Gamma-ray spectral unmixing of compositional end-members: A fresh look at lunar geochemistry
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Introduction: Global maps of the elemental composition of the lunar surface were determined from gamma ray and neutron data acquired by Lunar Prospector (LP) [1,2,3]. The chemical data were used for petrologic mapping and characterization of crustal terranes, providing insight into igneous processes that shaped the lunar surface [1-6]. Element spectral unmixing was used to determine the abundance of 10 elements (O, Mg, Al, Si, Ca, Ti, Fe, K, Th, and U) from gamma ray spectra binned on equal area pixels for three different map scales: 20°, 5°, and 2° [3]. The elemental abundances were found to be consistent with parameters independently measured by neutron spectroscopy, including atomic mass and macroscopic absorption.

Due in part to the large number of free parameters, some elements (esp. Ca and Si) were determined with poor precision for all but the coarsest (20°) scale. Some improvement in precision was achieved by fitting spectral components for oxides and correlating U with Th, thus reducing the number of free parameters from 10 to 8. Here, we take one step further and fit the spectral data with compositional end-members determined from lunar samples and meteorites.

The work is motivated in part by preparations for the Dawn mission at Vesta. The whole-rock compositions of the Howardite, Eucrite, and Diogenite (HED) meteorites, thought to originate from Vesta, are accurately represented by a mixing model with three end members [7,8]. Our approach can be used to determine the mixing ratios of the end members, basaltic eucrite, cumulate eucrite, and diogenite, directly from the spectral data. The statistical framework of least-squares spectral unmixing will also aid in the detection of compositional trends that are distinct from the HEDs. Since the gamma ray spectrometers used on Dawn and LP are similar [9], the LP data can be used to develop a common approach.

Lunar mixing model: End members were determined from a database of lunar meteorites, soils, and regolith breccias (MSRB), thought to be representative of the bulk regolith as seen by LP (ref. Fig. 5 of [3]). In matrix notation, the elemental abundance vector \( \mathbf{w} \) of length \( n = 10 \) is related to the end member mixing ratios \( \mathbf{r} \) of length \( m < n \) by \( \mathbf{w} = \mathbf{B} \mathbf{r} \) (Eq.1).

The columns of the matrix \( \mathbf{B} \) are the elemental compositions of the \( m \) end-members. Note that \( \mathbf{w} \), \( \mathbf{r} \), and the columns of \( \mathbf{B} \) are positive and have unit Euclidean norms. If \( \mathbf{w} \) is known, then a valid \( \mathbf{r} \) can be determined by constrained least squares. To determine \( \mathbf{B} \), we first searched over all permutations of \( m \) compositions in the MSRB database to find a combination that minimized the difference between the abundances in the database and those determined by Eq. 1. We then used a statistical optimization method to adjust the values of \( \mathbf{B} \) to improve the fit. The final end members, therefore, do not correspond to specific MSRB compositions.

For four end members (\( m = 4 \)), an Apollo (A) 14 KREEP-rich soil, a high-plagioclase bulk soil, an A17 high-Ti soil, and an A15 Fe-rich soil & green glass were selected as the starting point for the statistical optimization. For the optimal end-members, strong linear correlations between MSRB and fitted compositions were found for all elements (with Pearson coefficients ranging from 0.88 to 0.99), with the strongest correlations for Mg, Al, Ti, Fe, and Th and the weakest for Ca and Si. The addition of a fifth end member would improve the accuracy of the model; however, four end-members may be sufficient to characterize MSRB compositional trends considering the analytical uncertainties for spectral unmixing.

End-member spectral unmixing: The least squares spectral unmixing algorithm of [3] solves the linear system \( \mathbf{p} = \mathbf{H} \mathbf{w} \), where the columns of \( \mathbf{H} \) are the elemental response functions and \( \mathbf{p} \) is a vector containing the \( p \)-channel gamma ray spectrum for a selected pixel. Using Eq. 1, the linear system was recast in terms of mixing ratios as \( \mathbf{p} = \mathbf{Q} \mathbf{r} \), where \( \mathbf{Q} = \mathbf{HB} \). Mixing ratios and their propagated uncertainties were determined via constrained least squares for each pixel on each of the three map scales for data acquired in high altitude mapping orbit (100 km). Elemental and oxide weight fractions were then determined using Eq. 1 and compared with the MSRB data.

Results: Abundances for major oxides, Th and K, determined with high precision by end-member unmixing, were similar to those determined previously by elemental unmixing [3]. For example, the scatterplot of Th vs. FeO abundances in Fig. 1 reveals a collection of pixels (light blue circles) with intermediate Th and high FeO which map to regions in western Procellarum and Imbrium and that fall outside the set defined by the MSRB samples (triangle). While these compositions are not common in lunar samples, they are consistent with our mixing model, which follows lunar MSRB chemical trends.

For most highlands pixels, the goodness of fit (as measured by reduced chi-squared \( \chi^2 \)) for end-member spectral unmixing was similar to that obtained by elemental unmixing; however, a factor of two increase in
was observed for some mare pixels, in which case, a fifth end member could improve the fit.

Maps of end member (EM) mixing ratios are shown in Fig. 2. The map of the high-Ti EM0 is similar to maps of TiO2 (cf. [3,10,11]), and the KREEP-rich end member map (EM2) is similar to maps of Th and K (cf. [1,3]). The mixing ratio for the low-Ti, high-Fe and high-Mg EM1 is elevated along the western rim of the Procellarum basin, Imbrium, Serenitatis, and other basins, including south pole-Aitken. Together, EM0 and EM1 reveal the diversity of mare volcanism. The felsic EM3 illuminates the plagioclase-rich highlands.

Conclusions: We have demonstrated the use of lunar sample data to guide the analysis of nuclear spectroscopy data. The global lunar composition is accurately represented by a mixing model with four end members derived from MSRB compositions (cf. [5,12]). More end-members may be justified for some mare pixels or with the inclusion of additional compositional constraints, for example from neutron- or reflectance-spectroscopy. The young basalts of western Procellarum and Imbrium follow the same geochemical trends as basalts in the sample collection.

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