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Analysis of urinary stone based on a spectrum absorption FTIR-ATR

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Abstract. This research analysed the urinary stone by measuring samples using Fourier transform infrared-attenuated total reflection spectroscopy and black box analysis. The main objective of this study is to find kinds of urinary stone and determine a total spectrum, which is a simple model of the chemical and mineral composition urinary stone through black box analysis using convolution method. The measurements result showed that kinds of urinary stone were pure calcium oxalate monohydrate, ion amino acid calcium oxalate monohydrate, a mixture of calcium oxalate monohydrate with calcium phosphate, a mixture of ion amino acid calcium oxalate monohydrate and calcium phosphate,pure uric acid, ion amino acid uric acid, and a mixture of calcium oxalate monohydrate with ion amino acid uric acid. The results of analysis of black box showed characteristics as the most accurate and precise to confirm the type of urinary stones based on theregion absorption peak on a graph, the results of the convolution, and the shape of the total spectrum on each urinary stones.

1. Introduction

Urinary stone is is the most painful diseases that is found in developing countries. In Indonesia, it becomes the highest visiting number of patients in urology clinic. According to health research in 2013, the highest prevalence of urinary stone disease occurs in the age group of 55-64 years (1.3%), which slightly decreased in the age group of 65-74 years (1.2%) and lesser on ≥ 75 years (1.1%). Urinary stone occurs more frequently in male (0.8%) better than in female (0.4%). Urinary stone which was formed caused disturbances in the urinary system. Therefore, it is very important to remove it in order to treat the disease, to prevent, and to hamper the recurrence of the stone formation. The surgery methods extracorporeal shock wave lithotripsy (ESWL) and percutaneous nephrolithotomy (PCNL), have been established for stone removal [1]. The preference and indication of success using these methods are affected by several factors. One of them is based on the chemical and mineral composition of urinary stones. In Indonesia, most of the hospital such as Hasan Sadikin Hospital Bandung, determined the urinary stones by using CT-Scan. CT-Scan is one of techniques to determine the chemical and mineral composition urinary stones. However, the measurements result showed that CT-Scan had the least accuracy and precision. This was due to the overlaping in Hounsfield Unit value for some types of urinary stones. Therefore, to get the most accurate and precise types of urinary stones by using CT-Scan. It is necessary to manufacture a standard operating procedure (SOP) to determine the types of urinary stones. Making the SOP was conducted with a CT-scan method and combined with other methods such as Fourier transform infrared spectroscopy (FTIR) method. The first stage to build the SOP was the determination of chemical and mineral composition model on urinary stone. The present study was conducted earlier by determining a total spectrum of a simple model of chemical and mineral composition in urinary stone through a black box analysis using convolution method.

2. Method and experiment

2.1. FTIR-ATR characterization

This research was performed using FTIR-ATR Alpha-P by Bruker. FTIR-ATR spectra were recorded in the range 4000-500 cm^{-1}. The evaluation menu that was provided in the OPUS software performed the entire process automatically.

A total of 25 urinary stones for the present study had been collected from Hasan Sadikin Hospital Bandung and it had dimension range from 0.7 cm – 3.2 cm. All together, the external layer of different parts of urinary stones were recorded and analyzed.

2.2. Black box analysis

Black box analysis was conducted by convolution method. Convolution is a mathematical way of combining two signals to form a third signal. Convolution is important because it relates the three signal of interest that is the input signal, the output signal, and the impulse response. On this research the impulse response signal was spectrum as a results of FTIR characterization and the input signal was infrared spectrum. The convolution was conducted using Matlab R2009a.

3. Results and discussion

3.1. Results of FTIR characterization

The information that was obtained from the infrared spectral pattern of samples is shown on figure 1-6, where BU is the number of samples urinary stone.

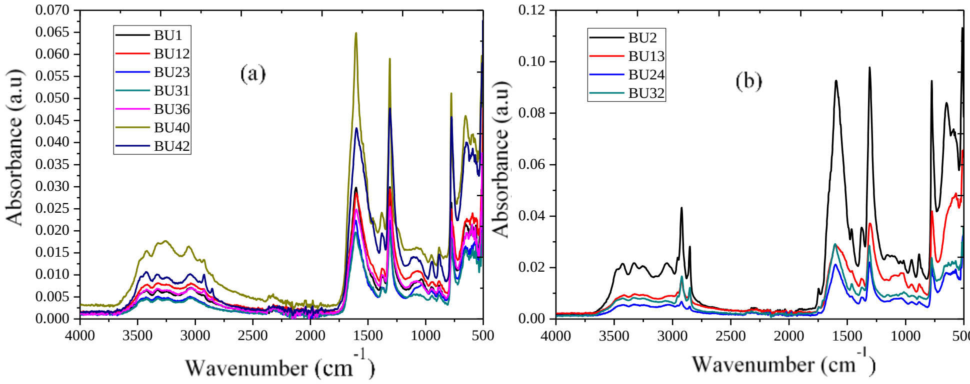

Figure 1. FTIR spectrum of urinary stone containing (a) pure calcium oxalate monohydrate, (b) ion amino acid calcium oxalate monohydrate.

The spectrum of a pure calcium oxalate monohydrate showed a high absorbance at 1616 - 1600 cm^{-1} and 1314 - 1302 cm^{-1} belonged to C=O and C-O stretching vibration, respectively. The frequency region was 779 - 775 cm^{-1} corresponding to C-H bending. The absorption band observed at 3446 - 3021 cm^{-1} which happened due to symmetric and asymmetric O-H bending. The absorption band at 1387– 1364 cm^{-1} was happened due to C-C dan C-O stretching, 891 - 874 cm^{-1} was due to C-C *stretching*, and 693 - 687 cm^{-1} was due to O-H bending. Visually spectrum of ion amino acid calcium oxalate monohydrate had shown similarity with figure 1a. However, in figure 1b, it showed absorbance at 2924 - 2850 cm^{-1} corresponding to N-H stretching vibration, which was the area that indicated ion amino acid. Spectrum in figure 1b, showed the chemical composition of urinary stone that consisted of ion amino acid and calcium oxalate monohydrate [1-5].

The spectrum mixture of calcium oxalate monohydrate and calcium phosphate showed a high absorbance at 1028 - 1001 cm^{-1} related to P-O stretching, the area indicated ion PO_4^{3-} [4, 5, 7]. The absorption at 3430 - 3043 cm^{-1} indicated symmetric and asymmetric O-H *stretching*, 1618 cm^{-1} - 1604 cm^{-1} indicated C=O stretching, 1316 - 1311 cm^{-1} indicated C-O stretching, 781 - 776 cm^{-1} indicated C-H bending, 886 - 872 cm^{-1} indicated C-C stretching [1,3].

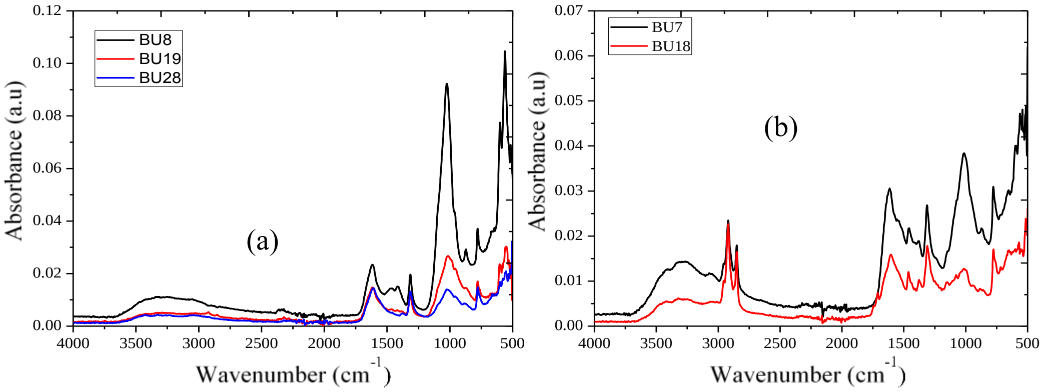

Figure 2. FTIR spectrum of urinary stone containing (a) mixture of calcium oxalate monohydrate with calcium phosphate, (b) mixture of ion amino acid calcium oxalate monohydrate and calcium phosphate.

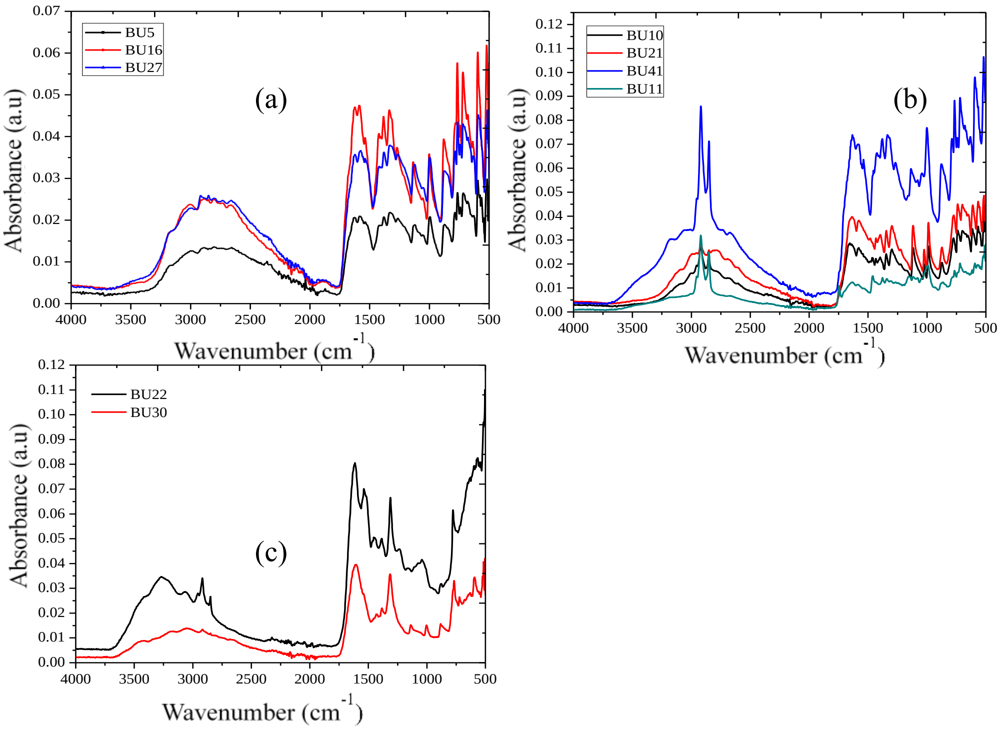

Figure 3. FTIR spectrum of urinary stone containing (a) pure uric acid, (b) ion amino acid uric acid, (c) mixture of calcium oxalate monohydrate with ion amino acid uric acid.

Visually, the spectrum of the mixture of amino acid calcium oxalate monohydrate ion with calcium phosphate showed similarity with figure 2a. However, figure 2b showed absorbance at 2922 - 2849 cm^{-1} related to N-H stretching, the area indicated amino acid ion. Spectrum in figure 2b showed that the chemical compositions of urinary stone consisted of amino acid ion, calcium oxalate monohydrate, and calcium phosphate.

The spectrum of thepure uric acid showed N-H bending vibration in the frequency region 1635 - 1622 cm^{-1}. In frequency region 1589 - 1574 cm^{-1} related to C-N stretching vibration. The absorption band that was observed at 1542 - 1538 cm^{-1} was due to N-O stretching. The absorption band at 1424 - 1417 cm^{-1} was due to O-H bending. The absorption band at 1385 - 1380 cm^{-1} was due to C-N stretching. The absorption band at 1337 - 1322 cm^{-1} was due to N-H stretching, 1137 - 1120 cm^{-1} was due to C-O stretching. C-N stretching and C-N bending vibration in frequency region 1057 - 993 cm^{-1} and 882 - 871 cm^{-1} respectively [3, 6]. Visually, the spectrum of amino acid and uric acid ion were similar with figure 3a. However, figure 3b showed absorbance at 2923 - 2850 cm^{-1} related to N-H stretching vibration indicated amino acid ion. Spectrum in figure 3b showed that the chemical composition of urinary stone consisted of amino acid and uric acid ion. And the figure 3c showed a mixture of amino acid and uric acid ion with calcium oxalate monohydrate. The spectrum of calcium oxalate monohydrate shows O-H stretching vibration in the frequency region was 3276 - 3252 cm^{-1}. In frequency region 1315 - 1311 cm^{-1} related C-O stretching, 778 - 776 cm^{-1} related to C-H bending. The spectrum of amino acid and uric acid ion showed N-H stretching vibration in the frequency region 2920 - 2849 cm^{-1}, the region indicated ion NH_3^+. The absorption band observed at 1627 - 1622 cm^{-1} was due to N-H bending, 1538 - 1537 cm^{-1} was due to N-O stretching, 1455 - 1436 cm^{-1} was due to O-H bending, 1388 - 1385 cm^{-1} was due to C-N stretching, and 1045 - 1041 cm^{-1} was due to C-N stretching [1, 3, 6].

3.2. *Results of convolution method*

The results of convolution from the infrared spectral pattern of samples were given in figure 4-5, where n is the number of convolution urinary stone.

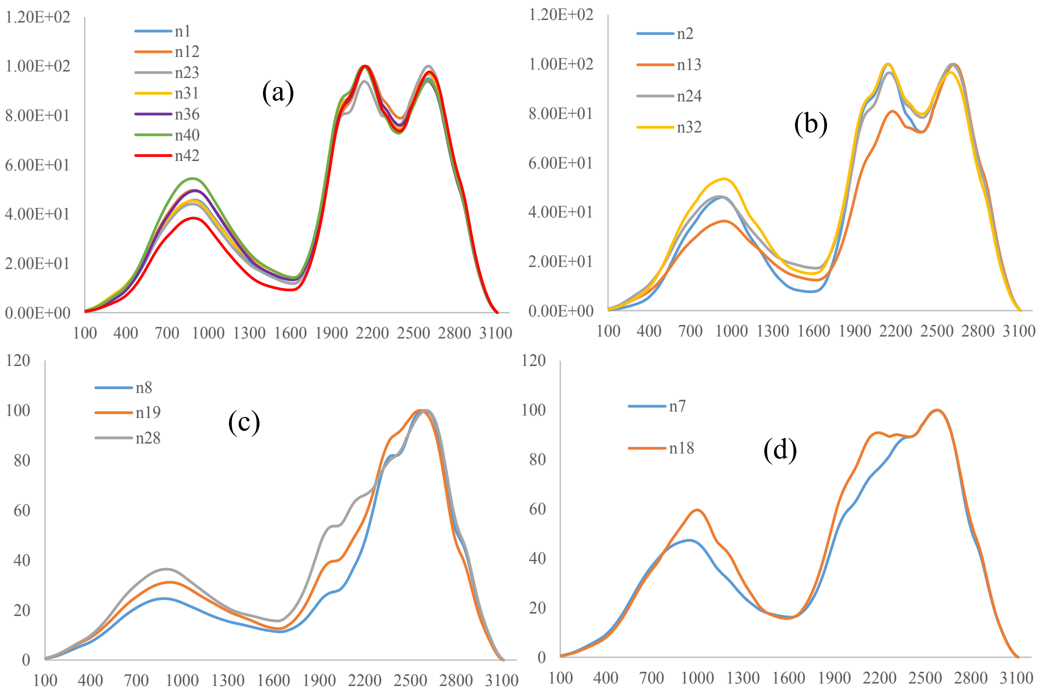

Figure 4. Result of convolution method (a) pure calcium oxalate monohydrate, (b) ion amino acid calcium oxalate monohydrate. (c) mixture of calcium oxalate monohydrate with calcium phosphate, (d) mixture of ion amino acid calcium oxalate monohydrate and calcium phosphate.

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Figure 4 and 5 are the normalization of convolution results for urinary stone. The convolution pattern of the samples under investigation were analyzed, for each samples of urinary stone had a different intensity, this indicated a functional group density had different amounts. The normalization of the results for kinds of urinary stones had a different shape and maximum intensity.

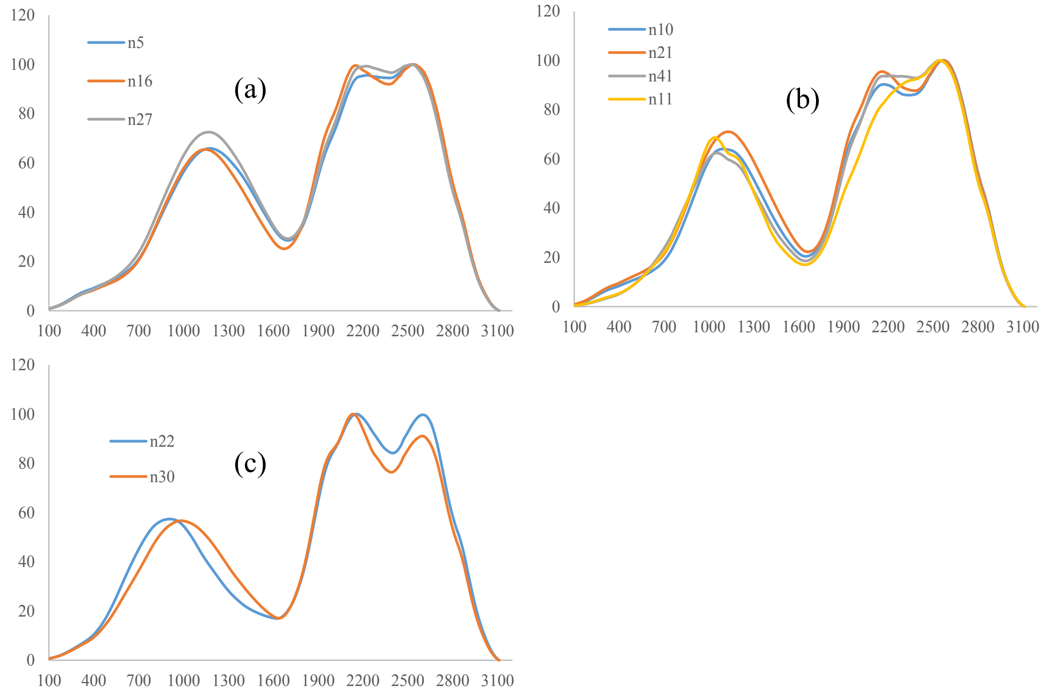

Figure 5. (a) Pure uric acid, (b) ion amino acid uric acid, (c) mixture of calcium oxalate monohydrate with ion amino acid uric acid.

4. Conclusions

The present study indicated that the information on chemical composition of urinary stone mostly varied. Generally, the results of analysis of black box showed the characteristics at the most accurate and precise to confirm the type of urinary stones by the shape of the total spectrum of each urinary stones as the result of convolution.

References

[1] Kanchana G, Sundaramoorthi P and Jeyanthi G P 2009 Bio-Chemical Analysis and FTIR-Spectral Studies of Artificially Removed Renal Stone Mineral Constituents *Journal of Minerals & Materials Characterization & Engineering* **8** 161-170

[2] Mandel I and Mandel N 2007 Structure and compositional analysis of kidney stones Totowa New Jersy Humana Press Inc

[3] Sekkoum K, Cheriti A, Taleb S and Belboukhari N 2011 FTIR Spectroscopic study of human *urinary* stones from El Bayadh District (Algeria) *Arabian Journal of Chemistry*

[4] Khaskheli M H, Sherazi S T H, Ujan H M and Mahesar S A 2012 Transmission FTIR spectroscopic analysis of human kidney stones in the Hyderabad Region of Pakistan *Turk Journal Chemical* **36** 477-483

[5] Shamema A A, Arul K T, Kumar R S and Kalkura S N 2014 Physicochemical analysis of *urinary* stones from Dharmapuri District *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* **134** 442-448

[6] Selvaraju R, Thiruppathi G and Raja A 2011 FT-IR Spectral studies on certain human urinary stones in the patients of rural area *Spectrochimica Acta Part A: Molecular and Biomolecular* **93** 260-265