CHEMICAL VERSUS MINERALOGICAL INFLUENCE ON REFLECTANCE SPECTRA OF ANDESITIC WHOLE ROCK POWDERS


Introduction: Multispectral remote sensing in the visible and near infrared is an important tool for investigating the composition of planetary surfaces. The spectral signature of the reflected electromagnetic radiation yields information on the chemical and mineralogical constituents. Most absorptions are attributed to intra- and interatomic transitions caused by the elements of the first transition series according to their oxidation state, crystallographic site and the mineralogical configuration. Qualitative and quantitative analyzing techniques of multispectral data are based on comparable laboratory measurements. Extensive studies focused on the determination of the presence and amount of minerals by analyzing reflectance spectra (e.g. 1, 2, 3, 4, 5). In addition, the spectrophotometric analysis of multispectral data of lunar samples results in the quantitative estimation of chemical parameters (6). Proceeding from these results we performed laboratory measurements in order to compare the relation between the spectral reflectance and the chemical and mineralogical constituents, respectively.

Samples: Whole rock samples of the calcalkaline igneous complex of Ballachulish, GBR (mainly dikes) were crushed and sieved to a grain size <63 µm. Parts of the bulk powder have been used to determine the chemical composition by XRF and wet chemical analysis in order to distinguish Fe²⁺ and Fe³⁺ (7). The modal mineralogy was examined by thin section petrography with a point counter of 1500 up to 6500 (7). The mineral assemblage includes plagioclase, orthopyroxene, clinopyroxene, amphibole, and biotite.

Method: Bidirectional reflectance data were obtained in the wavelength region from 0.5-2.5 µm with a spectral resolution of 0.002-0.006 µm. The experimental configuration was held constant with a viewing angle of 0° and an illumination angle of 30°. The measurements were performed with an IRIS Mark IV double-IFOV spectroradiometer operated in a single-IFOV mode. Each sample was measured eight times against a halon standard.

Results: The spectral signatures are dominated by absorption features due to iron which occurs in the form of Fe²⁺ and Fe³⁺ mainly in Op/ Cpx, Am, and Bi. Absorption bands between 2.2-2.4 µm and at 1.4 µm are related to overtone vibrations of the OII⁻ ion. A high amount of iron in addition with a high amount of hydrated minerals results in a steepening of the continuum (reddening). Based on the determination of absorption features and the slope of the continuum it is possible to distinguish distinct spectral rock-groups. The differences in the reflectance spectra can be explained satisfactorily only by considering both the chemical and the mineralogical constituents.

As a first approximation to quantify the relation between composition and spectral signature the correlation between the average reflectance (from 0.5-2.5 µm) and a single chemical or mineralogical component respectively was determined (Table 1). With the exception of Al₂O₃, there exists a strong correlation with the main chemical constituents while the relation with the main mineral phases is poor. Regarding the average reflectance as a multiple linear combination of all the coexisting chemical components or minerals, respectively (Table 1), the results indicate that it is justified to interpret the spectral reflectance as well in terms of chemical as of mineralogical composition.

<table>
<thead>
<tr>
<th>chemistry</th>
<th>SiO₂</th>
<th>Al₂O₃</th>
<th>MgO</th>
<th>CaO</th>
<th>FeO</th>
<th>Fe₂O₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>concentration in wt %</td>
<td>50-74</td>
<td>14-18</td>
<td>0.2-7</td>
<td>0.7-9</td>
<td>0.5-5</td>
<td>0.5-3</td>
</tr>
<tr>
<td>R²</td>
<td>0.91</td>
<td>0.38</td>
<td>0.76</td>
<td>0.87</td>
<td>0.84</td>
<td>0.78</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>mineralogy</th>
<th>Plag</th>
<th>Op/</th>
<th>Cpx</th>
<th>Am</th>
<th>Bi</th>
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</thead>
<tbody>
<tr>
<td>concentration in wt %</td>
<td>0.26</td>
<td>41-68</td>
<td>0.11</td>
<td>0.19</td>
<td>0.25</td>
</tr>
<tr>
<td>R²</td>
<td>0.85</td>
<td>0.60</td>
<td>0.26</td>
<td>0.44</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Table 1. Correlation (R²) between average reflectance and main compositional constituents. The column at the right gives the values for multiple linear regression with chemical and mineralogical components, respectively.
Nevertheless it remains a crude approximation to consider only the average reflectance neglecting the spectral distribution of the reflected electromagnetic radiation. Therefore the reflectances at every wavelength were fitted by a multiple linear regression with the chemical or mineralogical composition. Figure 1 shows the accuracy of the fit against the wavelength for both. The chemical influence dominates near 0.6 and between 0.75-1.6 μm, where intratonic crystal field transitions mainly determine the reflectance spectra. At longer wavelengths the mineralogy becomes more pronounced while bond vibrations becomes more effective on the spectral reflection behaviour. Near 0.7 μm Fe\(^{2+}\) → Fe\(^{3+}\) charge transfers occur coinciding with a deterioration of both fits.

The experiment strongly suggests that multispectral reflection data in the visible and near infrared can be used not only to determine the mineralogy of a natural surface but also can be interpreted in terms of the chemical composition as already demonstrated for lunar samples (6). Regressions with normalized reflectance data clearly demonstrate that the chemical information is masked by neglecting the reflection intensity while the relation with the mineralogical composition remains fairly unaltered.

![Figure 1. Multiple linear regression between reflectance spectra and chemical and mineralogical composition, respectively, for whole rock powders of the igneous Ballachulish-complex.](image)

Acknowledgement:
We thank Dr. S. Weiss for making available the samples and the analyses.

References: