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Identification of mineral compositions in some *renal calculi* by
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Highlights

- Identification of mineral constituents in nine *renal calculi* (kidney stone samples) by Raman and IR technique is presented.
- Whewellite, weddellite, struvite, brushite, hydroxyapatite and uric acid are identified.
- Raman alone can differentiate whewellite from weddellite and hydroxyapatite from struvite.
- One sample is composed of uric acid as a single component.

Abstract

We present in this paper accurate and reliable Raman and IR spectral identification of mineral constituents in nine samples of *renal calculi* (kidney stones) removed from patients suffering from nephrolithiasis. The identified mineral components include Calcium Oxalate Monohydrate (COM, whewellite), Calcium Oxalate Dihydrate (COD, weddellite), Magnesium Ammonium Phosphate Hexahydrate (MAPH, struvite), Calcium Hydrogen Phosphate Dihydrate (CHPD, brushite), Pentacalcium Hydroxy Triphosphate (PCHT, hydroxyapatite) and Uric Acid (UA). The identification is based on a satisfactory assignment of all the observed IR and Raman bands ($3500\text{--}400\text{ cm}^{-1}$) to chemical functional groups of mineral components in the samples, aided by spectral analysis of pure materials of COM, MAPH, CHPD and UA. It is found that the eight samples are composed of COM as the common component, the other mineral species as common components are: MAPH in five samples, PCHT in three samples, COD in three samples, UA in three samples and CHPD in two samples. One sample is wholly composed of UA as a single component; this inference is supported by the good agreement between ab initio density functional theoretical spectra and experimental spectral measurements of both sample and pure material. A combined application of Raman and IR techniques has shown that, where the IR is ambiguous, the Raman analysis can differentiate COD from COM and PCHT from MAPH.

Graphical abstract

Accurate and highly reliable identification of mineral constituents in a batch of nine *renal calculi* (kidney stone samples) taken from nephrolithiasis-struck patients is analyzed by Raman and IR spectral analysis. Identified components include whewellite, weddellite, struvite, brushite, hydroxyapatite and uric acid spread over the nine samples. It is shown that the Raman analysis can differentiate whewellite from weddellite and hydroxyapatite from struvite. One sample is found to possess wholly uric acid and its spectrum is in agreement with a pure uric acid's and DFT's spectra.



Keywords

Renal calculi; IR; Raman; DFT

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