traceDs: What we have learned about the existing trace element partitioning data during the population phase

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Goals

Our goal in developing traceDs is to provide a transparent and accessible resource of experimental partitioning data for the community. traceDs now includes all* the experimental trace element partitioning data (>4700 experiments). We set a minimum standard for inclusion, with the threshold criteria being the inclusion of:

- Experimental conditions (T,P, capsule, device)
- Major element composition of the phases
- Trace element analyses of the phases

The data are stored using a schema derived from that of the Library of Experimental Phase Relations (LEPR), modified to account for additional metadata, and restructured to permit multiple analytical entries for various element/technique/standard combinations.

*we hope

Utility

Search methodologies – the current version of the site includes basic search protocols (by phase, conditions, etc.). However, the output is in approximately the same format as the published format. Therefore, care must be taken in processing the data from this raw form into a uniform format.

Template - Investigators are encouraged to use a common format for submitted data. A template for documenting experimental data is provided through the LEPR/trace interface. The data in that uniform format can then be submitted with the publication as supplementary materials and then uploaded to the database.

traceDs provides a resource for:

Experimentalists – The database facilitates experimental design, data management plans and data publication.

Reviewers – This resource may be used by reviewers to test models.

Modelers – traceDs may be used to create calibration datasets for trace element partitioning models.

Practitioners – For those who are attempting to calculate differentiation scenarios, the current form allows one to search for compositions that match the system of interest/

99% plagioclase 1% glass (D^{mix})

D^{true}		D^{mix}/D^{true}
1	1	1.00
0.5	0.505	1.01
0.1	0.109	1.09
0.05	0.0595	1.19
0.01	0.02	2.0
0.005	0.015	3.0
0.001	0.011	11.0

Table 4. Influence of analytical error related to the inclusion of glass in analyses of plagioclase on the values of the estimates of plagioclase/melt partition coefficients. The "true" D value (D^{true}) assumes that analyses of plagioclase in the mineral/glass pair is pure. D^{mix} is the estimated value of D assuming that the analytical volume includes 99 % plagioclase and 1% glass.

The impact on the "measured" partition coefficient of inclusion of glass in the analysis volume is directly related to the actual partition coefficient. The lower the actual partition coefficient, the greater the impact.

One method used to determine whether a phenocryst is in equilibrium is to calculate the liquid in equilibrium with the crystal, then compare that liquid with the host (see below).

	D plag Weinsteiger	ppm in plag assuming 100 ppm in melt	D plag Bedard	Calc ppm in liquid using Bedard	Ratio to original melt
Ti	0.025	2.5	0.04	63	0.63
La	0.031	3.1	0.09	34	0.34
Ce	0.025	2.5	0.075	33	0.33
Sm	0.015	1.5	0.06	25	0.25
Gd	0.0075	0.75	0.03	25	0.25
Y	0.006	0.6	0.03	20	0.20
Lu	0.003	0.3	0.02	15	0.15
Zr	0.0006	0.06	0.005	12	0.12

If we use the partition coefficients of Weinsteiger, then interpret those numbers in terms of Bedard, 2006, the plagioclase is modeled to not be in equilibrium with the model melt – in spite of the fact that the calculations were done based on the premise of equilibrium – in effect, using the Bedard expressions resulted in the wrong conclusion. This is due to fact that the data used in the calibration of the Bedard expressions included data that included "mixed" analyses. The values are offset to higher values as a function of D – the lower the D, the more they are offset to incorrect, and inflated values.

Observations

In the process of populating the database, we have learned a number of things about the existing published experimental partitioning data. Most important are:

- ~ 20% of experimental partitioning papers do not satisfy one or more of the threshold criteria.
- The standard format for presenting data is the average. This was developed as the standard during the time where there were space constraints for publication. We have continued to publish averages in spite of fact that all the information can be published as an electronic supplement.
- The uncertainties that are published with the compositional data are often not adequately explained. It is often unclear if the uncertainty/error represents 1 or 2 sigma, if it is the standard deviation of the average, or if it is the error based on signal/noise, etc.
- The distribution of data in compositional space is extremely uneven

Based on these findings, we propose a new set of publication standards for experimental data that include the minimum criteria described above, the use of a common template/metadata, and the publication of all analyses with error based on peak count rates and background.

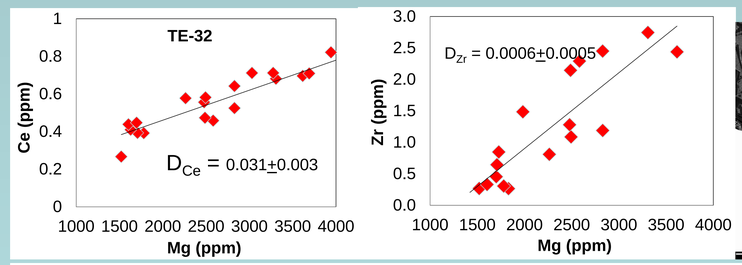
Issues and consequences

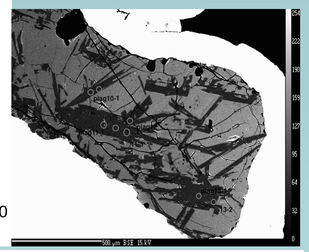
Distribution of data in compositional space – Even though we have conducted thousands of experiments – the coverage in compositional space is uneven – result is that we have a great deal of data for some elements/rock types/pressures and none for others – see example to right.

Over-processed data - We have rarely published the entire analytical dataset – rather, we have analysed the experimental charges, then averaged the results prior to interpretation and publication

Existing Experimental data for plagioclase/melt partitioning

Total # of experiments		276
# experiments that have data for each of these elements	Sr	167
	Ba	147
	La	79
	Ce	96
	Lu	25
	Ti	95
	Li	49
	Zr	41
	Pb	41
	Hf	10
	Re	1
	Os	0

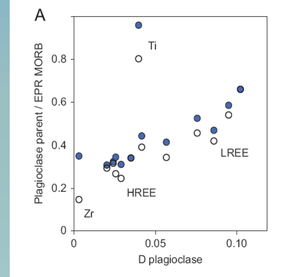




Above: BSE image of experimental charge TE-32 showing plagioclase and co-existing glass.

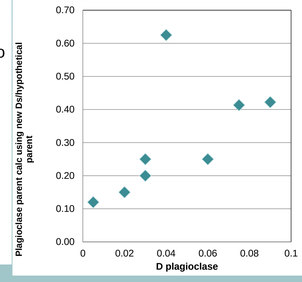
Note the correlation of Ce and Zr with Mg. Trend represented a "mixing" line between plagioclase and glass caused by inclusion of melt inclusions in the analysis volume. EMP analyses of the plagioclase (with a much smaller analysis volume) yield a value of 1500 ±250 ppm.

Typical selection criteria for "acceptable" mineral data are based on stoichiometry or concentration of what we assume is either a known (EMP values for Mg in plagioclase) or an excluded element (e.g. K in pyroxene). Therefore, the effective detection limit based on the analytical precision of EMP data and spatial resolution of SIMS or LA ICPMS for "mixed" data is approximately 1 %.



Left: from Lissenberg et al., 2013 "(iv) the degree of trace element depletion of plagioclase relative to MORB correlates strongly with plagioclase D's (Fig. 8A), which would require the D's to be increasingly erroneous with increasing incompatibility—an unlikely coincidence"

Right: modeled data using Weinsteiger partition coefficients interpreted using Bedard Ds



Future additions

- **Models – e.g. downloadable spreadsheets or programs from published investigations of partitioning behavior**
- **Enhanced interface, search and output formatting**
- **Workshop at Goldschmidt – Japan in June 2016**

Recommendations

- Publish all analyses – not averages
- Publish using a common template – available at the Earthchem portal and publish data as a supplementary file with common metadata
- Cite error in terms of counting statistics for each point
- Tie analyses to one another spatially – e.g. glass point nearest to pyroxene analytical point

CAVEATE – transcription of data is a human endeavor – there will be errors. If you find them, please contact Roger Nielsen and Gokce Ustunisik (roger.Nielsen@sdsmt.edu; gokce.ustunisik@sdsmt.edu) and provide details of where the errors lie.

Bedard, J.H. (2006) Trace element partitioning in plagioclase. Geochim Cosmochim Acta 70, 3717–3742
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Lissenberg, C.J. et al. (2013) Pervasive reactive melt migration through fast-spreading lower oceanic crust (Hess Deep, equatorial Pacific Ocean) Earth Planet. Sci. Lett.,
Weinsteiger, A.B. (2010) The origin of mid-ocean ridge basalts: insights from trace element contents in anorthite, anorthite hosted melt inclusions and ocean core complexes. PhD Thesis, Oregon State University, 403 pp.