

Application of Near-Infrared Spectroscopy for the identification of rock mineralogy

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Introduction

In the present study, a variety of different rock samples characterized by hydrous minerals, from Kos Island, South-East Aegean, were used to produce reflectance spectra in the VIS-NIR region. The spectroscopic analysis is supported with petrographic analysis accompanied with microphotography and X-Ray Powder Diffraction analysis, aiming at first level to classify the samples into the main rock types, and secondly to contribute to the mineralogical recognition. Through this study we attempt to examine the spectral characteristics of these different lithotypes and the way that the mineralogy could affect the absorption features of each spectrum. Even though the spectral data may be difficult sometimes to be interpreted due to lacking available extensive spectral libraries, the NIR spectroscopy can be a useful tool for direct and on-site identification of the rock mineralogy. The absorption features are a result of energy-matter interactions caused by molecular vibrations at specific frequencies. The evaluation of these features allows us to determine which functional group participates in the structure of the mineral. The major spectral features in the NIR region is a result mostly of water and hydroxyl groups vibrations such as Al-OH, Fe-OH, Mg-OH (Clark et al., 1990). However, several different parameters (such as grain size, color, mineralogy, texture, water content etc.) can affect the spectroscopic properties of the samples resulting in spectral variability (Clark, 1999).

Geological Setting

Kos Island (Dodecanese) is located in the eastern edge of the Aegean Volcanic Arc (Pe-Piper and Piper 2005). The geologic structure of the island is composed of various lithologies spanning the three main categories of rock classification: magmatic, metamorphosed and sedimentary rocks (Drinia et al. 2010, Soder et al. 2016, Kalt et al. 1998). Significant events for the petrologic evolution of Kos were the two episodes of magmatism, whose products are mainly found in the western part of the island (dating at ~ 3.5 Ma and ~ 161 ka, respectively). Particularly, the ~161 ka magmatic event caused the largest Quaternary eruption (>60 km³) in the Mediterranean and the formation of the voluminous, unwelded Kos Plateau Tuff (KPT; Allen, 2001).

Materials and Methods

The sampling performed on Kos (Iliopoulos et al., 2016) comprised a range of different lithologies and the main rock types included in this study are actinolite schist, clay schist, cataclasite, monzodiorite, diorite, and altered diorite. Petrographic thin sections were prepared and studied by means of polarizing microscope (Zeiss AxioScope A.1) in order to determine the mineral phases and classify them in the three main rock types. The detailed petrographic analysis provided additional information for the texture of the sample, the particle size and the metamorphic conditions. The mineralogy of the samples was verified by means of X-Ray Powder Diffraction (BRUKER D8 Advance). The reflectance spectroscopy (SM-3500 Spectral Evolution portable spectrometer) was applied in contact with a smooth, clean surface of the hand samples. The samples did not pre-processed in order to achieve as much as possible of the realistic conditions in the field. The methods discussed above were applied at the Research Laboratory of Minerals and Rocks, Department of Geology, University of Patras.

Data Analysis and Conclusions

Each sample from Kos Island for this study, was examined for its petrological characteristics and a semi-quantification was determined from the XRPD analysis (Table 1).

Table 1. Major mineral identification and the semi-quantitative analysis of the studied samples ('-': not detected; 'tr': traces; '+': few; '++': common; '+++': frequent; '++++': abundant; '+++++': dominant). Mineral abbreviations are according to Whitney & Evans, 2010.

	AS1	AS8	AS14	L4	SP3	PPY4	PPY6
Lithotype	altered diorite	altered diorite	actinolite schist	clay schist	cataclasite	monzodiorite	diorite
qz	tr	tr	Tr	++	++++	+	tr
pl	+	++	++	+	++	++++	++++
afs	-	-	-	tr	tr	+	+
hbl-act	+++++	+++++	++++	-	-	+++	++
ep-zo	+	++	tr	-	-	-	-
ilt-bt-ms	-	-	+	++++	++	+	++
chl	tr	tr	++	+++	tr	tr	tr

Monzodiorite is an inequigranular, coarse-grained sample (PPY4) with porphyroid, poikilitic texture, comprising quartz, plagioclase, alkali-feldspar, hornblende and minor biotite. Sample PPY6, has a more dioritic composition with biotite and hornblende being more abundant. The predominant mineral of altered diorites (samples AS1, AS8) is hornblende, forming coarse-grain phenocrysts (up to 6 mm) in a fine-grained matrix with plagioclase, and its saussuritization products epidote and chlorite. The cataclastic sample (SP3) has a cataclastic texture and consists of quartz, plagioclase, muscovite and minor alkali-feldspar and chlorite. The clay schist sample (L4) is fine-grained and has a grano-nematoblastic texture comprising chlorite, muscovite, quartz and plagioclase and minor alkali-feldspar. The L4 sample comes from pelitic protolith and has undertaken low grade metamorphism (chlorite zone according to Barrow metamorphism). The actinolite schist (sample AS14) has a grano-lepidoblastic texture forming hornblende and plagioclase porphyroblasts in a chlorite – mica matrix. The following conclusions were drawn during the preparation of the study:

- The NIR spectra of altered diorites (samples AS1, AS8) are dominated by the zoisite and amphibole absorption features, however the percentage participation of the minerals plays an important role.
- In the case of sample AS8, where the epidote is more abundant in the sample, the spectrum illustrates the epidote absorption features more detailed, whereas the spectrum of AS1 illustrates the amphiboles absorption features, with broader characteristics though, due to the presence of epidote.
- The epidotes are good reflectors for NIR spectroscopy even though they are fine-grained, saussuritization products.
- The spectra from PPY4 is characterized by the presence of hornblende which dominates the sample, with characteristic doublet features at ~2330 and ~2390 nm. As the biotite participation increases (PPY6 sample), even though the spectrum is characterized by the hornblende absorption features, it has a positive slope and a small sharp feature at ~2250 nm, indicative of biotite.
- The spectrum obtained from the cataclastic (SP4) is characterized by broad rounded absorption features at ~1900 and ~2200 nm and that could indicate the presence hydrous, Al-rich minerals, like illite and muscovite. However, due to small percentage of phyllosilicate minerals and their brittle crystallinity as opposed to the siliceous minerals (quartz and feldspars), the characteristic absorption features in higher wavelengths (> 2300 nm) are subdued. Only a small, sharp feature at ~2290 indicate the presence of chlorite.
- The clay schist spectrum (sample L4) is characterized by the absorption features of mica. The intense absorption feature at ~2200nm is characteristic for illite-muscovite.
- The actinolite schist spectrum (sample AS14) is characterized by absorption features both of amphibole (~2400 nm) and chlorite (~2250 and ~2300 nm).
- Relatively light colour to transparent siliceous minerals such as quartz and feldspars do not exhibit any intense absorption features. The most noticeable effect is the increasing reflectance of the sample respectively to the percentage participation of these minerals.
- The broad absorption feature at ~1100 nm is characteristic for the presence of iron in oxides and hydroxides.

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