INSTRUMENT REQUIREMENTS FOR GEOCHEMISTRY (ELEMENTAL ABUNDANCES): AN APPROACH.

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Introduction: Elemental abundances in glass and crystalline materials on planetary surfaces provide some of the strongest constraints on the origins of planets, asteroids, and other solar system materials. The importance of elemental analyses is clear from the presence of such instruments Mars and Venus rovers. However, it has been difficult to develop science-driven requirements on the performance of elemental analysis instruments, for many reasons.

First, the abundance of any individual element in a sample is rarely considered individually, but forms a component in a multidimensional space of possible compositions and inferences. For example, a given Al abundance might be evidence of feldspars if accompanied by elevated Si, K, Na, and Ca, of spinel if Mg is high, or of alunite is S is present. The web of overlapping possible material types and geological scenarios for their origins adds great complexity to development of instrument requirements. Second, limitations imposed by the scale of the geochemical sampling are also critical to this issue. The ratio of beam/probe size to grain size needs to be either very small (to analyze individual minerals) or very big (to get a representative whole rock analysis) [1]. Results must always be considered carefully within their spatial context, which must be supported by images acquired at appropriate resolution. Finally, geochemists can be quite ingeneous in analyzing available data.

The Onus is on Geochemists: Solutions to these problems must come from the geochemical community. Each instrument system has its own limitations, so accommodating instrument systems and geochemical requirements should be the basis of useful negotiations. However, the technologists and engineers will still need quantitative metrics against which to judge the success of their systems.

A Complex Metric: Ideally, a geochemist would like to specify that an elemental analysis would permit (with some uncertainty) a given geological inference. To a technologist, that would require a quantitative metric for the inference. One can take as an example the sort of quantitative metrics that have been proposed for sorting Earth basalts according to their tectonic settings. Several such metrics have been proposed, commonly from multiple element abundances with success criteria represented graphically [2-4]. For example here, we consider the classification of Verma et al. 2006 [3,5], in which the full major element analyses of a large suite of test basalts are transformed to log-ratios to remove effects of closure [6], and subjected to linear discriminant analysis to extract the two most significant factors (DF1 and DF2). These discriminants are reported to retrieve the tectonic settings of basalts with ~90% success rate.

To test the effects of analytical precision on classification by the [3] scheme, one basalt each was chosen from three tectonic groups [7,8]. Around each basalt composition, we calculated 25 compositions by applying normally-distributed uncertainties to each element's abundance. For the Venera/Vega uncertainties (Na estimated), no tectonic setting can be inferred from Verma's classifier. For the MER APXS uncertainties, the rocks are classified correctly in ~90% of cases. Thus, one would hope that a hypothetical elemental analysis system would be at least as precise as the MER APXS.

Further, the required levels of analytical precision can be refined with sensitivity analyses for each metric or classifier. For the Verma classifier, DF1 is strongly dependent on precision of Ti abundances. However, imprecision in Ti can be offset by greater precision in Fe. These uncertainty levels could be optimized (in theory) to trade instrument costs and complexity against scientific return.

Conclusions: Generating science-based requirements for elemental analyses from spacecraft instruments is complex, because of the many potential uses for the analyses. The responsibility for quantifying these requirements lies with geochemists, who will need to understand their scientific requirements, and develop achievable instrument requirements from them. For example, the capability of analyzing S in surface rocks is critically important to understanding surface-atmosphere interactions on Venus. But defining detection limits and precision levels will depend on laboratory experimentation on surface-atmosphere interactions to understand the rates, processes, and products of the interactions.

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