HOW GOOD IS GOOD ENOUGH? MAJOR ELEMENT CHEMICAL ANALYSES OF BASALT BY SPACECRAFT INSTRUMENTS.

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Elemental abundances are among the most useful data about surface materials (rock, regolith) on planetary bodies, but there has been little discussion of scientific requirements of accuracy & precision on such analyses [1]. Scientific requirements flow from the objectives and investigations of a spacecraft missions, which are usually vague, e.g. "*Determine elemental composition ... of surface samples in order to understand the compositional diversity and origin of the crust*" [2].

Here, we demonstrate a Monte Carlo approach to understanding relationships between analytical precision of major element chemical analyses, and the capability of addressing geochemical objectives [3].

Monte Carlo Method: For a basalt composition and a set of analytical uncertainties (Table 1), we calculated 1000-2000 compositions with 1-σ uncertainties applied randomly, element by element, in EXCEL spreadsheets. Uncertainties for APXS analyses are for the instrument on MER [4]. VET uncertainties are as proposed for a Venus In-Situ Explorer (VISE) lander spacecraft [5]. Uncertainties for 'LIBS' include both for RMSEP accuracy (calibration) and precision (reproducibility) from the June 2015 recalibration of ChemCam LIBS on MSL [6, *Clegg et al.* in preparation]. We take those RMSEP and reproducibility values as equivalent to 2σ and independent of each other, add them in quadrature, and divide by two to give 1σ uncertainties. For Cr_2O_3, MnO, and P_2O_5, uncertainties are not given and are set to zero.

Table 1. Uncertainties on Chemical Analyses of Basalt

Source (1σ)	APXS[4] %	VET[5] %	'LIBS'† %
SiO_2	0.4	0.9	2.9
TiO_2	0.06	0.06	0.5
Al_2O_3	0.14	1.1	3.5
Cr_2O_3	0.03	0.16	*0.0*
FeO*	0.12	0.6	4.8
MnO	0.01	0.1	*0.0*
MgO	0.13	0.4	2.1
CaO	0.06	0.3	2.0
Na_2O	0.25	0.1	0.8
K_2O	0.06	0.01	1.0
P_2O_5	0.07	0.1	*0.0*

Uncertainties are on abundances in an analysis, i.e. SiO_2 = 51.5 ± 0.4%. FeO* is total Fe calculated as ferrous oxide. † See text.

Results: Chemical compositions calculated using these uncertainties were used to calculate derived petrologic quantities, and their variations.

CIPW Norm. The CIPW norm is an idealized model of the minerals and their proportions that would form from a magma if it were allowed to crystallize and equilibrate fully in the absence of water. CIPW norms were calculated with the 'norm4.xls' (by K. Hollocher) for a terrestrial flood basalt [5]. Selected average norm values and standard deviations are given in Table 2 for a molar Fe^{3+}/Fe_{Tot} = 0.1 – some minor normative phases are not reported.

The basalt of Table 2 is critically saturated in silica – its norm has little Quartz and no Olivine. The APXS uncertainties lead to small and geochemically unimportant variations in normative mineral proportions and inferred compositions. VET uncertainties do not permit sure knowledge that the basalt is Quartz-normative, but do show that it is near silica-saturation with fairly precise compositional parameters. Applying the 'LIBS' uncertainties, it is no longer clear if the basalt is silica saturated, undersaturated (Ol-normative), or strongly undersaturated (Ne-normative), nor precisely what its Mg# nor An might be.

Table 2. CIPW Normative Mineralogy: Bulk Rock [5] and Derived Uncertainties

Norm Mineral	Rock Wt %	1-σ Uncertainties APXS ± wt%	VET wt%	'LIBS' wt%
Qz	0.9	0.2	1.2	4
Plag	52.4	0.1	3.7	10
Kspar	2.4	0.03	0.16	4
Ne	0	0	0	2
Di	21.6	0.1	4.4	12
Hy	19.7	0.1	2.4	10
Ol	0	0.0	1.7	7
Mt	1.4	0.0	0.04	0.6
Ap	0.23	0	0.04	0.02
Chr	1.2	0.0	0.02	0.1
Mg#	57.6	0.0	1	14
An	59.3	0. 1	4	14

Normative Minerals are: Quartz, Plagioclase, K feldspar, Nepheline, Diopside, Hypersthene, Olivine, Magnetite, Apatite, and Chromite. Mg# is molar Mg/(Mg+Fe) in rock, An is molar Ca/(Ca+Na) in Plagioclase.

Tectonic Classifier. Major element chemical compositions of basalts may be characteristic of their tectonic setting, at least on Earth. One such classifier [7] is taken as an example (without endorsement).

In Figure 2, we classify a terrestrial ocean island (plume) basalt from Mauritius [8] with applied uncertainties of Table 1. With the uncertainties of APXS,

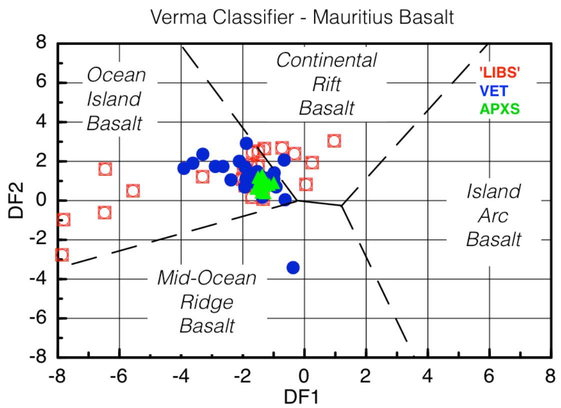

Figure 1. Tectonic classification [7] of an ocean island basalt from Mauritius [8], showing ~25 points for each set of uncertainties (Table 1). DF1 & DF2 are derived compositional components [7].

there is do doubt about inferred tectonic setting. With the VET uncertainties, points are spread out, but are nearly definitive; a few VET points fall outside this graph. However, applying 'LIBS' uncertainties gives a broad spread on this diagram (several points fall outside the diagram), and do not clearly define a tectonic setting for the basalt .

Mantle Equilibration P&T. If one assumes that a basalt magma last equilibrated with mantle peridotite (olivine + orthopyroxene) and assumes an Mg# for the peridotite, one can calculate the pressure (P) and temperature (T) of the average conditions under which the magma was generated [9,10].

For example, one can apply the analytical uncertainties of Table 1 to the martian Humphrey basalt of Gusev Crater [4,10], and see how its equilibration P&T are affected, Figure 2 [9,10]. Applying APXS uncertainties gives a tight cluster of points, and a fairly precise estimate of mantle equilibration. The VET points have double the uncertainties of the APXS points, but still are restrictive. The 'LIBS' uncertainties give compositions that span a large range of P&T (several points fall outside the diagram), so as to preclude useful geophysical inferences.

Implications: The adequacy of chemical elemental analyses of solid planetary materials depends critically on the science questions to be answered. Here, we show that major element analyses like to those of MER APXS [4] are adequate to distinguish among varieties of basalts, and to provide precise values for some geophysical parameters of their origins. Analyses with uncertainties like those suggested for a Venus lander [5] are nearly as good for basalt classification and understanding a planetary mantle. Analyses with 'LIBS'-

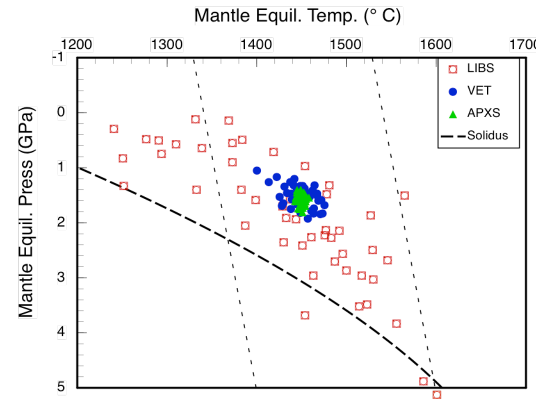

Figure 2. P & T at which Humphrey basalt (Gusev Crater) [4,10] last equilibrated with Mars' mantle, calculated as by [9], showing ~50 points for each set of uncertainties (Table 1). Heavy curve is mantle solidus; light lines are adiabats [10].

like uncertainties are not adequate for either purpose.

However, analyzes with 'LIBS'-like uncertainties could satisfy other science goals, e.g.: rapid surveys of rock and soil compositions [11]; determining if Venus' highlands are granitic or basaltic [12-14]; or determining if an asteroid is chondritic or differentiated [1]. For these goals, the tight analytical uncertainties of APXS and VET may not be necessary. (LIBS may yet become significantly more quantitative [6,15]).

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