Mineral identification of rocks from Pohon Batu hot springs in West Seram using FTIR spectroscopy

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Abstract. This study demonstrates the Fourier Transform Infrared (FTIR) spectroscopy which has been applied to identification of mineral rocks from Pohon Batu hot springs, West Seram regency, Province of Maluku. FTIR spectroscopic interpretation are absorbance or transmittance spectra as a function of wavelength that shows the content of organic compounds found in rocks. From the conditions of mineral formation and presence of various impurity ions and elements also influence the intensity and position of the IR absorption peaks. This study identified the strong peaks of minerals like kaolinite at 3618 cm⁻¹, montmorillonite at 1612 cm⁻¹, organic carbon at 2924 cm⁻¹, quartz at 1874 cm⁻¹, calcite at 1797 cm⁻¹, albite at 1026 cm⁻¹, illite at 756 cm⁻¹ and hematite at 532 cm⁻¹. From the result of FTIR analysis indicates that this area has undergone hydrothermal alteration thus becoming a secondary minerals. Rock-forming minerals in the hydrothermal alteration process are influenced by the presence of temperature, pressure in geothermal fluids and the decomposition of plants and animals.

1. Introduction

Geothermal is one of the utilization of renewable natural resources in the fulfillment of future energy. One indication of the existence of geothermal sources below the surface is the emergence of hot or warm springs. Hot or warm springs are formed due to the flow of hot or warm water from beneath the surface through rock fractures. The geothermal appearance appears in Pohon Batu area, West Seram Regency, Province of Maluku, in the form of hot springs that appear in several locations, especially along the Wai Pupukula river [1].

The geology of Pohon Batu area are grouped into filite rock units (Pf), schist (PTs), conglomerates (TQk), limestone (Qbt), and alluvium (Qa) (Figure 1). The geological structure in the area of inquiry is dominated by the trending structures of the northwest relative to the southeast and southwest - northeast. This fault structure is expected to facilitate the release of a number of hot springs at the survey site [2]. In this area has undergone hydrothermal alteration. Hydrothermal alteration occurs because fluids and reservoir rocks interact with one another to produce a collection of secondary minerals. Rock-forming minerals in the hydrothermal alteration process are influenced by the presence of temperature and pressure in geothermal fluids. Alteration mineral around the hot springs are very much dominated by...
clay, chlorite from the alteration mineral group of amphibol and pyroxene, and some feldspar groups [2,3].

To investigate the geothermal potential in the Pohon Batu hot springs area, it is necessary to identify the rock minerals around the hot springs using Fourier Transform Infrared (FTIR) spectroscopy [4,5]. Figure 2 schematically illustrates the components of a simple dispersive infrared spectrometer [6]. The infrared radiation beam is produced from the instrument by passing through a hot wire and mirrors, then the beam is divided into two parallel beams with the same radiation intensity. The sample to be tested is placed in one beam and the other beam is used as a reference. After that, the beams then pass into the monochromator, which disperses each into the continuous infrared frequency spectrum. The monochromator consists of a fast spinning sector (beam chopper) which passes two beams alternately into a diffraction grating (prism on older instruments). The diffusion grating rotates slowly to change the frequency or wavelength of radiation reaching the thermocouple detector. The detector detects the ratio between the reference intensity and the sample beam. In this way the detector can determine which frequencies have been absorbed by the sample and which frequencies are not affected by the light passing through the sample. After the signal received from the detector is amplified, the recorder takes the spectrum of the sample produced on the graph. It is important to realize that the spectrum recorded as the frequency of infrared radiation changes with diffraction lattice rotation. Dispersive instruments and said to record spectrum in the frequency domain [4-7].
Note that it is customary to plot frequency (wavenumber, cm\(^{-1}\)) versus light transmitted, not light absorbed. This is recorded as percent transmittance \(\%T\) because the detector records the ratio of the intensities of the two beams, and
\[
\%T = \frac{I_s}{I_r} \times 100
\]  
where \(I_s\) is the intensity of the sample beam and \(I_r\) is the intensity of the reference beam. For the transmittance spectrum almost 100%, it means that the sample being tested is almost transparent to the radiation frequency (does not absorb it). The maximum absorption is shown with a minimum on the graph, while the absorption that occurs in the sample is referred to as the absorption peak [6,7].

Identification of the molecular structure of the infrared (IR) spectrum output can be matched using information from the correlation table. Based on the correlation table, it can be seen the absorbance of the area of the spectrum of functional groups and the comparison of the spectrum obtained with known compounds or obtain samples of suspected suspected substances. The results of FTIR spectroscopic interpretation are absorbance or transmittance spectra as a function of wavelength that shows the content of organic compounds found in rocks [7-9].

2. Methods
The IR absorption spectra were recorded with a spectrometer in a region of 400 - 4000 cm\(^{-1}\) with a resolution of 0.01 cm\(^{-1}\). Samples were taken from Pohon Batu hot springs area in West Seram, Province of Maluku. This method uses mixing of finely ground solid samples with powdered potassium bromide, and then the mixture is pressed under high pressure. In addition, after that process, the potassium bromide and seals compounds into the matrix. By using the spectrometer, KBr pellet as the result of that mixture be inserted into a holder of spectrometer [7]. This broadband infrared energy is emitted by a hot bar in the FTIR spectrometer and directed by a mirror to "shine" on minerals or mineral powders, depending on the sample module. The mineral response to IR stimulation is to selectively absorb some energy / IR wavelengths and reflect back the energy / other IR wavelengths. Instead of a single composite infrared “color”, the FTIR spectrometer shows as a graph of the intensities of infrared energy reflection (the fraction of each wavelength that was not absorbed) as a function of wavenumber. By comparing the infrared spectrum of an unknown mineral to the infrared spectra of known minerals (standards), we will be able to identify many unknown minerals [8].

3. Results And Discussions
There were two sample were taken from internal (Int) hot springs and two sample from external (Ext) hot springs. FTIR results are summarized in Tables 1 and 2, where a series of analytical values wavenumber (in cm\(^{-1}\)) of the absorption bands of FTIR spectra of the powder samples.

![Figure 3. FTIR Spectrum of two sample from internal hot springs: Int-1 and Int-2](image)
From Figure 3 obtained mineral contained in rocks from internal hot springs. Kaolinite shows a sequence characteristic IR absorption in the range of 3700 to 3600 cm\(^{-1}\). The peak at \(\nu = 3618\) cm\(^{-1}\) is due to OH stretching frequencies associated with the hydroxyl and the band observed at approximately 3620 cm\(^{-1}\) for kaolinite is as a result of an inner hydroxyl stretch \([9,10]\). The most characteristic spectrum of montmorillonite is the broad absorption band that varies from 3300 to 3500 cm\(^{-1}\). Usually, this band centered at about 3400 cm\(^{-1}\) is due to stretching of the O-H molecule of water present in the interlayer region of montmorillonite. From Tables 1, the presence of peaks at 3425 cm\(^{-1}\) and 1612 cm\(^{-1}\) in all samples indicates the presence of montmorillonite. Organic carbon have frequencies at 2924 cm\(^{-1}\) and 2854 cm\(^{-1}\). The quartz mineral were detected at 1874 cm\(^{-1}\), 779 cm\(^{-1}\), 694 cm\(^{-1}\) and 462 cm\(^{-1}\). Calcite spectrum shows peaks at 1797 cm\(^{-1}\) due to the C−O stretching of carbonate. Albite spectrum shows strong peak at 1087 cm\(^{-1}\), illite peaks at 756 cm\(^{-1}\) and then hermatite shows the characteristic peaks at 540 cm\(^{-1}\) \([9,10]\).

### Table 1. Absorption Frequency the samples collected from internal Pohon Batu hot springs, together with minerals identification.

| Sample | Wavenumber (cm\(^{-1}\)) | Intensity (%T) | Functional Group | Mineral |
|--------|--------------------------|----------------|------------------|---------|
|        | 3672                     | 26,31          | O-H              | Kaolinite |
|        | 3425                     | 17,74          | N-H              | Montmorillonite |
|        | 1612                     | 4,91           |                  |          |
| Int-1  | 2924                     | 19,75          | C-H              | Organic Carbon |
|        | 2854                     | 21,26          |                  |          |
|        | 1874                     | 8,00           | C-H              | Quartz |
|        | 779                      | 0,55           |                  |          |
|        | 694                      | 3,53           |                  |          |
|        | 462                      | 0,10           |                  |          |
|        | 1797                     | 8,53           | C-O              | Calcite |
|        | 1087                     | 0,35           | C-N              | Albite |
|        | 3695                     | 26,11          | O-H              | Kaolinite |
|        | 3618                     | 19,37          |                  |          |
|        | 3425                     | 24,90          | N-H              | Montmorillonite |
|        | 1620                     | 18,58          |                  |          |
| Int-2  | 2924                     | 31,08          | C-H              | Organic Carbon |
|        | 2854                     | 31,22          |                  |          |
|        | 1874                     | 22,61          | C-H              | Quartz |
|        | 1797                     | 21,94          | C-O              | Calcite |
|        | 756                      | 10,63          | C-Cl             | Illite |
|        | 540                      | 4,53           | C-H              | Hematite |

**Figure 4.** FTIR Spectrum of two sample from external hot springs: Ext-1 and Ext-2.
In Figure 4 shows FTIR spectrum of sample were taken from external hot springs. Kaolinite shows a strong peak at $\nu = 3618$ cm$^{-1}$. Montmorillonite have strong peak at 1612 cm$^{-1}$. Organic carbon frequencies at 2924 cm$^{-1}$ and 2854 cm$^{-1}$. The quartz mineral were detected only at 1874 cm$^{-1}$ in two sample. Calcite spectrum shows peaks at 1797 cm$^{-1}$ due to the C–O stretching of carbonate. Albite spectrum shows strong peak at 1087 cm$^{-1}$, illite shows peak at 794 to 756 cm$^{-1}$ and hematite shows the characteristic peaks at 532 cm$^{-1}$[9,10].

| Sample | Wavenumber (cm$^{-1}$) | Intensity (%T) | Functional Group | Mineral |
|--------|------------------------|----------------|------------------|---------|
| Ext-1  | 3695                   | 8,27           | O-H              | Kaolinite |
|        | 3618                   | 5,87           |                  |          |
|        | 3448                   | 10,80          | N-H              | Montmorillonite |
|        | 1612                   | 4,91           |                  |          |
|        | 2924                   | 18,60          | C-H              | Organic Carbon |
|        | 2862                   | 19,50          |                  |          |
|        | 1874                   | 20,75          | C-H              | Quartz |
|        | 1774                   | 20,94          | C-O              | Calcite |
|        | 1026                   | 0,35           | C-N              | Albite |
|        | 756                    | 11,13          | C-Cl             | Illite |
|        | 532                    | 1,21           | C-H              | Hematite |
| Ext-2  | 3695                   | 16,34          | O-H              | Kaolinite |
|        | 3618                   | 11,10          |                  |          |
|        | 3425                   | 17,76          | N-H              | Montmorillonite |
|        | 1620                   | 22,28          |                  |          |
|        | 2924                   | 22,31          | C-H              | Organic Carbon |
|        | 2854                   | 23,04          |                  |          |
|        | 1874                   | 24,26          | C-H              | Quartz |
|        | 1797                   | 24,31          | C-O              | Calcite |
|        | 1033                   | 0,55           | C-N              | Albite |
|        | 794                    | 14,10          | C-Cl             | Illite |
|        | 532                    | 1,75           | C-H              | Hematite |

Based on FTIR analyses indicate that mineral of rocks from hot springs like kaolinite, montmorillonite, organic carbon, quartz, calcite, albite, illite and hematite. It was estimated that in this area has undergone hydrothermal alteration. Hydrothermal alteration occurs because fluids and reservoir rocks interact with one another to produce a collection of secondary minerals. In addition, temperature of hot springs is between 70-79°C, pH 6, conductivity (9,957-13,001) µS/m and water flow 1,10-1,56 L/min. It shows that geothermal system at Pohon Batu hot springs is water flow system from the subsurface or reservoir.

4. Conclusions
Determination of the type of minerals contained in rocks around hot springs has been carried out with a qualitative analysis approach based on the analysis of the absorption peak of FTIR. The intensity and peak position of IR absorption indicate the condition of mineral formation from rocks and the presence of various impurities and other elements. This study identified strong peaks of minerals such as kaolinite at 3618 cm$^{-1}$, montmorillonite at 1612 cm$^{-1}$, organic carbon at 2924 cm$^{-1}$, quartz at 1874 cm$^{-1}$, calcite at 1797 cm$^{-1}$, albite at 1026 cm$^{-1}$, light up at 756 cm$^{-1}$ and hematite at 532 cm$^{-1}$. FTIR analysis shows that this area has undergone hydrothermal changes so that it becomes a secondary mineral. Rock-
forming minerals in the process of hydrothermal change are influenced by temperature, pressure in geothermal fluids and decomposition of plants and animals.

5. References

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