SUBJECT INDEX

Papers are listed under subject headings based on symposia organised for the Goldschmidt Conference in Edinburgh in August-September, 1994. Sub-headings are used for the larger symposia, and often these sub-headings cover material which overlaps several symposia. The subject headings and their research areas are briefly outlined below, and these are followed by listings of the papers in alphabetical order under each subject heading or sub-heading.

- 1. Theoretical geochemistry applications of theoretical mineral physics to mineral chemistry and element distribution, including aspects of diffusion; ab initio methods.
- 2. Experimental geochemistry laboratory experimental studies across the full spectrum of P-T conditions.
- 3. Geochemical techniques developments in instrumentation and techniques; special applications and programmes.
- 4. Weathering and erosion, deposition and diagenesis geochemical processes in low temperature rock degradation and genesis.
- 5. Groundwater chemistry and palaeohydrology geochemical characterisation of groundwater systems and of time dependent hydrogeological changes, significance to palaeoenvironments, prognoses of future changes.
- **6.** Waste containment and pollutant transport geochemical assessment of the contols and risks of all types of waste and pollutant disposal.
- 7. Ocean composition and fluxes during the Quaternary high resolution documentation of changes in marine geochemistry, and geochemical indicators of recent events.
- **8.** Ocean palaeochemistry and the evolution of the ocean basins the goechemistry of ocean evolution in the pre-Quaternary.
- 9. Modern submarine hydrothermal processes contols on the geochemical reactions within sub-seafloor hydrothermal systems, and their spatial and temporal variability.
- 10. Mechanisms of isotopic and chemical communication in crust and mantle rocks application of new microanalytical (ion and laser probe) techniques to constrain micron to millimetre scale processes in rocks, and their relevance to macroscopic studies of mass and heat transport.
- 11. Partitioning of elements new data on partition coefficients for mineral, melt, fluid phases as determined by experiment or measurement of natural phases; including aspects of the distribution of precious metals.
- 12. Dehydration, partial melting and fluid distribution in the crust covering both the geochemistry of high-temperature processes in the continental crust and the modification of crust undergoing subduction.
- 13. Magma generation processes geochemical evidence of the generation and evolution of mantle-derived melts.
- **14.** Mantle development in space and time geochemical and mineralogical information on mantle constitution.
- 15. Geochronometry and thermal history quantitative thermal histories of rocks and metamorphic belts.

1. Theoretical geochemistry

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Ab initio study of the relative stability under pressure of MgSiO₃-ilmenite, -perovskite, and (periclase + stishovite)

Combined experimental and computer simulation studies of cation diffusion in silicate garnets

Empirical relations to estimate kinetic constants of silicates

A transferable interatomic potential model for crystals and melts in the system CaO-MgO-Al₂O₃-SiO₂

Atomistic simulation studies of mineral surfaces and the role of impurities on their structure and stability

Chemical bonds in minerals: Topological analysis of the electron localization function

Theoretical studies of the speciation of Sb in sulphidic solutions Absolute ionic diffusion in MgO: computer calculations via lattice dynamics

Ab initio constant pressure molecular dynamics study of silicate perovskites

Oxygen diffusion and water-related defects in feldspar minerals: information from experimental and modelling studies

Applications of ab initio quantum mechanical potential surfaces to mineral physics calculations

Oxygen isotope fractionation in metal monoxides

2. Experimental geochemistry

2a. Experimental constraints on melting in the mantle

See listing under section 13a

2b. Acidic and other melts and fluids at high P and T

Baker, D R, Vaillancourt, J

Ballhaus, C
Blencoe, J G
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Dinsdale, A, Gisby, J
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The viscosity of F+H₂O-bearing peralkaline and peraluminous rhyolitic melts

C-H-O fluid speciations under mantle conditions Calculated activities for species in albite-water melts

The thermodynamics of mineral-melt equilibria in the system CaO-MgO-Al₂O₃-SiO₂

Carbon dioxide fugacities at high temperature and pressure Experimental investigation of the Fe-Mg-partitioning between

garnet and biotite with respect to the influence of Ti in biotite The structure of Ti-silicate glasses by Raman spectros-copy:

Implications for the role of Ti in natural melts Disappearance of the liquid-liquid miscibility gap in the system

CaO-MgO-SiO₂ at high pressure

Diffusive growth of water bubbles in rhyolitic melts

The primary carbon and the formation of carbon species in terrestrial magmas

The effect of water on the solubility and speciation of CO₂ in aluminosilicate glasses along the join SiO₂-NaAlO₂

Phase relations and chemistry of richteritic amphiboles in the system K₂O-Na₂O-CaO-MgO-Al₂O₃-SiO₂-H₂O (KNCMASH)

Carbonation reactions in eclogites at high pressure: implications for carbonic fluids in the mantle

Experimental determination of the solubilities of quartz, kyanite and corundum in H_2O in the lower crust and mantle

Marr, R A, Baker, D R, Williams-Jones, A E Mungall, J E, Dingwell, D B

Popp, R K, Virgo, D, Yoder, H S, Hoering, T C, Phillips, M W

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Bassett, W A
Snyder, D, Gier, E,
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Alkali zirconosilicate speciation in halogen-rich, felsic, peralkaline magmas

Effects of water content, temperature and pressure on actinide tracer diffusion in melts of haplogranitic composition

The role of hydrogen fugacity in controlling Ferric-Ferrous ratio and volatile content of Kaersutitic amphibole: an experimental study

Experimental determination of PVTX relations of fluids in the diamond-anyil cell

Experimental measurements of the thermal conductivity of molten silicates

The sanidine - 'sanidine hydrate' reaction boundary The density of water to 25kbar/1873K

2c. Mantle mineralogy and the transition zone

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Harte, B, Harris, J W

Harte, B, Hutchison, M T, Harris, J W Irifune, T

Kesson, S E, FitzGerald, J, Shelley, J M Pawley, A R, Wood, B J

Ulmer, P, Trommsdorff, V, Reusser, E Wood, B J, Helffrich, G Experimentally determined melting relations in simple and complex chemical systems at pressures up to 23 GPa

A review of natural mineral assemblages from the mantle transition zone

Trace element characteristics of the lower mantle - An ion probe study of inclusions in diamonds from Sao Luie

Phase transformations in pyrolite and subducted crust compositions down to a depth of 800 km in the lower mantle.

Phase relations for the former basaltic crust of the slab in the perovskitite facies of the lower mantle

Talc dehydration to 50 kbar: constraints on the volume of H₂O at high pressure

Experimental investigation of antigorite stability to 80 kbar

Mantle stratification: constraints from mineral physics, seismological and phase equilibrium data

2d. Mineral dissolution, interfaces and hydrothermal solutions

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Gammons, CH, Williams-Jones, AE, Yu, Y

Fluid flow equipment for hydrothermal investigations: apparatus and preliminary results

Coupled flow and reaction: a modelling and experimental study of zeolite diagenesis

Thallium (1) chloride complexing in aqueous media to 200°C Gallium solubility and aqueous speciation in hydrothermal solutions (60–125°C). Experimental study and comparison with aluminium

Hydrosulphide complexes of gold (I) at high pressures and temperatures: equilibrium and kinetic problems

A new method for determining excess Gibbs energies in binary metal-carbonate solid solutions

Solubility of kaolinite in alkaline solutions at hydrothermal conditions

Experimental study of Na-Al complexing in hydrothermal solutions

Evaluation of the chemical model in WATEQ4F: 1. The major ion activity coefficients - Na, K, Ca, Mg, Cl

Comparison between actual and theoretical dissolution rates in a granite-water interaction experiment at 180°C and 14 bar

New data on the stability of gold(I) chloride complexes at 300°C

Gammons, C H, Wood, S A, Williams-Jones, A E Gehring, A U, Schosseler, P M, Luster, J Hellmann, R

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Valsami-Jones, E, Bailey, E H, Ragnarsdottir, K V Wogelius, R A, Refson, K, Fraser, D G, Goff, J P, Grime, G W Experimental investigation of the stability of neodymium chloride complexes at 300°C

The chemical form of Mn(II) and V(IV) in mineral phases as determined by EPR spectroscopy

A leached layer hydrolysis model: A better way to understanding feldspar dissolution at elevated temperatures and pressures

Implications of pseudomorphic replacement for reactiontransport modelling in rocks

The solubility of sparingly-soluble minerals at 25°C using a flow-through column

Experimental study of kyanite dissolution rates as a function of Al and Si concentration

Determination of the sodium-borate association constant NaB(OH)⁴ between 75 and 200°C using new sodium selective glass electrodes

Calculation of the effect of KAl(OH)O₄ formation on the solubility of corundum at high pressures and temperatures Migration of cement pore fluids from a radioactive waste respository: Experimental studies of chlorite dissolution rates

A synchrotron EXAFS study of hydrothermal AgNO₃ solutions

Competition between metal-carboxylate complexing, mineral precipitation, and carboxylate decomposition reactions

On-line monitoring of clay mineral precipitation in sandstone porespace under flow conditions

Experimental investigation of the solubility of uranium (VI) under hydrothermal conditions

Hydration reactions at the mineral-fluid interface: Experimental and computational studies

2e. Stable isotope partitioning.

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Rosenbaum, J M, Mattey, D P, Elphick, S Tennie, A, Hoffbauer, R, Hoernes, S Zheng, Y-F, Metz, P, Satir, M The above liquidus inhomogenity and cluster differentiation of fluid magmatic melts

Oxygen isotope exchange rates in mineral-fluid systems: correlations and predictions

Effects of dissolved salts on calcite-water oxygen stable isotope fractionation at elevated temperatures and pressures Equilibrium garnet-calcite oxygen istope fractionation

Experimental determination of the oxygen isotope fractionations in the systems kyanite-calcite and talc-carbonate-water

Experimental calibration of oxygen isotope fractionation between calcite and tremolite in the presence of CO₂-H₂O fluid and a new data processing method for three phase systems

3. Geochemical techniques, instrumentation and special applications.

Galer, S J G, Laue, H-J, Goldstein, S L, Mezger, K, Hofmann, A W Hallbauer, D K Concept of a new thermal isotope mass spectrometer

Geochemical trace element analysis for ionic species by capillary electrophoresis

Halliday, A N, Lee, D-C, Christensen, J N, Yi, W, Hall, C M, Jones, C E, Teagle, D, Walder, A J, Freedman, P A Holdham, M T, Jarvis, I

Lahtinen, R, Lestinen, P, Korkiakoski, E, Salminen, R, Sandstrom, H, Savolainen, H, Vallius, H Petit, J-C

Sackett, W van Moort, J C I.C.P. magnetic sector multicollector mass spectrometry and its applications to geochemistry

A new method for the determination of the platinum group elements in sedimentary materials

Rock geochemistry research project (RGRP) in the Geological Survey of Finland

Applying MeV ion beam techniques to geochemical issues: Cross-fertilizing nuclear physics and geosciences

The utility of sediment pyrolysis

The chemical composition and paramagnetism of auriferous quartz

4. Weathering and erosion, deposition and diagenesis

4a. Early diagenesis

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Davison, W, Zhang, H, Miller, S

Donahoe, R J, Liu, C, Dobson, K, Graham Furukawa, Y, Barnes, H L Gonzalez-Lopez, J M, Fernandez-Nieto, C, Lopez-Galindo, A, Torres-Ruiz, J Holdham, M T, Jarvis

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Krom, M, Davison, P, Zhang,
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Krupp, R E, Suleimenov, O M

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Markel, D, Kolodny, Y, Luz, B, Nishri, A Michel, C

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The use of ¹³⁷Cs and ²¹⁰Pb to model erosive processes in high altitude settings; The Muttsee (Switzerland) example

Diagenetic mineral formation in sediments of the Mississippi River delta plain

Mathematical models of diagenetic processes in marine sediments: iron and manganese redox cycling and nonsteady state diagenesis

Why diagenetic carbonate concretions form: localised microbial buffering

Geochemical studies of salt marsh sediments: Evidence for possible ²¹⁰Pb mobility

Developing and applying new techniques for measuring steep chemical gradients of trace metals and inorganic ions at the sediment-water interface

Cycling of iron and manganese in a Riparian wetland

Replacement mechanisms among iron sulphide minerals Carbonates associated with the Almazan sepiolite-palygorskite deposits (northern Spain)

A new method for the determination of the platinum group elements in sedimentary materials

Hydrogeochemistry of sulphur isotopes in the Kalix River catchment, northern Sweden

High resolution sampling of pore waters using a gel probe from Eshwaite Water, Lake District

Thermodynamics of aqueous H₂S solutions at elevated temperatures: solubility and first dissociation constant

Trace Pb, Zn, Cd, Tl contents and Pb-Sr radiogenic isotopes in the dissolved and particulate phases of a river during high-water stage: constraints on the origin(s) and transport of the metals

Tracing phosphorus sources and P-cycling by oxygen isotopes in phosphate; Laker Kinneret (Israel)

A regular pattern of chert within Lower Carboniferous limestones at the Benbulben Range, NW-Ireland

Tracing sedimentary textures and source materials in paragneisses from the Bohemian Massif (Germany)

Novak, M, Wieder, R K Pierre, C, Taberner, C, Urquiola, M M, Pueyo, J J

Postma, D Rickard, D Sackett, W Schaller, T, Wehrli, B

Sholkovitz, E Wehrli, B, Dinkel, C, Muller, B Sulphur diagenesis in freshwater peatlands

Sulphur and oxygen isotopic composition of sulphates in hypersaline environments, as markers of redox depositional versus diagenetic changes

Kinetics of Fe(III) reduction in a marine sediment

A new sedimentary pyrite formation model

The utility of sediment pyrolysis

Focusing patterns of transition metals in lake sediments - indicators for the reconstruction of deep-water mixing in the past?

Fractionation of Rare Earth Elements in rivers and estuaries Measurements of benthis gradients in deep lakes with ionselective electrodes and video endoscopy

4b. Weathering of geological systems

Bricker, O P Cochran, M F, Berner, R A Faure, G, Nishiizume, K

Gislason, S R, Arnorsson, S, Armannsson, H
Holland, H D, Kuo, P H, Rye, R O
Phillips, F M, Bowen, D Q, Elmore, D
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Weathering and mass-balance budgets in small catchments
Vegetative enhancement of chemical weathering
Exposure dating of quartz sandstone in the Transantarctic
Mountains by cosmogenic ¹⁰Be and ²⁶Al
Present chemical weathering of basalt in Iceland

O₂ and CO₂ in the Late Archaean and Early Proterozoic atmosphere

Surface exposure dating of glacial features in Great Britain

Biotic enhancement of weathering redux

Chemical weathering beneath Alpine glaciers: rates and implications for CO₂ drawdown

Effects of climate on chemical weathering in watersheds underlain by granitoid rocks

4c. Weathering of minerals

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The tetrad effect, a general effect in partitioning of REE between aqua and solid

An integrated model for feldspar dissolution under acid conditions The kinetics of smectite dissolution

Replacement reactions during weathering: macrokinetic approach

Field weathering rates versus laboratory dissolution rates: An update

The effects of oxalic acid on kaolinite dissolution rate The coprecipitation of Mg and Si with calcium carbonate Geochemical modeling of diagenetic reactions

Use of AFM in experimental surface geochemistry

Weathering or hydrothermal alteration? - Examples from the Rhenish Massif, Germany

The effect of pH, HClO₄, HNO₃ and delta Gr on the dissolution rate of natural gibbsite using column experiments

Experimental simulations of fluid-rock interaction: The effect of surface area on the rate of alteration

An experimental study of fluid-rock interaction: application to groundwater aquifers

Kinetics and mechanisms of dissolution of silica at room temperature and pressure

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4d. Diagenesis of rocks

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Kinetics of CaCO₃ homogeneous precipitation in seawater Dissolution rates and alteration of muscovite, phlogopite and biotite at pH 1 to 4, room temperature

An alternative approach to assess the true nature of 2:1 mixedlayer silicates in diagenetic and weathering environments

Does redistribution of rare earth elements in turbidites of the Appalachian foreland basin compromise provenance information?

REE study in Jurassic radiolarites from the subbetic, Betic Cordillera, Spain

A comparison of shale compositions from the Western Canada sedimentary basis and the US Gulf coast: the importance of depositional composition on shale diagenesis

Multi-stage illite evolution in Upper Proterozoic shales: Rb-Sr, XRD and TEM studies

Crustal evolution in the source region of the Witwatersrand sediments, South Africa - evidence from quartz

Geochemistry of Proterozoic (~1.9 Ga) sedimentary rocks from the Labrador district, Canada

Rock porosity and element distribution in an extremely acid sulphate altered Tertiary Latite, Styria, Austria: a comparison

Geochemical traces and sequence stratigraphy analysis during the Upper Jurassic in South Iberia

The Cretaceous-Tertiary boundary in the Betic Cordilleras and Basque Cantabrian Basin; a study of the platinum group elements anomalies

Stable isotopic constraints on palaeoenvironment, temperatures and fluids, from silica and carbonate phases; East Kirkton, West Lothian, Scotland

Genesis of banded, fibrous and twisted quartz by 'catalysis', unstable crystallization fronts, and substitution: self-organisation in agates

Diagenetic and thermal history of a fore-arc basin sequence -The Himalia Ridge Formation, Alexander Island, Antarctica

Fluid-rock interactions in chalk groundwater systems: an initial investigation into geochemical composition of Upper Cretaceous chalks from SE England

REE behaviour across the Cretaceous-Tertiary boundary

Diagenesis of Miocene vitric tuffs to zeolites, Mexican Highlands, Mexico

Geochemical characteristics of Toarcian sedimentation in Alpine geological domains

Growth and dissolution characteristics of dolomite studied in ultrathin section: a new TEM approach

REE distribution as an indicator of the origin of carbonates and silicates in basaltic rocks

Stable isotopes, minor elements and diagenetic alteration associated with Tono sandstone-type uranium deposits in Japan

Geochemistry and mineralogy of some British coals

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Isotopic indicators of epigenetic alteration of Upper Proterozoic sediments on Siberian platform

4e. Experimental studies of mineral dissolution, interfaces and hydrothermal solutions

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5. Groundwater chemistry and palaeohydrology

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Okrugin, V M, Kokarev, S G, Okrugina, A M, Chubarov, V N, Shuvalov, R A

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Ruotsalainen, PH, Snellman, MV

A chromatographic model for water quality variations in the Aquia aquifer (Maryland, USA)

Hydrogeochemical investigation of the passive margin of the south east basin of France. GPF Programme

Chromatographic pattern in a freshening aquifer (Tertiary Ledo-Paniselian aquifer, Flanders-Belgium)

Time-dependent variations in groundwater chemistry: the Norwegian groundwater monitoring network

Chemical characterisation of core pore-waters for deep borehole investigations at Sellafield, Cumbria

Baseline hydrogeochemical study of shallow groundwaters in N E England

Tritium variability of repeated samplings of well waters in south Ontario

Isotopic and geochemical evidence for old groundwaters in a granite on the Canadian shield

¹³C in low temperature, CO₂-charged waters: a need for consistency with carbonate chemistry

Isotopic evidence for age of intense spring activity in the Arava Valley, Israel, during Quaternary times

The influence of open-cast lignite mining on adjacent ground water systems

The origins of deep groundwaters in Cumbria, northwest England: hydrochemical constraints

Chemical evolution of waters in long term interaction with granitic rocks: example of waters from Nagra boreholes, North Switzerland

An unusual example of the interaction of modern hydrothermal system with Au-Ag veins (South Kamchatka)

Mercury as pathfinder in geochemical exploration of hydrothermal gold-silver deposits in Kamchatka

Natural denitrification in groundwater in the presence of pyrite: Preliminary results obtained at Naizin (Brittany, France)

Strontium isotope characterization of flow systems in southern Nevada, USA

Applying MeV ion beam techniques to geochemical issues: Cross-fertilizing nuclear physics and geosciences

Modelling of hydrochemical evolution in coastal regression area in Finland: a mass balance approach

Groundwater chemistry in some Italian seismic areas: space and time correlations with tectonic features and seismic activity

The hydrogeochemical characterization of deep groundwaters in crystalline bedrock: investigations in boreholes with multipackers

Sanjuan, B, Mossmann, J.R, Merceron, T Stepanov, I I

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Wallin, B G K, Peterman, Z E

Walraevens, K, Cardenal, J

Modelling boom clay formation porewater chemistry: Ion exchange versus dissolution precipitation mechanisms

Distribution of mercury concentrations in the atmosphere over the Western part of the Pacific Ocean

The origin of nitrogen in aquifer systems in the great plain, Hungary

Stable and radiogenic isotope systematics in ground water and fracture fillings at Aspo, Sweden

Aquifer recharge and exchangeable cations in a Tertiary clay layer (Bartonian clay, Flanders-Belgium)

6. Waste containment and pollutant transport

Albrecht, A, Beer, J, Gloor, M, Fischer, A, Mattle, N Atkins, M, Glasser, F P

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Berry, JA, Bishop, HE, Cowper, MM, Fozard, PR, McMillan, JW, Mountfort, SA Birke, M, Rauch, U Chudaeva, VA Cidu, R, Caboi, R, Fanfani, L, Frau, F Cooper, GI, Cox, GA, Perutz, RN

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Rodriguez-Navarro, C, Sebastian, E Sigg, L, Nowack, B, Xue, H Aquatic transport behaviour of Cobalt deduced from nuclear reactor derived ⁶⁰Co

Modelling the geochemical degradation of cements in a waste repository

Heavy metals and lead isotopes in mollusks from a coastal pont (Thau, South France) and adjacent Mediterranean Sea

The application of nuclear microprobe analysis and secondary ion mass spectrometry to radioactive waste disposal studies

Geochemical investigations in the urban areas of Berlin Metal contamination of surface waters of Primorye

Hydrogeochemistry around an epithermal system hosting gold mineralisation

An assessment of experimental glass corrosion by comparison with ancient analogues

The geochemical development of mine waters in the former Uranium - mine Konigstein, Saxony, Germany

Trace elements in the neighbourhood of a coal-fired power station

Heavy metals content in sediments of the continental shelf of Cadiz (SW of Spain)

The Synroc strategy of HLW management

Chemistry and mineralogy of fly ash and filter cakes from the incineration of municipal solid wastes

Potential groundwater contamination from pulverised fuel ash (PFA)

Alteration of noble metal geochemical cycles due to sewage disposal

Modeling of hydro-geochemical processes in waste disposal systems

On ecological-geochemical monitoring in Kamchatka (The Mutnovsky-Asachinsky ore region)

Ejection of trace metals from volcanoes

Geochemistry and radioactive waste management - issues and conflicts

Pollution-derived heavy-metal enrichment on building stones

Role of strong ligands for the infiltration of trace metals into groundwater

Starostin, V I, Sobolev, R N, Volkov, A B

Sterpenich, J, Le Forestier, L, Libourel, G, Chaussidon, M, Barbey, P

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Taubald, H, Satir, M

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Forecast of changing migration condition of harmful solutions (on base of study of geological structures development)

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10a. Small-scale evidence of geochemical processes in mantle rocks and ultrabasic complexes
See section 14g

10b. Spatial distribution of isotope and trace element variations in rocks and magmas, and their implications

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11. Partitioning of elements

11a. Partition coefficients for silicate melts, minerals and associated fluids

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13d. Mafic-ultramafic rocks and complexes

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14. Mantle development in space and time

14a. Experimental constraints on melting in the mantle See section 13a

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14d. Large scale mantle to terrestrial geochemistry

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14e. Rare gases

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