	7.49
8a	37	$3.94 \cdot 10^{-11}$	$7.31 \cdot 10^{-13}$	-12.14	3.0	4.25	7.82
b	37	$3.94 \cdot 10^{-11}$	$7.33 \cdot 10^{-13}$	-12.13	3.0	4.25	7.51

Tab. D-10: Experimental data for Th on sample BUL-955 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.76 \cdot 10^{-7}$	$3.64 \cdot 10^{-10}$	-9.44	3.0	5.21	7.48
b	37	$1.76 \cdot 10^{-7}$	$3.54 \cdot 10^{-10}$	-9.45	3.0	5.22	7.51
2a	37	$5.28 \cdot 10^{-8}$	$1.17 \cdot 10^{-10}$	-9.93	3.0	5.18	4.47
b	37	$5.28 \cdot 10^{-8}$	$1.17 \cdot 10^{-10}$	-9.93	3.0	5.18	4.48
3a	37	$1.76 \cdot 10^{-8}$	$5.09 \cdot 10^{-11}$	-10.29	3.0	5.07	7.50
b	37	$1.76 \cdot 10^{-8}$	$4.63 \cdot 10^{-11}$	-10.33	3.0	5.11	7.50
4a	37	$5.31 \cdot 10^{-9}$	$2.08 \cdot 10^{-11}$	-10.68	3.0	4.93	7.49
b	37	$5.31 \cdot 10^{-9}$	$1.74 \cdot 10^{-11}$	-10.76	3.0	5.01	7.48
5a	37	$1.80 \cdot 10^{-9}$	$5.82 \cdot 10^{-12}$	-11.23	3.0	5.01	7.49
b	37	$1.80 \cdot 10^{-9}$	$6.27 \cdot 10^{-12}$	-11.20	3.0	4.98	7.52
6a	37	$5.67 \cdot 10^{-10}$	$1.71 \cdot 10^{-12}$	-11.77	3.0	5.05	7.45
b	37	$5.67 \cdot 10^{-10}$	$1.95 \cdot 10^{-12}$	-11.71	3.0	4.99	7.46
7a	37	$2.15 \cdot 10^{-10}$	$9.75 \cdot 10^{-13}$	-12.01	3.0	4.87	7.51
b	37	$2.15 \cdot 10^{-10}$	$9.83 \cdot 10^{-13}$	-12.01	3.0	4.86	7.45
8a	37	$3.94 \cdot 10^{-11}$	$6.72 \cdot 10^{-13}$	-12.17	3.0	4.29	7.47
b	37	$3.94 \cdot 10^{-11}$	$6.87 \cdot 10^{-13}$	-12.16	3.0	4.28	7.49

Tab. D-11: Experimental data for Th on sample BUL-995 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.76 \cdot 10^{-7}$	$5.68 \cdot 10^{-11}$	-10.25	2.4	6.10	7.62
b	37	$1.76 \cdot 10^{-7}$	$1.49 \cdot 10^{-10}$	-9.83	2.4	5.69	7.58
2a	37	$5.28 \cdot 10^{-8}$	$3.67 \cdot 10^{-11}$	-10.44	2.4	5.77	7.62
b	37	$5.28 \cdot 10^{-8}$	$3.65 \cdot 10^{-11}$	-10.44	2.4	5.77	7.63
3a	37	$1.76 \cdot 10^{-8}$	$1.38 \cdot 10^{-11}$	-10.86	2.4	5.72	7.61
b	37	$1.76 \cdot 10^{-8}$	$1.42 \cdot 10^{-11}$	-10.85	2.4	5.71	7.59
4a	37	$5.31 \cdot 10^{-9}$	$1.58 \cdot 10^{-11}$	-10.80	2.4	5.14	7.62
b	37	$5.31 \cdot 10^{-9}$	$4.71 \cdot 10^{-12}$	-11.33	2.4	5.66	7.62
5a	37	$1.80 \cdot 10^{-9}$	$2.26 \cdot 10^{-12}$	-11.65	2.4	5.51	7.59
b	37	$1.80 \cdot 10^{-9}$	$4.03 \cdot 10^{-12}$	-11.40	2.4	5.26	7.64
6a	37	$5.67 \cdot 10^{-10}$	$1.03 \cdot 10^{-12}$	-11.99	2.4	5.35	7.57
b	37	$5.67 \cdot 10^{-10}$	$9.36 \cdot 10^{-13}$	-12.03	2.4	5.39	7.57
7a	37	$2.15 \cdot 10^{-10}$	$4.88 \cdot 10^{-13}$	-12.31	2.4	5.26	7.56
b	37	$2.15 \cdot 10^{-10}$	$4.77 \cdot 10^{-13}$	-12.32	2.4	5.27	7.53
8a	37	$3.94 \cdot 10^{-11}$	$6.76 \cdot 10^{-13}$	-12.17	2.4	4.37	7.46
b	37	$3.94 \cdot 10^{-11}$	$5.09 \cdot 10^{-13}$	-12.29	2.4	4.50	7.53

Tab. D-12: Experimental data for Th on sample BUL-1002 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.76 \cdot 10^{-7}$	$8.56 \cdot 10^{-11}$	-10.07	2.6	5.89	7.64
b	37	$1.76 \cdot 10^{-7}$	$2.41 \cdot 10^{-10}$	-9.62	2.6	5.44	7.68
2a	37	$5.28 \cdot 10^{-8}$	$2.81 \cdot 10^{-11}$	-10.55	2.6	5.85	7.72
b	37	$5.28 \cdot 10^{-8}$	$5.94 \cdot 10^{-11}$	-10.23	2.6	5.53	7.70
3a	37	$1.76 \cdot 10^{-8}$	$2.03 \cdot 10^{-11}$	-10.69	2.6	5.52	7.66
b	37	$1.76 \cdot 10^{-8}$	$2.59 \cdot 10^{-11}$	-10.59	2.6	5.41	7.69
4a	37	$5.31 \cdot 10^{-9}$	$1.42 \cdot 10^{-11}$	-10.85	2.6	5.15	7.69
b	37	$5.31 \cdot 10^{-9}$	$8.64 \cdot 10^{-12}$	-11.06	2.6	5.37	7.70
5a	37	$1.80 \cdot 10^{-9}$	$3.98 \cdot 10^{-12}$	-11.40	2.6	5.23	7.66
b	37	$1.80 \cdot 10^{-9}$	$5.06 \cdot 10^{-12}$	-11.30	2.6	5.13	7.64
6a	37	$5.67 \cdot 10^{-10}$	$9.98 \cdot 10^{-13}$	-12.00	2.6	5.33	7.70
b	37	$5.67 \cdot 10^{-10}$	$1.13 \cdot 10^{-12}$	-11.95	2.6	5.28	7.69
7a	37	$2.15 \cdot 10^{-10}$	$4.69 \cdot 10^{-13}$	-12.33	2.6	5.24	7.61
b	37	$2.15 \cdot 10^{-10}$	$4.81 \cdot 10^{-13}$	-12.32	2.6	5.23	7.66
8a	37	$3.94 \cdot 10^{-11}$	$5.29 \cdot 10^{-13}$	-12.28	2.6	4.44	7.71
b	37	$3.94 \cdot 10^{-11}$	$5.11 \cdot 10^{-13}$	-12.29	2.6	4.46	7.67

Tab. D-13: Experimental data for Th on sample BUL-1017 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.76 \cdot 10^{-7}$	$1.33 \cdot 10^{-10}$	-9.88	1.8	5.86	7.71
b	37	$1.76 \cdot 10^{-7}$	$1.60 \cdot 10^{-10}$	-9.80	1.8	5.78	7.74
2a	37	$5.28 \cdot 10^{-8}$	$9.20 \cdot 10^{-11}$	-10.04	1.8	5.50	7.74
b	37	$5.28 \cdot 10^{-8}$	$1.22 \cdot 10^{-10}$	-9.91	1.8	5.37	7.75
3a	37	$1.76 \cdot 10^{-8}$	$5.36 \cdot 10^{-11}$	-10.27	1.8	5.25	7.72
b	37	$1.76 \cdot 10^{-8}$	$9.26 \cdot 10^{-11}$	-10.03	1.8	5.02	7.72
4a	37	$5.31 \cdot 10^{-9}$	$1.46 \cdot 10^{-11}$	-10.84	1.8	5.30	7.73
b	37	$5.31 \cdot 10^{-9}$	$1.95 \cdot 10^{-11}$	-10.71	1.8	5.17	7.76
5a	37	$1.80 \cdot 10^{-9}$	$4.08 \cdot 10^{-12}$	-11.39	1.8	5.38	7.72
b	37	$1.80 \cdot 10^{-9}$	$5.00 \cdot 10^{-12}$	-11.30	1.8	5.29	7.74
6a	37	$5.67 \cdot 10^{-10}$	$1.39 \cdot 10^{-12}$	-11.86	1.8	5.35	7.66
b	37	$5.67 \cdot 10^{-10}$	$1.49 \cdot 10^{-12}$	-11.83	1.8	5.32	7.68
7a	37	$2.15 \cdot 10^{-10}$	$1.20 \cdot 10^{-12}$	-11.92	1.8	4.99	7.65
b	37	$2.15 \cdot 10^{-10}$	$1.14 \cdot 10^{-12}$	-11.94	1.8	5.01	7.70
8a	37	$3.94 \cdot 10^{-11}$	$1.12 \cdot 10^{-12}$	-11.95	1.8	4.27	7.57
b	37	$3.94 \cdot 10^{-11}$	$1.14 \cdot 10^{-12}$	-11.94	1.8	4.26	7.73

D.3 Experimental data for Th on TRU1-1 samples

Tab. D-14: Experimental data for Th on sample TRU-748 in its corresponding SPW (cf. Tab. 2-4).

Sample	Vol (10^{-3} L)	Th_{in} (M)	Th_{aq} (M)	Log Th_{aq} (M)	S/L ratio (10^{-3} kg/L)	log R_d (L/kg)	pH
1a	37	$1.76 \cdot 10^{-7}$	$1.48 \cdot 10^{-10}$	-9.83	2.4	5.69	7.65
b	37	$1.76 \cdot 10^{-7}$	$1.35 \cdot 10^{-10}$	-9.87	2.4	5.73	7.67
2a	37	$5.28 \cdot 10^{-8}$	$4.91 \cdot 10^{-11}$	-10.31	2.4	5.65	7.65
b	37	$5.28 \cdot 10^{-8}$	$6.65 \cdot 10^{-11}$	-10.18	2.4	5.52	7.64
3a	37	$1.76 \cdot 10^{-8}$	$1.78 \cdot 10^{-11}$	-10.75	2.4	5.61	7.65
b	37	$1.76 \cdot 10^{-8}$	$1.69 \cdot 10^{-11}$	-10.77	2.4	5.64	7.67
4a	37	$5.32 \cdot 10^{-9}$	$6.83 \cdot 10^{-12}$	-11.17	2.4	5.51	7.67
b	37	$5.32 \cdot 10^{-9}$	$1.09 \cdot 10^{-11}$	-10.96	2.4	5.30	7.69
5a	37	$1.80 \cdot 10^{-9}$	$2.21 \cdot 10^{-12}$	-11.66	2.4	5.53	7.67
b	37	$1.80 \cdot 10^{-9}$	$1.70 \cdot 10^{-12}$	-11.77	2.4	5.64	7.64
6a	37	$5.67 \cdot 10^{-10}$	$1.03 \cdot 10^{-12}$	-11.99	2.4	5.36	7.66
b	37	$5.67 \cdot 10^{-10}$	$1.14 \cdot 10^{-12}$	-11.94	2.4	5.31	7.66
7a	37	$2.15 \cdot 10^{-10}$	$3.70 \cdot 10^{-13}$	-12.43	2.4	5.38	7.71
b	37	$2.15 \cdot 10^{-10}$	$5.74 \cdot 10^{-13}$	-12.24	2.4	5.19	7.70
8a	37	$3.94 \cdot 10^{-11}$	$5.56 \cdot 10^{-14}$	-13.25	2.4	5.47	7.67
b	37	$3.94 \cdot 10^{-11}$	$6.07 \cdot 10^{-14}$	-13.22	2.4	5.43	7.65

Tab. D-15: Experimental data for Th on sample TRU-794 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.76 \cdot 10^{-7}$	$2.89 \cdot 10^{-10}$	-9.54	2.4	5.41	7.65
b	37	$1.76 \cdot 10^{-7}$	$1.73 \cdot 10^{-10}$	-9.76	2.4	5.63	7.67
2a	37	$5.28 \cdot 10^{-8}$	$7.87 \cdot 10^{-11}$	-10.10	2.4	5.45	7.65
b	37	$5.28 \cdot 10^{-8}$	$8.69 \cdot 10^{-11}$	-10.06	2.4	5.41	7.64
3a	37	$1.76 \cdot 10^{-8}$	$1.64 \cdot 10^{-11}$	-10.79	2.4	5.65	7.65
b	37	$1.76 \cdot 10^{-8}$	$2.80 \cdot 10^{-11}$	-10.55	2.4	5.42	7.67
4a	37	$5.32 \cdot 10^{-9}$	$9.77 \cdot 10^{-12}$	-11.01	2.4	5.36	7.67
b	37	$5.32 \cdot 10^{-9}$	$6.83 \cdot 10^{-12}$	-11.17	2.4	5.51	7.69
5a	37	$1.80 \cdot 10^{-9}$	$3.25 \cdot 10^{-12}$	-11.49	2.4	5.36	7.67
b	37	$1.80 \cdot 10^{-9}$	$1.87 \cdot 10^{-12}$	-11.73	2.4	5.60	7.64
6a	37	$5.67 \cdot 10^{-10}$	$1.07 \cdot 10^{-12}$	-11.97	2.4	5.35	7.66
b	37	$5.67 \cdot 10^{-10}$	$1.80 \cdot 10^{-12}$	-11.75	2.4	5.12	7.66
7a	37	$2.15 \cdot 10^{-10}$	$5.80 \cdot 10^{-13}$	-12.24	2.4	5.19	7.71
b	37	$2.15 \cdot 10^{-10}$	$4.60 \cdot 10^{-13}$	-12.34	2.4	5.29	7.70
8a	37	$3.94 \cdot 10^{-11}$	$7.12 \cdot 10^{-14}$	-13.15	2.4	5.36	7.67
b	37	$3.94 \cdot 10^{-11}$	$8.61 \cdot 10^{-14}$	-13.06	2.4	5.28	7.65

Tab. D-16: Experimental data for Th on sample TRU-815 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.76 \cdot 10^{-7}$	$2.23 \cdot 10^{-10}$	-9.65	1.7	5.67	7.49
b	37	$1.76 \cdot 10^{-7}$	$2.49 \cdot 10^{-10}$	-9.60	1.7	5.63	7.48
2a	37	$5.28 \cdot 10^{-8}$	$6.59 \cdot 10^{-11}$	-10.18	1.7	5.68	7.49
b	37	$5.28 \cdot 10^{-8}$	$1.15 \cdot 10^{-10}$	-9.94	1.7	5.44	7.50
3a	37	$1.76 \cdot 10^{-8}$	$2.35 \cdot 10^{-11}$	-10.63	1.7	5.65	7.47
b	37	$1.76 \cdot 10^{-8}$	$1.56 \cdot 10^{-11}$	-10.81	1.7	5.83	7.48
4a	37	$5.32 \cdot 10^{-9}$	$7.01 \cdot 10^{-12}$	-11.15	1.7	5.66	7.46
b	37	$5.32 \cdot 10^{-9}$	$9.01 \cdot 10^{-12}$	-11.05	1.7	5.55	7.49
5a	37	$1.80 \cdot 10^{-9}$	$3.49 \cdot 10^{-12}$	-11.46	1.7	5.49	7.45
b	37	$1.80 \cdot 10^{-9}$	$3.78 \cdot 10^{-12}$	-11.42	1.7	5.45	7.46
6a	37	$5.67 \cdot 10^{-10}$	$7.95 \cdot 10^{-13}$	-12.10	1.7	5.63	7.47
b	37	$5.67 \cdot 10^{-10}$	$7.31 \cdot 10^{-13}$	-12.14	1.7	5.67	7.48
7a	37	$2.15 \cdot 10^{-10}$	$3.93 \cdot 10^{-13}$	-12.41	1.7	5.52	7.48
b	37	$2.15 \cdot 10^{-10}$	$3.92 \cdot 10^{-13}$	-12.41	1.7	5.52	7.50
8a	37	$3.94 \cdot 10^{-11}$	$6.57 \cdot 10^{-14}$	-13.18	1.7	5.55	7.45
b	37	$3.94 \cdot 10^{-11}$	$7.52 \cdot 10^{-14}$	-13.12	1.7	5.50	7.45

Tab. D-17: Experimental data for Th on sample TRU-831 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.76 \cdot 10^{-7}$	$6.82 \cdot 10^{-11}$	-10.17	2.3	6.04	7.49
b	37	$1.76 \cdot 10^{-7}$	$7.87 \cdot 10^{-11}$	-10.10	2.3	5.98	7.49
2a	37	$5.28 \cdot 10^{-8}$	$3.63 \cdot 10^{-11}$	-10.44	2.3	5.79	7.46
b	37	$5.28 \cdot 10^{-8}$	$3.20 \cdot 10^{-11}$	-10.50	2.3	5.85	7.47
3a	37	$1.76 \cdot 10^{-8}$	$1.13 \cdot 10^{-11}$	-10.95	2.3	5.82	7.47
b	37	$1.76 \cdot 10^{-8}$	$9.66 \cdot 10^{-12}$	-11.02	2.3	5.89	7.46
4a	37	$5.32 \cdot 10^{-9}$	$4.09 \cdot 10^{-12}$	-11.39	2.3	5.74	7.48
b	37	$5.32 \cdot 10^{-9}$	$4.09 \cdot 10^{-12}$	-11.39	2.3	5.74	7.46
5a	37	$1.80 \cdot 10^{-9}$	$1.40 \cdot 10^{-12}$	-11.85	2.3	5.74	7.46
b	37	$1.80 \cdot 10^{-9}$	$1.53 \cdot 10^{-12}$	-11.82	2.3	5.70	7.45
6a	37	$5.67 \cdot 10^{-10}$	$4.70 \cdot 10^{-13}$	-12.33	2.3	5.71	7.45
b	37	$5.67 \cdot 10^{-10}$	$5.36 \cdot 10^{-13}$	-12.27	2.3	5.66	7.47
7a	37	$2.15 \cdot 10^{-10}$	$1.72 \cdot 10^{-13}$	-12.76	2.3	5.73	7.45
b	37	$2.15 \cdot 10^{-10}$	$1.47 \cdot 10^{-13}$	-12.83	2.3	5.80	7.46
8a	37	$3.94 \cdot 10^{-11}$	$3.55 \cdot 10^{-14}$	-13.45	2.3	5.68	7.43
b	37	$3.94 \cdot 10^{-11}$	$5.37 \cdot 10^{-14}$	-13.27	2.3	5.50	7.43

Tab. D-18: Experimental data for Th on sample TRU-882 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.81 \cdot 10^{-7}$	$2.41 \cdot 10^{-10}$	-9.62	2.2	5.53	7.56
b	37	$1.81 \cdot 10^{-7}$	$1.74 \cdot 10^{-10}$	-9.76	2.2	5.67	7.44
2a	37	$5.43 \cdot 10^{-8}$	$1.22 \cdot 10^{-10}$	-9.91	2.2	5.30	7.58
b	37	$5.43 \cdot 10^{-8}$	$1.12 \cdot 10^{-10}$	-9.95	2.2	5.34	7.54
3a	37	$1.82 \cdot 10^{-8}$	$2.38 \cdot 10^{-11}$	-10.62	2.2	5.54	7.51
b	37	$1.82 \cdot 10^{-8}$	$2.70 \cdot 10^{-11}$	-10.57	2.2	5.48	7.51
4a	37	$5.49 \cdot 10^{-9}$	$3.45 \cdot 10^{-11}$	-10.46	2.2	4.85	7.54
b	37	$5.49 \cdot 10^{-9}$	$3.47 \cdot 10^{-11}$	-10.46	2.2	4.85	7.54
5a	37	$1.87 \cdot 10^{-9}$	$1.21 \cdot 10^{-11}$	-10.92	2.2	4.84	7.52
b	37	$1.87 \cdot 10^{-9}$	$1.36 \cdot 10^{-11}$	-10.87	2.2	4.79	7.51
6a	37	$6.04 \cdot 10^{-10}$	$1.28 \cdot 10^{-12}$	-11.89	2.2	5.33	7.44
b	37	$6.04 \cdot 10^{-10}$	$1.05 \cdot 10^{-12}$	-11.98	2.2	5.41	7.58
7a	37	$2.42 \cdot 10^{-10}$	$5.52 \cdot 10^{-13}$	-12.26	2.2	5.29	7.51
b	37	$2.42 \cdot 10^{-10}$	$6.51 \cdot 10^{-13}$	-12.19	2.2	5.22	7.51
8a	37	$6.07 \cdot 10^{-11}$	$1.67 \cdot 10^{-13}$	-12.78	2.2	5.21	7.44
b	37	$6.07 \cdot 10^{-11}$	$2.10 \cdot 10^{-13}$	-12.68	2.2	5.11	7.62

Tab. D-19: Experimental data for Th on sample TRU-923 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.81 \cdot 10^{-7}$	$1.84 \cdot 10^{-10}$	-9.73	1.9	5.71	7.62
b	37	$1.81 \cdot 10^{-7}$	$2.43 \cdot 10^{-10}$	-9.61	1.9	5.59	7.60
2a	37	$5.43 \cdot 10^{-8}$	$1.31 \cdot 10^{-10}$	-9.88	1.9	5.34	7.56
b	37	$5.43 \cdot 10^{-8}$	$1.25 \cdot 10^{-10}$	-9.90	1.9	5.36	7.57
3a	37	$1.82 \cdot 10^{-8}$	$2.65 \cdot 10^{-11}$	-10.58	1.9	5.55	7.57
b	37	$1.82 \cdot 10^{-8}$	$2.11 \cdot 10^{-11}$	-10.68	1.9	5.65	7.59
4a	37	$5.49 \cdot 10^{-9}$	$3.36 \cdot 10^{-11}$	-10.47	1.9	4.93	7.57
b	37	$5.49 \cdot 10^{-9}$	$3.71 \cdot 10^{-11}$	-10.43	1.9	4.89	7.62
5a	37	$1.87 \cdot 10^{-9}$	$9.98 \cdot 10^{-12}$	-11.00	1.9	4.99	7.57
b	37	$1.87 \cdot 10^{-9}$	$1.19 \cdot 10^{-11}$	-10.92	1.9	4.91	7.60
6a	37	$6.04 \cdot 10^{-10}$	$9.18 \cdot 10^{-13}$	-12.04	1.9	5.54	7.56
b	37	$6.04 \cdot 10^{-10}$	$1.02 \cdot 10^{-12}$	-11.99	1.9	5.49	7.62
7a	37	$2.42 \cdot 10^{-10}$	$7.80 \cdot 10^{-13}$	-12.11	1.9	5.21	7.55
b	37	$2.42 \cdot 10^{-10}$	$6.02 \cdot 10^{-13}$	-12.22	1.9	5.32	7.57
8a	37	$6.07 \cdot 10^{-11}$	$1.93 \cdot 10^{-13}$	-12.71	1.9	5.21	7.50
b	37	$6.07 \cdot 10^{-11}$	$2.01 \cdot 10^{-13}$	-12.70	1.9	5.20	7.59

Tab. D-20: Experimental data for Th on sample TRU-938 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**Th_{in}** (M)	**Th_{aq}** (M)	**Log Th_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	37	$1.81 \cdot 10^{-7}$	$5.64 \cdot 10^{-10}$	-9.25	2.1	5.18	7.66
b	37	$1.81 \cdot 10^{-7}$	$3.11 \cdot 10^{-10}$	-9.51	2.1	5.44	7.67
2a	37	$5.43 \cdot 10^{-8}$	$1.41 \cdot 10^{-10}$	-9.85	2.1	5.26	7.67
b	37	$5.43 \cdot 10^{-8}$	$2.35 \cdot 10^{-10}$	-9.63	2.1	5.04	7.68
3a	37	$1.82 \cdot 10^{-8}$	$3.90 \cdot 10^{-11}$	-10.41	2.1	5.34	7.65
b	37	$1.82 \cdot 10^{-8}$	$3.93 \cdot 10^{-11}$	-10.41	2.1	5.34	7.69
4a	37	$5.49 \cdot 10^{-9}$	$4.76 \cdot 10^{-11}$	-10.32	2.1	4.73	7.71
b	37	$5.49 \cdot 10^{-9}$	$4.45 \cdot 10^{-11}$	-10.35	2.1	4.76	7.73
5a	37	$1.87 \cdot 10^{-9}$	$1.50 \cdot 10^{-11}$	-10.83	2.1	4.77	7.68
b	37	$1.87 \cdot 10^{-9}$	$1.64 \cdot 10^{-11}$	-10.79	2.1	4.73	7.68
6a	37	$6.04 \cdot 10^{-10}$	$1.45 \cdot 10^{-12}$	-11.84	2.1	5.29	7.66
b	37	$6.04 \cdot 10^{-10}$	$1.33 \cdot 10^{-12}$	-11.88	2.1	5.33	7.67
7a	37	$2.42 \cdot 10^{-10}$	$9.08 \cdot 10^{-13}$	-12.04	2.1	5.10	7.67
b	37	$2.42 \cdot 10^{-10}$	$1.06 \cdot 10^{-12}$	-11.97	2.1	5.03	7.66
8a	37	$6.07 \cdot 10^{-11}$	$2.83 \cdot 10^{-13}$	-12.55	2.1	5.00	7.69
b	37	$6.07 \cdot 10^{-11}$	$2.58 \cdot 10^{-13}$	-12.59	2.1	5.04	7.70

App. E Experimental data for uranium

E.1 Experimental data for U on BOZ1-1 samples

Tab. E-1: Experimental data for U on sample BOZ-323 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$7.51 \cdot 10^{-6}$	$6.68 \cdot 10^{-6}$	-5.17	52.5	0.37	8.03
b	30.00	$7.51 \cdot 10^{-6}$	$6.58 \cdot 10^{-6}$	-5.18	52.5	0.43	8.06
2a	30.00	$2.77 \cdot 10^{-6}$	$2.36 \cdot 10^{-6}$	-5.63	52.5	0.52	8.00
b	30.00	$2.77 \cdot 10^{-6}$	$2.32 \cdot 10^{-6}$	-5.63	52.5	0.57	8.02
3a	30.00	$7.68 \cdot 10^{-7}$	$6.19 \cdot 10^{-7}$	-6.21	52.5	0.66	8.02
b	30.00	$7.68 \cdot 10^{-7}$	$6.13 \cdot 10^{-7}$	-6.21	52.5	0.68	8.05
4a	30.00	$2.93 \cdot 10^{-7}$	$2.27 \cdot 10^{-7}$	-6.64	52.5	0.75	8.02
b	30.00	$2.93 \cdot 10^{-7}$	$2.27 \cdot 10^{-7}$	-6.64	52.5	0.74	8.01
5a	30.00	$9.15 \cdot 10^{-8}$	$7.01 \cdot 10^{-8}$	-7.15	52.5	0.76	7.97
b	30.00	$9.15 \cdot 10^{-8}$	$6.73 \cdot 10^{-8}$	-7.17	52.5	0.84	8.03
6a	30.00	$4.61 \cdot 10^{-8}$	$3.33 \cdot 10^{-8}$	-7.48	52.5	0.86	7.96
b	30.00	$4.61 \cdot 10^{-8}$	$3.26 \cdot 10^{-8}$	-7.49	52.5	0.90	7.95
7a	30.00	$1.99 \cdot 10^{-8}$	$1.37 \cdot 10^{-8}$	-7.86	52.5	0.94	7.89
b	30.00	$1.99 \cdot 10^{-8}$	$1.33 \cdot 10^{-8}$	-7.87	52.5	0.98	7.92

Tab. E-2: Experimental data for U on sample BOZ-440 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$2.75 \cdot 10^{-5}$	$2.50 \cdot 10^{-5}$	-4.60	53.4	0.26	8.09
b	30.00	$2.75 \cdot 10^{-5}$	$2.53 \cdot 10^{-5}$	-4.60	53.4	0.21	8.09
2a	30.00	$7.51 \cdot 10^{-6}$	$6.00 \cdot 10^{-6}$	-5.22	53.4	0.68	8.06
b	30.00	$7.51 \cdot 10^{-6}$	$6.09 \cdot 10^{-6}$	-5.22	53.4	0.64	8.03
3a	30.00	$2.77 \cdot 10^{-6}$	$2.09 \cdot 10^{-6}$	-5.68	53.4	0.78	8.00
b	30.00	$2.77 \cdot 10^{-6}$	$2.12 \cdot 10^{-6}$	-5.67	53.4	0.76	8.02
4a	30.00	$7.68 \cdot 10^{-7}$	$5.16 \cdot 10^{-7}$	-6.29	53.4	0.96	8.02
b	30.00	$7.68 \cdot 10^{-7}$	$5.12 \cdot 10^{-7}$	-6.29	53.4	0.97	8.05
5a	30.00	$2.93 \cdot 10^{-7}$	$1.79 \cdot 10^{-7}$	-6.75	53.4	1.08	8.02
b	30.00	$2.93 \cdot 10^{-7}$	$1.71 \cdot 10^{-7}$	-6.77	53.4	1.13	8.01
6a	30.00	$9.15 \cdot 10^{-8}$	$4.78 \cdot 10^{-8}$	-7.32	53.4	1.23	7.97
b	30.00	$9.15 \cdot 10^{-8}$	$4.75 \cdot 10^{-8}$	-7.32	53.4	1.24	8.03
7a	30.00	$4.61 \cdot 10^{-8}$	$2.03 \cdot 10^{-8}$	-7.69	53.4	1.38	7.96
b	30.00	$4.61 \cdot 10^{-8}$	$2.10 \cdot 10^{-8}$	-7.68	53.4	1.35	7.95
8a	30.00	$1.99 \cdot 10^{-8}$	$8.15 \cdot 10^{-9}$	-8.09	53.4	1.43	7.89
b	30.00	$1.99 \cdot 10^{-8}$	$7.75 \cdot 10^{-9}$	-8.11	53.4	1.47	7.92

Tab. E-3: Experimental data for U on sample BOZ-493 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$2.75 \cdot 10^{-5}$	$1.59 \cdot 10^{-5}$	-4.80	55.7	1.12	8.03
b	30.00	$2.75 \cdot 10^{-5}$	$1.61 \cdot 10^{-5}$	-4.79	55.7	1.10	8.03
2a	30.00	$7.51 \cdot 10^{-6}$	$5.68 \cdot 10^{-6}$	-5.25	55.7	0.76	8.00
b	30.00	$7.51 \cdot 10^{-6}$	$5.71 \cdot 10^{-6}$	-5.24	55.7	0.75	8.03
3a	30.00	$2.77 \cdot 10^{-6}$	$2.21 \cdot 10^{-6}$	-5.65	55.7	0.65	7.96
b	30.00	$2.77 \cdot 10^{-6}$	$2.29 \cdot 10^{-6}$	-5.64	55.7	0.57	7.97
4a	30.00	$7.68 \cdot 10^{-7}$	$5.44 \cdot 10^{-7}$	-6.26	55.7	0.87	7.93
b	30.00	$7.68 \cdot 10^{-7}$	$5.22 \cdot 10^{-7}$	-6.28	55.7	0.93	7.94
5a	30.00	$2.93 \cdot 10^{-7}$	$1.83 \cdot 10^{-7}$	-6.74	55.7	1.03	7.99
b	30.00	$2.93 \cdot 10^{-7}$	$1.83 \cdot 10^{-7}$	-6.74	55.7	1.04	7.97
6a	30.00	$9.15 \cdot 10^{-8}$	$5.12 \cdot 10^{-8}$	-7.29	55.7	1.15	7.99
b	30.00	$9.15 \cdot 10^{-8}$	$5.03 \cdot 10^{-8}$	-7.30	55.7	1.17	7.98
7a	30.00	$4.61 \cdot 10^{-8}$	$2.20 \cdot 10^{-8}$	-7.66	55.7	1.29	7.99
b	30.00	$4.61 \cdot 10^{-8}$	$2.33 \cdot 10^{-8}$	-7.63	55.7	1.24	7.98
8a	30.00	$1.99 \cdot 10^{-8}$	$8.59 \cdot 10^{-9}$	-8.07	55.7	1.38	7.98
b	30.00	$1.99 \cdot 10^{-8}$	$8.78 \cdot 10^{-9}$	-8.06	55.7	1.36	7.96

Tab. E-4: Experimental data for U on sample BOZ-521 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$2.75 \cdot 10^{-5}$	$2.62 \cdot 10^{-5}$	-4.58	43.6	0.04	7.98
b	30.00	$2.75 \cdot 10^{-5}$	$2.44 \cdot 10^{-5}$	-4.61	43.6	0.47	7.99
2a	30.00	$7.51 \cdot 10^{-6}$	$6.61 \cdot 10^{-6}$	-5.18	43.6	0.50	7.96
b	30.00	$7.51 \cdot 10^{-6}$	$6.49 \cdot 10^{-6}$	-5.19	43.6	0.56	7.98
3a	30.00	$2.77 \cdot 10^{-6}$	$2.37 \cdot 10^{-6}$	-5.63	43.6	0.58	7.90
b	30.00	$2.77 \cdot 10^{-6}$	$2.35 \cdot 10^{-6}$	-5.63	43.6	0.61	7.85
4a	30.00	$7.68 \cdot 10^{-7}$	$6.24 \cdot 10^{-7}$	-6.20	43.6	0.72	7.88
b	30.00	$7.68 \cdot 10^{-7}$	$6.17 \cdot 10^{-7}$	-6.21	43.6	0.75	7.91
5a	30.00	$2.93 \cdot 10^{-7}$	$2.17 \cdot 10^{-7}$	-6.66	43.6	0.90	7.97
b	30.00	$2.93 \cdot 10^{-7}$	$2.24 \cdot 10^{-7}$	-6.65	43.6	0.85	7.98
6a	30.00	$9.15 \cdot 10^{-8}$	$6.37 \cdot 10^{-8}$	-7.20	43.6	1.00	7.88
b	30.00	$9.15 \cdot 10^{-8}$	$6.16 \cdot 10^{-8}$	-7.21	43.6	1.05	7.89
7a	30.00	$4.61 \cdot 10^{-8}$	$2.90 \cdot 10^{-8}$	-7.54	43.6	1.13	7.84
b	30.00	$4.61 \cdot 10^{-8}$	$2.95 \cdot 10^{-8}$	-7.53	43.6	1.11	7.88
8a	30.00	$1.99 \cdot 10^{-8}$	$1.13 \cdot 10^{-8}$	-7.95	43.6	1.24	7.88

Tab. E-5: Experimental data for U on sample BOZ-572 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$2.75 \cdot 10^{-5}$	$1.33 \cdot 10^{-5}$	-4.88	57.9	1.27	7.91
b	30.00	$2.75 \cdot 10^{-5}$	$1.34 \cdot 10^{-5}$	-4.87	57.9	1.26	7.90
2a	30.00	$7.51 \cdot 10^{-6}$	$4.54 \cdot 10^{-6}$	-5.34	57.9	1.05	7.83
b	30.00	$7.51 \cdot 10^{-6}$	$4.73 \cdot 10^{-6}$	-5.33	57.9	1.01	7.80
3a	30.00	$2.77 \cdot 10^{-6}$	$2.15 \cdot 10^{-6}$	-5.67	57.9	0.70	7.92
b	30.00	$2.77 \cdot 10^{-6}$	$2.05 \cdot 10^{-6}$	-5.69	57.9	0.78	7.85
4a	30.00	$7.68 \cdot 10^{-7}$	$4.78 \cdot 10^{-7}$	-6.32	57.9	1.02	7.79
b	30.00	$7.68 \cdot 10^{-7}$	$4.73 \cdot 10^{-7}$	-6.33	57.9	1.03	7.80
5a	30.00	$2.93 \cdot 10^{-7}$	$1.52 \cdot 10^{-7}$	-6.82	57.9	1.20	7.80
b	30.00	$2.93 \cdot 10^{-7}$	$1.48 \cdot 10^{-7}$	-6.83	57.9	1.23	7.81
6a	30.00	$9.15 \cdot 10^{-8}$	$4.41 \cdot 10^{-8}$	-7.36	57.9	1.27	7.81
b	30.00	$9.15 \cdot 10^{-8}$	$3.85 \cdot 10^{-8}$	-7.41	57.9	1.38	7.82
7a	30.00	$4.61 \cdot 10^{-8}$	$1.61 \cdot 10^{-8}$	-7.79	57.9	1.51	7.83
b	30.00	$4.61 \cdot 10^{-8}$	$1.67 \cdot 10^{-8}$	-7.78	57.9	1.48	7.82
8a	30.00	$1.99 \cdot 10^{-8}$	$5.35 \cdot 10^{-9}$	-8.27	57.9	1.67	7.82
b	30.00	$1.99 \cdot 10^{-8}$	$6.14 \cdot 10^{-9}$	-8.21	57.9	1.59	7.81

Tab. E-6: Experimental data for U on sample BOZ-681 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$2.75 \cdot 10^{-5}$	$1.08 \cdot 10^{-5}$	-4.97	42.3	1.56	7.99
b	30.00	$2.75 \cdot 10^{-5}$	$1.09 \cdot 10^{-5}$	-4.96	42.3	1.55	7.95
2a	30.00	$7.51 \cdot 10^{-6}$	$2.17 \cdot 10^{-6}$	-5.66	42.3	1.76	7.99
b	30.00	$7.51 \cdot 10^{-6}$	$2.21 \cdot 10^{-6}$	-5.65	42.3	1.75	7.98
3a	30.00	$2.77 \cdot 10^{-6}$	$1.47 \cdot 10^{-6}$	-5.83	42.3	1.32	8.03
b	30.00	$2.77 \cdot 10^{-6}$	$1.55 \cdot 10^{-6}$	-5.81	42.3	1.27	7.99
4a	30.00	$7.68 \cdot 10^{-7}$	$3.62 \cdot 10^{-7}$	-6.44	42.3	1.42	7.89
b	30.00	$7.68 \cdot 10^{-7}$	$3.54 \cdot 10^{-7}$	-6.45	42.3	1.44	7.93
5a	30.00	$2.93 \cdot 10^{-7}$	$9.31 \cdot 10^{-8}$	-7.03	42.3	1.71	7.92
b	30.00	$2.93 \cdot 10^{-7}$	$1.04 \cdot 10^{-7}$	-6.98	42.3	1.63	7.94
6a	30.00	$9.15 \cdot 10^{-8}$	$2.49 \cdot 10^{-8}$	-7.60	42.3	1.80	7.88
b	30.00	$9.15 \cdot 10^{-8}$	$2.51 \cdot 10^{-8}$	-7.60	42.3	1.79	7.92
7a	30.00	$4.61 \cdot 10^{-8}$	$1.06 \cdot 10^{-8}$	-7.98	42.3	1.90	7.86
b	30.00	$4.61 \cdot 10^{-8}$	$1.10 \cdot 10^{-8}$	-7.96	42.3	1.88	7.89
8a	30.00	$1.99 \cdot 10^{-8}$	$3.89 \cdot 10^{-9}$	-8.41	42.3	1.99	7.83
b	30.00	$1.99 \cdot 10^{-8}$	$3.96 \cdot 10^{-9}$	-8.40	42.3	1.98	7.84

E.2 Experimental data for U on BUL1-1 samples

Tab. E-7: Experimental data for U on sample BUL-851 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1	30.00	$9.99 \cdot 10^{-5}$	$5.39 \cdot 10^{-5}$	-4.27	166.3	0.71	7.55
2	30.00	$3.00 \cdot 10^{-5}$	$1.66 \cdot 10^{-5}$	-4.78	165.3	0.69	7.62
3	30.00	$1.00 \cdot 10^{-5}$	$5.44 \cdot 10^{-6}$	-5.26	165.3	0.71	7.64
4	30.00	$3.03 \cdot 10^{-6}$	$1.51 \cdot 10^{-6}$	-5.82	166.9	0.78	7.61
5	30.00	$1.03 \cdot 10^{-6}$	$4.97 \cdot 10^{-7}$	-6.30	165.6	0.81	7.63
6	30.00	$3.33 \cdot 10^{-7}$	$1.55 \cdot 10^{-7}$	-6.81	165.6	0.84	7.56
7	30.00	$1.34 \cdot 10^{-7}$	$5.88 \cdot 10^{-8}$	-7.23	165.8	0.89	7.60
8	30.00	$4.28 \cdot 10^{-8}$	$1.95 \cdot 10^{-8}$	-7.71	167.5	0.85	7.75

Tab. E-8: Experimental data for U on sample BUL-861 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	33.00	$5.45 \cdot 10^{-5}$	$3.82 \cdot 10^{-5}$	-4.42	43.9	0.99	7.69
b	33.00	$5.45 \cdot 10^{-5}$	$3.82 \cdot 10^{-5}$	-4.42	43.9	0.99	7.68
2a	33.00	$1.64 \cdot 10^{-5}$	$1.01 \cdot 10^{-5}$	-5.00	43.9	1.16	7.67
b	33.00	$1.64 \cdot 10^{-5}$	$1.02 \cdot 10^{-5}$	-4.99	43.9	1.14	7.65
3a	33.00	$5.48 \cdot 10^{-6}$	$3.13 \cdot 10^{-6}$	-5.50	43.9	1.23	7.65
b	33.00	$5.48 \cdot 10^{-6}$	$3.18 \cdot 10^{-6}$	-5.50	43.9	1.22	7.64
4a	33.00	$1.67 \cdot 10^{-6}$	$8.56 \cdot 10^{-7}$	-6.07	43.9	1.33	7.63
b	33.00	$1.67 \cdot 10^{-6}$	$8.47 \cdot 10^{-7}$	-6.07	43.9	1.34	7.65
5a	33.00	$5.79 \cdot 10^{-7}$	$2.69 \cdot 10^{-7}$	-6.57	43.9	1.42	7.64
b	33.00	$5.79 \cdot 10^{-7}$	$2.65 \cdot 10^{-7}$	-6.58	43.9	1.43	7.63
6a	33.00	$1.96 \cdot 10^{-7}$	$8.35 \cdot 10^{-8}$	-7.08	43.9	1.49	7.68
b	33.00	$1.96 \cdot 10^{-7}$	$8.28 \cdot 10^{-8}$	-7.08	43.9	1.49	7.70
7a	33.00	$8.79 \cdot 10^{-8}$	$3.61 \cdot 10^{-8}$	-7.44	43.9	1.52	7.65
b	33.00	$8.79 \cdot 10^{-8}$	$3.59 \cdot 10^{-8}$	-7.45	43.9	1.52	7.68
8a	33.00	$3.82 \cdot 10^{-8}$	$1.52 \cdot 10^{-8}$	-7.82	43.9	1.54	7.66
b	33.00	$3.82 \cdot 10^{-8}$	$1.52 \cdot 10^{-8}$	-7.82	43.9	1.54	7.63

Tab. E-9: Experimental data for U on sample BUL-921 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$3.33 \cdot 10^{-5}$	$2.36 \cdot 10^{-5}$	-4.63	36.7	1.05	7.21
b	30.00	$3.33 \cdot 10^{-5}$	$2.21 \cdot 10^{-5}$	-4.66	36.7	1.14	7.18
2a	30.00	$1.00 \cdot 10^{-5}$	$7.53 \cdot 10^{-6}$	-5.12	36.7	0.96	7.13
b	30.00	$1.00 \cdot 10^{-5}$	$7.47 \cdot 10^{-6}$	-5.13	36.7	0.97	7.18
3a	30.00	$3.37 \cdot 10^{-6}$	$2.37 \cdot 10^{-6}$	-5.62	36.7	1.06	7.29
b	30.00	$3.37 \cdot 10^{-6}$	$2.26 \cdot 10^{-6}$	-5.65	36.7	1.12	7.13
4a	30.00	$1.03 \cdot 10^{-6}$	$6.75 \cdot 10^{-7}$	-6.17	36.7	1.16	7.14
b	30.00	$1.03 \cdot 10^{-6}$	$6.08 \cdot 10^{-7}$	-6.22	36.7	1.28	7.18
5a	30.00	$3.68 \cdot 10^{-7}$	$2.17 \cdot 10^{-7}$	-6.66	36.7	1.28	7.09
b	30.00	$3.68 \cdot 10^{-7}$	$2.18 \cdot 10^{-7}$	-6.66	36.7	1.28	7.13
6a	30.00	$1.35 \cdot 10^{-7}$	$6.86 \cdot 10^{-8}$	-7.16	36.7	1.42	7.15
b	30.00	$1.35 \cdot 10^{-7}$	$6.95 \cdot 10^{-8}$	-7.16	36.7	1.41	7.09
7a	30.00	$6.88 \cdot 10^{-8}$	$3.18 \cdot 10^{-8}$	-7.50	36.7	1.50	7.10
b	30.00	$6.88 \cdot 10^{-8}$	$3.26 \cdot 10^{-8}$	-7.49	36.7	1.48	7.14
8a	30.00	$3.61 \cdot 10^{-8}$	$1.86 \cdot 10^{-8}$	-7.73	36.7	1.41	7.10
b	30.00	$3.61 \cdot 10^{-8}$	$1.50 \cdot 10^{-8}$	-7.82	36.7	1.58	7.13

Tab. E-10: Experimental data for U on sample BUL-955 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$3.33 \cdot 10^{-5}$	$2.21 \cdot 10^{-5}$	-4.66	36.7	1.14	7.15
b	30.00	$3.33 \cdot 10^{-5}$	$2.02 \cdot 10^{-5}$	-4.70	36.7	1.25	7.32
2a	30.00	$1.00 \cdot 10^{-5}$	$6.95 \cdot 10^{-6}$	-5.16	36.7	1.08	7.13
b	30.00	$1.00 \cdot 10^{-5}$	$6.70 \cdot 10^{-6}$	-5.17	36.7	1.13	7.24
3a	30.00	$3.37 \cdot 10^{-6}$	$2.10 \cdot 10^{-6}$	-5.68	36.7	1.22	7.28
b	30.00	$3.37 \cdot 10^{-6}$	$2.08 \cdot 10^{-6}$	-5.68	36.7	1.23	7.36
4a	30.00	$1.03 \cdot 10^{-6}$	$5.56 \cdot 10^{-7}$	-6.25	36.7	1.37	7.20
b	30.00	$1.03 \cdot 10^{-6}$	$5.43 \cdot 10^{-7}$	-6.26	36.7	1.39	7.13
5a	30.00	$3.68 \cdot 10^{-7}$	$1.87 \cdot 10^{-7}$	-6.73	36.7	1.42	7.25
b	30.00	$3.68 \cdot 10^{-7}$	$1.74 \cdot 10^{-7}$	-6.76	36.7	1.48	7.24
6a	30.00	$1.35 \cdot 10^{-7}$	$6.18 \cdot 10^{-8}$	-7.21	36.7	1.51	7.09
b	30.00	$1.35 \cdot 10^{-7}$	$5.29 \cdot 10^{-8}$	-7.28	36.7	1.63	7.13
7a	30.00	$6.88 \cdot 10^{-8}$	$2.69 \cdot 10^{-8}$	-7.57	36.7	1.63	7.16
b	30.00	$6.88 \cdot 10^{-8}$	$2.69 \cdot 10^{-8}$	-7.57	36.7	1.63	7.09
8a	30.00	$3.61 \cdot 10^{-8}$	$1.51 \cdot 10^{-8}$	-7.82	36.7	1.58	7.13
b	30.00	$3.61 \cdot 10^{-8}$	$1.67 \cdot 10^{-8}$	-7.78	36.7	1.50	7.14

Tab. E-11: Experimental data for U on sample BUL-995 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	38.00	$2.84 \cdot 10^{-4}$	$1.21 \cdot 10^{-4}$	-3.92	23.7	1.76	7.78
b	38.00	$2.84 \cdot 10^{-4}$	$1.28 \cdot 10^{-4}$	-3.89	23.7	1.71	7.77
2a	38.00	$1.42 \cdot 10^{-4}$	$8.16 \cdot 10^{-5}$	-4.09	23.7	1.50	7.76
b	38.00	$1.42 \cdot 10^{-4}$	$8.34 \cdot 10^{-5}$	-4.08	23.7	1.47	7.76
3a	38.00	$4.75 \cdot 10^{-5}$	$3.49 \cdot 10^{-5}$	-4.46	23.7	1.18	7.77
b	38.00	$4.75 \cdot 10^{-5}$	$3.49 \cdot 10^{-5}$	-4.46	23.7	1.18	7.70
4a	38.00	$1.43 \cdot 10^{-5}$	$1.09 \cdot 10^{-5}$	-4.96	23.7	1.12	7.65
b	38.00	$1.43 \cdot 10^{-5}$	$1.07 \cdot 10^{-5}$	-4.97	23.7	1.15	7.70
5a	38.00	$1.43 \cdot 10^{-5}$	$1.09 \cdot 10^{-5}$	-4.96	23.7	1.12	7.66
b	38.00	$1.43 \cdot 10^{-5}$	$1.08 \cdot 10^{-5}$	-4.97	23.7	1.13	7.69
6a	38.00	$4.83 \cdot 10^{-6}$	$3.54 \cdot 10^{-6}$	-5.45	23.7	1.18	7.65
b	38.00	$4.83 \cdot 10^{-6}$	$3.51 \cdot 10^{-6}$	-5.46	23.7	1.20	7.65
7a	38.00	$1.51 \cdot 10^{-6}$	$1.01 \cdot 10^{-6}$	-5.99	23.7	1.32	7.65
b	38.00	$1.51 \cdot 10^{-6}$	$1.02 \cdot 10^{-6}$	-5.99	23.7	1.31	7.65
8a	38.00	$5.65 \cdot 10^{-7}$	$3.62 \cdot 10^{-7}$	-6.44	23.7	1.37	7.64
b	38.00	$5.65 \cdot 10^{-7}$	$3.44 \cdot 10^{-7}$	-6.46	23.7	1.43	7.66
9a	38.00	$2.33 \cdot 10^{-7}$	$1.50 \cdot 10^{-7}$	-6.82	23.7	1.37	7.64
b	38.00	$2.33 \cdot 10^{-7}$	$1.36 \cdot 10^{-7}$	-6.87	23.7	1.48	7.63
10a	38.00	$1.39 \cdot 10^{-7}$	$7.97 \cdot 10^{-8}$	-7.10	23.7	1.49	7.63
b	38.00	$1.39 \cdot 10^{-7}$	$8.20 \cdot 10^{-8}$	-7.09	23.7	1.46	7.63
11a	38.00	$1.01 \cdot 10^{-7}$	$5.30 \cdot 10^{-8}$	-7.28	23.7	1.58	7.60
b	38.00	$1.01 \cdot 10^{-7}$	$5.29 \cdot 10^{-8}$	-7.28	23.7	1.58	7.60
12a	38.00	$8.62 \cdot 10^{-8}$	$5.00 \cdot 10^{-8}$	-7.30	23.7	1.48	7.68
b	38.00	$8.62 \cdot 10^{-8}$	$4.98 \cdot 10^{-8}$	-7.30	23.7	1.49	7.63

Tab. E-12: Experimental data for U on sample BUL-1002 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$3.33 \cdot 10^{-5}$	$2.20 \cdot 10^{-5}$	-4.66	32.5	1.20	7.40
b	30.00	$3.33 \cdot 10^{-5}$	$2.41 \cdot 10^{-5}$	-4.62	32.5	1.07	7.46
2a	30.00	$1.00 \cdot 10^{-5}$	$6.91 \cdot 10^{-6}$	-5.16	32.5	1.14	7.32
b	30.00	$1.00 \cdot 10^{-5}$	$7.81 \cdot 10^{-6}$	-5.11	32.5	0.94	7.36
3a	30.00	$3.37 \cdot 10^{-6}$	$1.98 \cdot 10^{-6}$	-5.70	32.5	1.33	7.35
b	30.00	$3.37 \cdot 10^{-6}$	$2.31 \cdot 10^{-6}$	-5.64	32.5	1.15	7.48
4a	30.00	$1.04 \cdot 10^{-6}$	$5.61 \cdot 10^{-7}$	-6.25	32.5	1.42	7.43
b	30.00	$1.04 \cdot 10^{-6}$	$5.95 \cdot 10^{-7}$	-6.23	32.5	1.36	7.46
5a	30.00	$3.69 \cdot 10^{-7}$	$1.71 \cdot 10^{-7}$	-6.77	32.5	1.55	7.42
b	30.00	$3.69 \cdot 10^{-7}$	$1.86 \cdot 10^{-7}$	-6.73	32.5	1.48	7.45
6a	30.00	$1.36 \cdot 10^{-7}$	$5.28 \cdot 10^{-8}$	-7.28	32.5	1.69	7.42
b	30.00	$1.36 \cdot 10^{-7}$	$5.79 \cdot 10^{-8}$	-7.24	32.5	1.62	7.44
7a	30.00	$6.80 \cdot 10^{-8}$	$3.00 \cdot 10^{-8}$	-7.52	32.5	1.59	7.31
b	30.00	$6.80 \cdot 10^{-8}$	$3.01 \cdot 10^{-8}$	-7.52	32.5	1.59	7.41
8a	30.00	$3.61 \cdot 10^{-8}$	$1.22 \cdot 10^{-8}$	-7.91	32.5	1.78	7.33
b	30.00	$3.61 \cdot 10^{-8}$	$1.56 \cdot 10^{-8}$	-7.81	32.5	1.61	7.36

Tab. E-13: Experimental data for U on sample BUL-1017 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$3.33 \cdot 10^{-5}$	$3.08 \cdot 10^{-5}$	-4.51	22.5	0.55	7.35
b	30.00	$3.33 \cdot 10^{-5}$	$3.01 \cdot 10^{-5}$	-4.52	22.5	0.68	7.32
2a	30.00	$1.00 \cdot 10^{-5}$	$5.70 \cdot 10^{-6}$	-5.24	22.5	1.53	7.33
b	30.00	$1.00 \cdot 10^{-5}$	$6.64 \cdot 10^{-6}$	-5.18	22.5	1.36	7.41
3a	30.00	$3.37 \cdot 10^{-6}$	$2.07 \cdot 10^{-6}$	-5.68	22.5	1.44	7.36
b	30.00	$3.37 \cdot 10^{-6}$	$2.08 \cdot 10^{-6}$	-5.68	22.5	1.44	7.31
4a	30.00	$1.04 \cdot 10^{-6}$	$6.94 \cdot 10^{-7}$	-6.16	22.5	1.34	7.35
b	30.00	$1.04 \cdot 10^{-6}$	$6.99 \cdot 10^{-7}$	-6.16	22.5	1.33	7.45
5a	30.00	$3.69 \cdot 10^{-7}$	$2.54 \cdot 10^{-7}$	-6.60	22.5	1.31	7.28
b	30.00	$3.69 \cdot 10^{-7}$	$2.94 \cdot 10^{-7}$	-6.53	22.5	1.06	7.33
6a	30.00	$1.36 \cdot 10^{-7}$	$1.06 \cdot 10^{-7}$	-6.98	22.5	1.11	7.42
b	30.00	$1.36 \cdot 10^{-7}$	$1.05 \cdot 10^{-7}$	-6.98	22.5	1.12	7.41
7a	30.00	$6.80 \cdot 10^{-8}$	$5.68 \cdot 10^{-8}$	-7.25	22.5	0.94	7.38
b	30.00	$6.80 \cdot 10^{-8}$	$5.89 \cdot 10^{-8}$	-7.23	22.5	0.84	7.36
8a	30.00	$3.61 \cdot 10^{-8}$	$1.96 \cdot 10^{-8}$	-7.71	22.5	1.57	7.32
b	30.00	$3.61 \cdot 10^{-8}$	$1.95 \cdot 10^{-8}$	-7.71	22.5	1.58	7.24

E.3 Experimental data for U on TRU1-1 samples

Tab. E-14: Experimental data for U on sample TRU-748 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$2.86 \cdot 10^{-5}$	$2.41 \cdot 10^{-5}$	-4.62	31.8	0.76	7.64
b	35.00	$2.86 \cdot 10^{-5}$	$2.49 \cdot 10^{-5}$	-4.60	31.8	0.66	7.69
2a	35.00	$8.58 \cdot 10^{-6}$	$6.21 \cdot 10^{-6}$	-5.21	31.8	1.08	7.63
b	35.00	$8.58 \cdot 10^{-6}$	$6.03 \cdot 10^{-6}$	-5.22	31.8	1.12	7.58
3a	35.00	$2.87 \cdot 10^{-6}$	$2.05 \cdot 10^{-6}$	-5.69	31.8	1.10	7.52
b	35.00	$2.87 \cdot 10^{-6}$	$2.24 \cdot 10^{-6}$	-5.65	31.8	0.94	7.64
4a	35.00	$8.75 \cdot 10^{-7}$	$6.06 \cdot 10^{-7}$	-6.22	31.8	1.14	7.56
b	35.00	$8.75 \cdot 10^{-7}$	$5.45 \cdot 10^{-7}$	-6.26	31.8	1.28	7.61
5a	35.00	$3.04 \cdot 10^{-7}$	$1.72 \cdot 10^{-7}$	-6.76	31.8	1.38	7.57
b	35.00	$3.04 \cdot 10^{-7}$	$1.72 \cdot 10^{-7}$	-6.76	31.8	1.38	7.61
6a	35.00	$1.03 \cdot 10^{-7}$	$4.84 \cdot 10^{-8}$	-7.32	31.8	1.55	7.50
b	35.00	$1.03 \cdot 10^{-7}$	$4.80 \cdot 10^{-8}$	-7.32	31.8	1.56	7.55
7a	35.00	$4.78 \cdot 10^{-8}$	$2.12 \cdot 10^{-8}$	-7.67	31.8	1.59	7.55
b	35.00	$4.78 \cdot 10^{-8}$	$2.03 \cdot 10^{-8}$	-7.69	31.8	1.63	7.49
8a	35.00	$2.01 \cdot 10^{-8}$	$7.91 \cdot 10^{-9}$	-8.10	31.8	1.68	7.51
b	35.00	$2.01 \cdot 10^{-8}$	$8.84 \cdot 10^{-9}$	-8.05	31.8	1.60	7.58

Tab. E-15: Experimental data for U on sample TRU-794 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$2.86 \cdot 10^{-5}$	$2.38 \cdot 10^{-5}$	-4.62	31.5	0.81	7.61
b	35.00	$2.86 \cdot 10^{-5}$	$2.44 \cdot 10^{-5}$	-4.61	31.5	0.73	7.58
2a	35.00	$8.60 \cdot 10^{-6}$	$6.58 \cdot 10^{-6}$	-5.18	31.5	0.99	7.63
b	35.00	$8.60 \cdot 10^{-6}$	$6.65 \cdot 10^{-6}$	-5.18	31.5	0.97	7.66
3a	35.00	$2.89 \cdot 10^{-6}$	$2.12 \cdot 10^{-6}$	-5.67	31.5	1.06	7.70
b	35.00	$2.89 \cdot 10^{-6}$	$1.92 \cdot 10^{-6}$	-5.72	31.5	1.21	7.70
4a	35.00	$8.92 \cdot 10^{-7}$	$5.41 \cdot 10^{-7}$	-6.27	31.5	1.31	7.62
b	35.00	$8.92 \cdot 10^{-7}$	$5.71 \cdot 10^{-7}$	-6.24	31.5	1.25	7.58
5a	35.00	$3.20 \cdot 10^{-7}$	$2.08 \cdot 10^{-7}$	-6.68	31.5	1.23	7.67
b	35.00	$3.20 \cdot 10^{-7}$	$1.92 \cdot 10^{-7}$	-6.72	31.5	1.33	7.61
6a	35.00	$1.19 \cdot 10^{-7}$	$5.84 \cdot 10^{-8}$	-7.23	31.5	1.51	7.72
b	35.00	$1.19 \cdot 10^{-7}$	$6.18 \cdot 10^{-8}$	-7.21	31.5	1.46	7.71
7a	35.00	$6.51 \cdot 10^{-8}$	$3.09 \cdot 10^{-8}$	-7.51	31.5	1.55	7.62
b	35.00	$6.51 \cdot 10^{-8}$	$3.15 \cdot 10^{-8}$	-7.50	31.5	1.53	7.63
8a	35.00	$3.56 \cdot 10^{-8}$	$1.63 \cdot 10^{-8}$	-7.79	31.5	1.58	7.63
b	35.00	$3.56 \cdot 10^{-8}$	$1.72 \cdot 10^{-8}$	-7.76	31.5	1.53	7.63

Tab. E-16: Experimental data for U on sample TRU-815 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$2.86 \cdot 10^{-5}$	$2.79 \cdot 10^{-5}$	-4.56	22.0	0.06	7.70
2a	35.00	$8.58 \cdot 10^{-6}$	$7.54 \cdot 10^{-6}$	-5.12	22.0	0.79	7.65
b	35.00	$8.58 \cdot 10^{-6}$	$7.39 \cdot 10^{-6}$	-5.13	22.0	0.87	7.68
3a	35.00	$2.87 \cdot 10^{-6}$	$2.52 \cdot 10^{-6}$	-5.60	22.0	0.80	7.66
b	35.00	$2.87 \cdot 10^{-6}$	$2.49 \cdot 10^{-6}$	-5.60	22.0	0.84	7.66
4a	35.00	$8.75 \cdot 10^{-7}$	$6.86 \cdot 10^{-7}$	-6.16	22.0	1.10	7.67
b	35.00	$8.75 \cdot 10^{-7}$	$7.21 \cdot 10^{-7}$	-6.14	22.0	0.99	7.66
5a	35.00	$3.04 \cdot 10^{-7}$	$2.46 \cdot 10^{-7}$	-6.61	22.0	1.03	7.65
b	35.00	$3.04 \cdot 10^{-7}$	$2.35 \cdot 10^{-7}$	-6.63	22.0	1.12	7.65
6a	35.00	$1.03 \cdot 10^{-7}$	$7.62 \cdot 10^{-8}$	-7.12	22.0	1.20	7.64
b	35.00	$1.03 \cdot 10^{-7}$	$7.25 \cdot 10^{-8}$	-7.14	22.0	1.28	7.64
7a	35.00	$4.77 \cdot 10^{-8}$	$3.58 \cdot 10^{-8}$	-7.45	22.0	1.18	7.65
b	35.00	$4.77 \cdot 10^{-8}$	$3.28 \cdot 10^{-8}$	-7.48	22.0	1.31	7.64
8a	35.00	$2.01 \cdot 10^{-8}$	$1.76 \cdot 10^{-8}$	-7.76	22.0	0.81	7.53
b	35.00	$2.01 \cdot 10^{-8}$	$1.40 \cdot 10^{-8}$	-7.85	22.0	1.29	7.66

Tab. E-17: Experimental data for U on sample TRU-831 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	35.00	$2.86 \cdot 10^{-5}$	$2.46 \cdot 10^{-5}$	-4.61	30.9	0.72	7.45
b	35.00	$2.86 \cdot 10^{-5}$	$2.49 \cdot 10^{-5}$	-4.60	30.9	0.68	7.54
2a	35.00	$8.60 \cdot 10^{-6}$	$6.50 \cdot 10^{-6}$	-5.19	30.9	1.02	7.55
b	35.00	$8.60 \cdot 10^{-6}$	$6.23 \cdot 10^{-6}$	-5.21	30.9	1.09	7.57
3a	35.00	$2.89 \cdot 10^{-6}$	$1.90 \cdot 10^{-6}$	-5.72	30.9	1.22	7.50
b	35.00	$2.89 \cdot 10^{-6}$	$1.83 \cdot 10^{-6}$	-5.74	30.9	1.27	7.48
4a	35.00	$8.92 \cdot 10^{-7}$	$4.93 \cdot 10^{-7}$	-6.31	30.9	1.42	7.43
b	35.00	$8.92 \cdot 10^{-7}$	$4.75 \cdot 10^{-7}$	-6.32	30.9	1.45	7.51
5a	35.00	$3.21 \cdot 10^{-7}$	$1.49 \cdot 10^{-7}$	-6.83	30.9	1.57	7.56
b	35.00	$3.21 \cdot 10^{-7}$	$1.46 \cdot 10^{-7}$	-6.84	30.9	1.59	7.50
6a	35.00	$1.18 \cdot 10^{-7}$	$4.75 \cdot 10^{-8}$	-7.32	30.9	1.68	7.55
b	35.00	$1.18 \cdot 10^{-7}$	$4.43 \cdot 10^{-8}$	-7.35	30.9	1.73	7.55
7a	35.00	$6.49 \cdot 10^{-8}$	$2.44 \cdot 10^{-8}$	-7.61	30.9	1.73	7.56
b	35.00	$6.49 \cdot 10^{-8}$	$2.53 \cdot 10^{-8}$	-7.60	30.9	1.71	7.50
8a	35.00	$3.56 \cdot 10^{-8}$	$1.33 \cdot 10^{-8}$	-7.88	30.9	1.74	7.52
b	35.00	$3.56 \cdot 10^{-8}$	$1.30 \cdot 10^{-8}$	-7.89	30.9	1.75	7.54

Tab. E-18: Experimental data for U on sample TRU-882 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$2.75 \cdot 10^{-5}$	$1.99 \cdot 10^{-5}$	-4.70	41.1	0.97	7.63
b	30.00	$2.75 \cdot 10^{-5}$	$1.96 \cdot 10^{-5}$	-4.71	41.1	0.99	7.59
2a	30.00	$7.51 \cdot 10^{-6}$	$4.85 \cdot 10^{-6}$	-5.31	41.1	1.13	7.55
b	30.00	$7.51 \cdot 10^{-6}$	$4.94 \cdot 10^{-6}$	-5.31	41.1	1.10	7.68
3a	30.00	$2.76 \cdot 10^{-6}$	$1.61 \cdot 10^{-6}$	-5.79	41.1	1.24	7.67
b	30.00	$2.76 \cdot 10^{-6}$	$1.60 \cdot 10^{-6}$	-5.80	41.1	1.25	7.68
4a	30.00	$7.66 \cdot 10^{-7}$	$3.76 \cdot 10^{-7}$	-6.42	41.1	1.40	7.66
b	30.00	$7.66 \cdot 10^{-7}$	$3.64 \cdot 10^{-7}$	-6.44	41.1	1.43	7.58
5a	30.00	$2.92 \cdot 10^{-7}$	$1.21 \cdot 10^{-7}$	-6.92	41.1	1.53	7.68
b	30.00	$2.92 \cdot 10^{-7}$	$1.05 \cdot 10^{-7}$	-6.98	41.1	1.63	7.65
6a	30.00	$9.26 \cdot 10^{-8}$	$3.20 \cdot 10^{-8}$	-7.50	41.1	1.66	7.66
b	30.00	$9.26 \cdot 10^{-8}$	$3.23 \cdot 10^{-8}$	-7.49	41.1	1.66	7.67
7a	30.00	$4.40 \cdot 10^{-8}$	$1.41 \cdot 10^{-8}$	-7.85	41.1	1.71	7.56
b	30.00	$4.40 \cdot 10^{-8}$	$1.42 \cdot 10^{-8}$	-7.85	41.1	1.71	7.68
8a	30.00	$1.89 \cdot 10^{-8}$	$5.75 \cdot 10^{-9}$	-8.24	41.1	1.74	7.66
b	30.00	$1.89 \cdot 10^{-8}$	$5.93 \cdot 10^{-9}$	-8.23	41.1	1.73	7.66

Tab. E-19: Experimental data for U on sample TRU-923 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$2.75 \cdot 10^{-5}$	$1.97 \cdot 10^{-5}$	-4.71	35.4	1.05	7.67
b	30.00	$2.75 \cdot 10^{-5}$	$1.99 \cdot 10^{-5}$	-4.70	35.4	1.03	7.68
2a	30.00	$7.51 \cdot 10^{-6}$	$4.71 \cdot 10^{-6}$	-5.33	35.4	1.23	7.66
b	30.00	$7.51 \cdot 10^{-6}$	$4.95 \cdot 10^{-6}$	-5.31	35.4	1.16	7.65
3a	30.00	$2.76 \cdot 10^{-6}$	$1.54 \cdot 10^{-6}$	-5.81	35.4	1.35	7.65
b	30.00	$2.76 \cdot 10^{-6}$	$1.59 \cdot 10^{-6}$	-5.80	35.4	1.32	7.67
4a	30.00	$7.66 \cdot 10^{-7}$	$3.41 \cdot 10^{-7}$	-6.47	35.4	1.55	7.64
b	30.00	$7.66 \cdot 10^{-7}$	$3.74 \cdot 10^{-7}$	-6.43	35.4	1.47	7.64
5a	30.00	$2.92 \cdot 10^{-7}$	$1.12 \cdot 10^{-7}$	-6.95	35.4	1.66	7.63
b	30.00	$2.92 \cdot 10^{-7}$	$1.10 \cdot 10^{-7}$	-6.96	35.4	1.67	7.59
6a	30.00	$9.26 \cdot 10^{-8}$	$3.03 \cdot 10^{-8}$	-7.52	35.4	1.76	7.66
b	30.00	$9.26 \cdot 10^{-8}$	$3.08 \cdot 10^{-8}$	-7.51	35.4	1.75	7.65
7a	30.00	$4.40 \cdot 10^{-8}$	$1.45 \cdot 10^{-8}$	-7.84	35.4	1.76	7.67
b	30.00	$4.40 \cdot 10^{-8}$	$1.26 \cdot 10^{-8}$	-7.90	35.4	1.85	7.66
8a	30.00	$1.89 \cdot 10^{-8}$	$6.13 \cdot 10^{-9}$	-8.21	35.4	1.77	7.63
b	30.00	$1.89 \cdot 10^{-8}$	$7.06 \cdot 10^{-9}$	-8.15	35.4	1.67	7.69

Tab. E-20: Experimental data for U on sample TRU-938 in its corresponding SPW (cf. Tab. 2-4).

Sample	**Vol** (10^{-3} L)	**U_{in}** (M)	**U_{aq}** (M)	**Log U_{aq}** (M)	**S/L ratio** (10^{-3} kg/L)	**log R_d** (L/kg)	**pH**
1a	30.00	$2.75 \cdot 10^{-5}$	$1.56 \cdot 10^{-5}$	-4.81	39.4	1.29	7.72
b	30.00	$2.75 \cdot 10^{-5}$	$1.35 \cdot 10^{-5}$	-4.87	39.4	1.42	7.73
2a	30.00	$7.51 \cdot 10^{-6}$	$3.64 \cdot 10^{-6}$	-5.44	39.4	1.43	7.73
b	30.00	$7.51 \cdot 10^{-6}$	$3.65 \cdot 10^{-6}$	-5.44	39.4	1.43	7.74
3a	30.00	$2.76 \cdot 10^{-6}$	$1.36 \cdot 10^{-6}$	-5.87	39.4	1.42	7.72
b	30.00	$2.76 \cdot 10^{-6}$	$1.16 \cdot 10^{-6}$	-5.94	39.4	1.55	7.76
4a	30.00	$7.66 \cdot 10^{-7}$	$3.36 \cdot 10^{-7}$	-6.47	39.4	1.51	7.75
b	30.00	$7.66 \cdot 10^{-7}$	$3.14 \cdot 10^{-7}$	-6.50	39.4	1.56	7.74
5a	30.00	$2.92 \cdot 10^{-7}$	$1.37 \cdot 10^{-7}$	-6.86	39.4	1.46	7.74
b	30.00	$2.92 \cdot 10^{-7}$	$1.39 \cdot 10^{-7}$	-6.86	39.4	1.45	7.75
6a	30.00	$9.26 \cdot 10^{-8}$	$3.34 \cdot 10^{-8}$	-7.48	39.4	1.65	7.74
b	30.00	$9.26 \cdot 10^{-8}$	$3.92 \cdot 10^{-8}$	-7.41	39.4	1.54	7.75
7a	30.00	$4.40 \cdot 10^{-8}$	$1.77 \cdot 10^{-8}$	-7.75	39.4	1.58	7.73
b	30.00	$4.40 \cdot 10^{-8}$	$1.52 \cdot 10^{-8}$	-7.82	39.4	1.68	7.75
8a	30.00	$1.89 \cdot 10^{-8}$	$8.35 \cdot 10^{-9}$	-8.08	39.4	1.51	7.76
b	30.00	$1.89 \cdot 10^{-8}$	$6.89 \cdot 10^{-9}$	-8.16	39.4	1.64	7.76