Geochemical data of crystalline target lithologies of the Ries impact crater, Germany

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Abstract

This data set comprises major (XRF) and trace (XRF, ICP-MS, ICP-AES) element geochemistry of 185 samples of crystalline target lithologies of the Nördlinger Ries impact crater in Southern Germany.
The sample set was originally collected by D. Stöffler for the investigation of shock metamorphism and Schmitt and Siebenschock for a research project on the occurrence of impact diamonds in the Nördlinger Ries crater.
Repository samples and thin sections are available for more or less the whole sample set of Stöffler and selected samples from Schmitt and Siebenschock, and are stored in the impactite collection of the Museum für Naturkunde Berlin.

Keywords

Geology, Ries impact crater, target rock geochemistry, X-ray fluorescence, ICP-MS, ICP-AES

Samples

This compilation contains chemical data of 185 rocks from different crystalline basement lithologies of the Nördlinger Ries impact crater, Bavaria/Baden-Württemberg, Germany. This sample set represents a good overview about the various crystalline target lithologies (Engelhardt and Graup 1984), and extended their major element chemical data substantially by trace elements. The crystalline rocks were collected in outcrops of the megablock zone (Alerheim, Appetshofen, Bissingen, Hürnheim, Langenmühle, Lehberg, Maihingen, Minderoffingen, Möttingen, Nördlingen, Schmähingen, Schrattenhofen, Wengenhausen, Wennenberg, Wörnitzostheim) and as fragments from the suevite (Alte Bürg, Amerdingen, Aumühle, Bollstadt, Otting, Seelbronn, Zipplingen) or the impact melt breccia (Polsingen).
The following abbreviations for collectors were used: Sie = Siebenschock, M., Sch = Schmitt, R. T. and St = Stöffler, D.
The sample set originally collected by Stöffler was utilized for the investigation of shock metamorphism within the Nördlinger Ries impact crater. Petrographic details on selected samples are published in Stöffler (1970, 1971a, b, 1972). The samples collected by Schmitt and Siebenschock in 1996 and 1997 were applied to a research project on the occurrence of impact diamonds in the Nördlinger Ries crater (Schmitt et al. 2005).
Repository samples and thin sections are available under the given inventory numbers for more or less the whole sample set of Stöffler and selected samples from Schmitt and

Siebenschock, and are stored in the impactite collection of the Museum für Naturkunde Berlin.

Rock classification

The rock classification was carried out for the sample set collected by Stöffler by his own based on thin section investigations, and for the set collected by Schmitt and Siebenschock by Siebenschock based also on thin section inspection supported by major element chemistry data. Nevertheless, for samples of shock stage III a rock classification is prevented in many cases due to the intensive shock metamorphism destroying primary rock textures and mineral constituents. Such samples were classified “target rock, undifferentiated” in the compilation. Additionally, such highly shocked rocks are often influenced by post-impact hydrothermal alteration leading to alteration and/or carbonization.

Shock classification

The shock classification of the rocks is based on the classification system for quartzo-feldspathic rocks by Stöffler (1971a) and Stöffler and Grieve (2007). For the sample set collected by Stöffler the shock classification was done by him based on thin section inspection. For the sample set by Schmitt and Siebenschock the shock classification was carried out by Siebenschock. For these samples the shock stage was established by macroscopic (shock stage III, easily recognizable due to the pumice like texture) or thin section inspections (shock stages 0 to II).

Sample preparation

The samples were crushed with a RETSCH Jaw Crusher BB 100 with stainless steel grinding tools and afterwards milled with a RETSCH Vibratory Disc Mill RS 100 with stainless steel grinding devices. A slight contamination of the samples with Fe, Cr, and Ni could not be excluded due to these grinding materials.

XRF methodology

Major and trace element analyses were carried out in the years 1997-1999 by x-ray fluorescence spectroscopy (XRF). Therefore, a SRS 3000 spectrometer of SIEMENS AG (Karlsruhe, Germany) was used. The major elements (SiO_2, TiO_2, Al_2O_3, Fe_2O_3 [total-Fe as Fe_2O_3], MnO, MgO, CaO, Na_2O, K_2O, P_2O_5 and SO_3 [total-S as SO_3]) as well as the trace elements (Ba, Ce, Co, Cr, Cu, Mo, Nb, Ni, Pb, Rb, Sr, Th, U, V, Y, Zn and Zr) were measured on glass tablets composed of 0.600 g of pulverized sample material, which was dried for four hours at 105 °C, 3.600 g of Di-lithiumtetraborate (BRA A10 Specflux), and, depending on the oxidation grade of the sample, approximately 0.5 – 2.0 g NH_4NO_3 for the oxidation of the sample material. Glass tablets were produced using Pt/Au-crucibles (950/50) on a OXIFLUX burner chain (CRB ANALYSE SERVICE, Hardegsen, Germany).

For measurement and data analysis, a modified GEOQUANT program (SIEMENS) based on international rock standards (CERAM 2CAS11, CCRMP MRG-1, CCRMP SY-3, HUN BaH, IGEM 2e-10 [VS 813-89], IGEM MK-1 [VS 2125-81], IGEM MO-2 [VS 2116-81], IGEM MO-3 [VS 2117-81], IGEM MO-5 [VS 2119-81], IGEM MO-6 [VS 2120-81], IGEM MW-1 [VS 2121-81], IGEM MW-2 [VS 2122-81], IGEM MW-3 [VS 2123-81], IGEM MO-7 [VS 1046-94], IGEM MO-13 [VS 1044-94], IGEM MO-15 [VS 1017-94], IGEM VS-2889-84, IGI BIL-1 [VS 7126-95], IGI BIL-2 [VS 7176-95], MINTEK NIM-D [SARM 6], MINTEK NIM-G [SARM 1], MINTEK NIM-L [SARM 3], MINTEK NIM-N [SARM 4], MINTEK NIM-P [SARM 5], MINTEK NIM-S [SARM 2], MINTEK SARM 39 [X-39], MINTEK SARM 41 [X-41], MINTEK SARM 44 [X-44], MINTEK SARM 45 [X-45], MINTEK SARM 48 [X-48], MINTEK SARM 50 [X-50], RIAP OOPE401 [VS 5370-90], UNS SpS, ZGI AN, ZGI BM, ZGI FK, ZGI GM, ZGI GNA, ZGI KH, ZGI SW, ZGI TB, ZGI TS; see Govindaraju 1994 for description and analytical data), and 10 reference standards (SIEM-01 - SIEM-10; delivered by SIEMENS AG, Karlsruhe) was used.

Accuracy values on data presented here are 0.5 wt% for SiO_2, 0.1 wt% for Al_2O_3 and SO_3, 0.05 wt% for Fe_2O_3, MgO, CaO, Na_2O, K_2O, 0.01 wt% for TiO_2, MnO, and P_2O_5, 30 ppm for Ba, 25 ppm for Cu and Zn, 20 ppm for Ce and Pb, 10 ppm for Mo and U, and 5 ppm for Co, Cr, Nb, Ni, Rb, Sr, Th, V, Y and Zr. The precision values on these data are of about the same order or lower. Detection limits are as follows: 1.0 wt% for SiO_2, 0.5 wt% for Al_2O_3, 0.1 wt% for SO_3, 0.05 wt% for Fe_2O_3; 0.01 wt% for TiO_2, MnO, MgO, CaO, Na_2O, K_2O, and P_2O_5, 30 ppm for Ba, Ce, Cu and Zn, 15 ppm for Co, Cr, Ni, Rb, Sr, V and Zr, and 10 ppm for Mo, Nb, Th, U and Y.

During the analytical work an improvement of the measurement program for trace elements was established, which extended the original measured set of trace elements (Ba, Co, Cr, Mo, Ni, Rb, Sr, U, V and Zr) by Ce, Cu, Nb, Pb, Th, Y and Zn. Therefore, not all of the given analyses covered the complete set of trace elements.

Loss on ignition (LOI)

For loss on ignition (LOI), about 1 g of pulverized sample material, dried for four hours at 105 °C, was used. The sample material was heated in porcelain crucibles for four hours at 1000 °C. LOI was calculated using the weight difference from before and after heating. Detection limit, precision, and accuracy values for LOI are about 0.1 wt%.

CO_2 measurement

The CO_2 concentration of the samples was measured by infrared spectroscopy with a ROSEMOUNT CWA 5003 analyzer. Depending on the LOI between 0.2 to 2 g of pulverized sample material, which was dried for four hours at 105 °C, was used for the analyses. The temperature for the thermal decomposition and/or oxidation of the sample to release CO_2 was set to 990 °C and synthetically $CaCO_3$ p. aq. Was used as standard material. The detection limit of this method was 0.1 wt% CO_2, and the precision and accuracy values for are also about 0.1 wt% CO_2.

ICP-MS and ICP-AES methodology

Additional trace element analyses were determined for selected samples at ALS Geochemistry, North Vancouver, Canada, in 2015 by using inductively coupled plasma mass spectrometry (ICP-MS) for the elements Ba, Ce, Cr, Cs, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Nb, Nd, Pr, Rb, Sm, Sn, Sr, Ta, Tb, Th, Tm, U, V, W, Y, Yb, and Zr, and inductively coupled plasma atomic emission spectroscopy (ICP-AES) for the elements Ag, As, Cd, Co, Cu, Li, Mo, Ni, Pb, Sc, Tl, and Zn on lithium borate fusions prior to acid dissolution. Information about the measuring range and the analytical error are given in Table 1 and 2.

Table 1: Precision expectation method ICP-MS

Analyte	Units	Sig Figs	Lower Limit	Upper Limit	Tolerance (%)
Ba	ppm	3	0.5	10000	10
Ce	ppm	3	0.5	10000	10
Cr	ppm	3	10	10000	10
Cs	ppm	3	0.01	10000	10
Dy	ppm	3	0.05	1000	10
Er	ppm	3	0.03	1000	10
Eu	ppm	3	0.03	1000	10
Ga	ppm	3	0.1	1000	10
Gd	ppm	3	0.05	1000	10
Hf	ppm	3	0.2	10000	10
Ho	ppm	3	0.01	1000	10
La	ppm	3	0.5	10000	10
Lu	ppm	3	0.01	1000	10
Nb	ppm	3	0.2	2500	10
Nd	ppm	3	0.1	10000	10
Pr	ppm	3	0.03	1000	10
Rb	ppm	3	0.2	10000	10
Sm	ppm	3	0.03	1000	10
Sn	ppm	3	1	10000	10
Sr	ppm	3	0.1	10000	10
Ta	ppm	3	0.1	2500	10
Tb	ppm	3	0.01	1000	10
Th	ppm	3	0.05	1000	10
Tm	ppm	3	0.01	1000	10
U	ppm	3	0.05	1000	10
V	ppm	3	5	10000	10
W	ppm	3	1	10000	10
Y	ppm	3	0.5	10000	10
Yb	ppm	3	0.03	1000	10
Zr	ppm	3	2	10000	10

Table 2: Precision expectation method ICP-AES

Analyte	Unit	Sig Figs	Lower limit	Upper Limit	Tolerance (%)
Ag	ppm	3	0.5	100	10
As	ppm	3	5	10000	10
Cd	ppm	3	0.5	1000	10
Co	ppm	3	1	10000	10
Cu	ppm	3	1	10000	7
Li	ppm	3	10	10000	10
Mo	ppm	3	1	10000	10
Ni	ppm	3	1	10000	10
Pb	ppm	3	2	10000	10
Sc	ppm	3	1	10000	10
Tl	ppm	3	10	10000	10
Zn	ppm	3	2	10000	10

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