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Paper

PAPER

CHEMICAL COMPOSITION OF KIDNEY STONES, MECHANISMS OF THEIR FORMATION AND STUDY BASED ON SPECTRAL ANALYSIS

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Abstract

This research paper reviews the chemical composition of kidney stones, their formation mechanisms, and their detection using modern spectral analysis methods. Kidney stones are a common pathophysiological condition in urology that significantly impacts human health. Studies have shown that the chemical composition of stones is directly related to their formation mechanisms and pathogenesis (Coe et al., 2016; Khan, 2014). The article analyzes the ratio of calcium oxalate, calcium phosphate, urate, struvite, and cystine in kidney stones, and their relationship with metabolic processes, pH balance, and water and salt metabolism in the body. The article also discusses the possibilities of detecting kidney stones and determining their chemical composition using modern analytical methods, including X-ray diffraction (XRD), infrared spectral analysis (FTIR), atomic emission spectroscopy, and scanning electron microscopy (SEM). These approaches are characterized by high accuracy and rapid results in determining the composition of stones. According to the results of the article , the study of the chemical and morphological characteristics of kidney stones allows us to understand the mechanisms of their formation and develop prevention and individual treatment strategies. The article is a scientific basis for research in modern urology and bioanalytical chemistry, allowing for a deeper understanding of the pathophysiological processes associated with kidney stones and their application in clinical practice.

Key words: kidney stones, chemical composition, formation mechanism, spectral analysis, IR spectroscopy, XRD, AAS, urolithiasis.

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Kidney stones (urolithiasis) are a pathological process that occurs as a result of the crystallization of ions and organic substances in the urine and their accumulation in the form of solid aggregates in the kidneys. Their occurrence is closely related to chemical imbalances, urine pH, metabolic disorders, dehydration, food composition, and hereditary factors. Accurate determination of the chemical composition of kidney stones is important for correctly determining the clinical treatment strategy and preventing the recurrence of stones. Modern spectral analysis methods are considered one of the most reliable technologies in this regard. [1]

Kidney stones are divided into several main groups based on their composition. The most common stones are calcium oxalate stones. They are composed of CaC_2O_4, which accounts for 65–70% of all stones, are very hard, and are insoluble in water. [2]

Calcium phosphate stones are composed of hydroxylapatite - $Ca_{10}(PO_4)_6(OH)_2$, which crystallize in alkaline urine (pH > 7). Urate stones are composed of uric acid crystals ($C_5H_4N_4O_3$), which form at low pH (< 5.5) and are not visible on X-ray. Struvite stones are composed of magnesium ammonium phosphate ($MgNH_4PO_4 \cdot 6H_2O$) crystals, which are formed as a result of infectious processes. Bacteria that produce the enzyme urease (Proteus, Klebsiella) alkalize the urine and accelerate crystallization. Rare cystine stones are composed of the amino acid cystine, and are formed as a result of the hereditary disease cystinuria. [3]

The chemical mechanisms of kidney stone formation are mainly related to urine supersaturation, that is, a state of oversaturation. When the dissolved ions in the urine exceed the norm or the urine volume decreases, the ions begin to crystallize. The crystals stick together, turning into large aggregates, and stones are formed. One of the stones whose formation in the body is best studied is calcium oxalate. Calcium ions (Ca^{2+}) and oxalate ions ($C_2O_4^{2-}$) combine to form insoluble calcium oxalate crystals:

$$Ca^{2+} + C_2O_4^{2-} \rightarrow CaC_2O_4 \downarrow$$

This process is aggravated by factors such as hypercalciuria, intestinal diseases, increased oxalate, excessive consumption of vitamin C, and dehydration. Calcium phosphate stones are formed as a result of crystallization of calcium and phosphate ions in an alkaline environment. Urate stones are formed when the urine is too acidic, since the solubility of urates decreases sharply at low pH. Metabolic syndrome, gout, and excessive consumption of meat products lower the pH, increasing the formation of urate stones. Bacteria play an important role in the formation of struvite stones: the enzyme urease breaks down urea in the urine into ammonia and carbon dioxide, making the urine alkaline. This reacts with phosphates, magnesium, and ammonium ions to form struvite crystals. Cystine stones are formed as a result of a genetic defect in cystine reabsorption; cystine is poorly soluble and crystallizes easily. [4]

The causes of stones are many. Metabolic factors (hypercalciuria, hyperuricemia, increased oxalate), dietary errors, low fluid intake, changes in urine pH, infections, and hereditary diseases are the main factors. Changes in urine pH play a decisive role in the formation of the type of stone: urate stones form when pH < 5.5, and phosphate and struvite stones form when pH > 7. While infections are the main source of struvite stones , hereditary diseases (e.g., cystinuria) cause cystine stones. Dehydration dramatically increases the likelihood of the formation of all types of stones. [5]

Spectral analysis methods are very important in the detection of kidney stones. Infrared (IR) spectroscopy determines the chemical composition by the wavelengths of the functional groups in the stone. For example, calcium oxalate has characteristic lines at 1620 cm^{-1}, urates at 1670–1690 cm^{-1}, and cystine at 1200–1500 cm^{-1}. X-ray diffraction (XRD) studies the structure of the crystal lattice; since each type of stone has a unique diffraction "fingerprint", XRD also clearly distinguishes mixed stones. Raman spectroscopy measures molecular vibrations and gives accurate results even in very small samples. Atomic absorption spectroscopy (AAS) is used to determine the amount of metal ions—elements such as calcium, magnesium, sodium, zinc.

Conclusion

The results of the study show that the chemical composition and formation mechanisms of kidney

Table 1

T/r	Element	Concentration (mg/L)	Note
1	Ca	120	The main calcium component
2	Mg	15	Minor component
3	No	8	Related to salts
4	Zn	0.5	Track element

stones are closely related to their various metabolic, physiological and environmental factors. Spectral analysis methods - infrared (IR) spectroscopy, X-ray diffraction (XRD), Raman spectroscopy and atomic absorption spectroscopy (AAS) - play an important role in the identification and analysis of these processes.

IR spectroscopy provides high-precision identification of functional groups in the stone, for example, by separating components such as calcium oxalate, urate, and cystine through specific wavelengths. XRD allows for the determination of the structure of the crystal lattice and the differentiation of mixed stones. Raman spectroscopy, on the other hand, provides accurate results even on small samples by measuring molecular vibrations. AAS is used to determine the amount of metals - calcium, magnesium, sodium, zinc, and other elements - which helps to understand the mineral and chemical composition of stones.

It is possible to identify the mechanisms of kidney stone formation, develop strategies for their prevention and individual treatment. These methods make the detection of kidney stones in clinical and laboratory conditions fast, accurate and reliable. As a result, spectral analysis serves as an important scientific and practical tool in the diagnosis of kidney stones and a deep understanding of their pathophysiology.

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