International Journal of Multidisciplinary Research and Development
www.allsubjectjournal.com
ISSN Online: 2349-4182
Received: 19-01-2026; Accepted: 18-02-2026; Published: 05-03-2026
Volume 13, Issue 1, 2026, Page No. 497-501

# Chemical composition of α-amino acids determined by IR spectroscopy

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**Abstract**
α-Amino acids are the fundamental structural units of proteins and are characterized by the presence of a central carbon atom (α carbon) linked to four distinct groups: an amino group ($–NH_2$), a carboxyl group (–COOH), a hydrogen atom and a side group specific to each amino acid (the R chain). This structure gives amino acids amphoteric properties, allowing them to function as both acids and bases, and determines their behavior in biological solutions. The R side group is what differentiates the 20 proteinogenic amino acids, influencing their solubility, polarity and reactivity. Most natural α-amino acids have the L configuration, essential for the three-dimensional structure of proteins. Their common structure, combined with the variability of the R chains, allows them to form complex polypeptide chains through peptide bonds, underlying the functional diversity of biological proteins.

**Keywords:** Amino acids, spectroscopy, IR

## Introduction

Amino acids are building blocks of proteins, with numerous roles in vital processes, from hormone synthesis to neurotransmitter synthesis. Some of them can also be administered as dietary supplements to support athletic performance.

From a chemical point of view, amino acids are organic compounds with mixed function, whose molecules contain the $-NH_2$ and -COOH (amino and carboxyl) groups.

The human body needs 20 amino acids to function properly. 11 of them are synthesized by the body, and the other 9, the essential amino acids, can only be obtained through a balanced diet. In the case of amino acid deficiencies, protein synthesis suffers, but the assimilation of other nutrients, as well as immunity, can also be affected.

Amino acids are also necessary for the production of enzymes. That is why they are considered some of the most important nutrients [1, 5].

Amino acids join together to form proteins, and their main function is to build the building blocks of proteins. These typically contain between 50 and 2,000 amino acids, joined together in various combinations. Each protein has a unique amino acid sequence and a distinct configuration. Proteins have many functions, playing an important role in all cellular processes of normal physiological functioning.

20 different amino acids combine to build the impressive, chemically unique matrix of proteins. Amino acids can be essential, non-essential, and conditionally essential. Essential amino acids are those that we must obtain from our diet, while non-essential amino acids are produced naturally in the human body. Conditionally essential amino acids are only needed under certain circumstances, such as stress or illness.

The way or sequence in which these amino acids combine to form proteins determines their three-dimensional structure and function, which is distinct for each protein. Some functions of proteins include their role as antibodies, enzymes, messengers or transporters/storage and structural capacities.

Here are the most important roles of proteins made up of amino acids:

Antibodies - these are proteins produced by the immune system and play a key role in detecting antigens, considered by the body as foreign and harmful. Viruses, bacteria, fungi and parasites are such examples of antigens. Sometimes, however, the body can confuse healthy tissues with antigens and produce antibodies to defend the uncontaminated body - this happens in the case of autoimmune diseases.

Enzymes - proteins that function as biological catalysts are called enzymes. They are responsible for catalyzing and accelerating chemical reactions in the body, acting on molecules called substrates and stimulating their production. Unlike other catalysts, enzymes are highly specific macromolecules whose activity can be stimulated by molecules called activators and reduced by molecules called inhibitors. For enzymes to function properly, optimal temperature conditions and a balanced pH are necessary. Enzymes are found in every organ and cell of the human body, including the blood and the gastrointestinal tract.

Other roles - proteins can exhibit numerous patterns of chemical messenger reactions in the form of hormones, neurotransmitters and neuropeptides. They regulate the behavior and physiology of organs and systems, enable communication between nerve cells and glandular or muscle cells, are a constituent part of cellular structure and support (collagen, keratin and elastin are such proteins). Furthermore, proteins transport atoms and small molecules inside cells and throughout the body. Therefore, we can say that they have both a storage and a transport role. One such example of a protein is hemoglobin, which, with the help of iron, transports oxygen. An intracellular storage protein is ferritin, necessary for iron storage [6, 12].

As mentioned, there are three types of amino acids: essential, nonessential, and conditionally essential. Below, you will learn all about these types of amino acids and their role in the body:

Essential amino acids, which can be obtained strictly from food, support anabolic muscle growth and reduce catabolic muscle breakdown by synthesizing the proteins necessary for these processes. Here are the essential amino acids and what you need to know about each:

Lysine plays an important role in increasing muscle mass, maintaining bone health, contributing to recovery from injury or surgery, and regulating hormones, antibodies, and enzymes. Lysine may also have antiviral effects. One study indicates that lysine deficiency can cause stress-induced anxiety.

Histidine is an amino acid that the body also produces, but in small, insufficient quantities, so it is included in the same category of essential acids. Histidine facilitates growth, blood cell creation and tissue regeneration. It helps maintain the protective membranes of nerve cells (myelin sheath). The body metabolizes histidine into histamine, which is important for the immune system, reproductive health and digestion. Deficiency can cause anemia, especially among people suffering from arthritis and kidney diseases.

Threonine is necessary for skin and tooth health, being a component of tooth enamel, collagen and elastin. It helps metabolize fats and may be beneficial for patients suffering from indigestion, anxiety and depression. Deficiency can cause lower resistance to other diseases, according to a study published in Science Direct.

Methionine plays, along with a non-essential amino acid - cysteine - an important role in the health and flexibility of skin, hair and nails. It contributes to the proper absorption of selenium and zinc and to the elimination of heavy metals such as lead and mercury from the body.

Valine is essential for mental focus, muscle coordination and emotional calm. Valine supplements are often used to increase muscle mass, repair tissue and provide extra energy. Valine deficiency can cause insomnia and reduce mental functioning.

Isoleucine helps heal injuries and wounds, strengthens the immune system, regulates blood sugar levels and balances hormone production. It is present predominantly in muscle tissue. As we age, isoleucine deficiencies can occur, causing loss of muscle mass and symptoms such as tremors.

Leucine helps regulate blood glucose levels and contributes to the growth and repair of muscle and bone tissue. It is also important for the healing of superficial injuries and wounds and plays an important role in the production of growth hormones. Leucine deficiency can lead to skin rashes, hair loss and can also manifest itself through fatigue.

Phenylalanine helps the body use other amino acids, proteins and enzymes. It is converted into tyrosine by the body, a compound necessary for certain brain functions. Phenylalanine deficiency occurs only in exceptional cases and can lead to growth problems in children, and to eczema, fatigue and memory difficulties in adults. On the other hand, excesses can cause anxiety, irritability and nervousness and sleep disorders; these symptoms can occur in the case of excessive consumption of sweets and diet soft drinks sweetened with aspartame, which contains large amounts of phenylalanine.

Tryptophan is necessary for the growth of children and is the precursor of serotonin and melatonin. While melatonin has the role of regulating sleep, serotonin also contributes to this mission, in addition to regulating appetite, mood and pain. Tryptophan acts as a sedative and, when taken as a dietary supplement, can improve mental energy and emotional processing, according to a study in the British Journal of Nutrition. Deficiencies can cause pellagra, which can lead to dementia, digestive problems, and eczema.

Nonessential amino acids are produced by the body, even if they are not assimilated from dietary sources, unless a condition or high stress levels prevent their natural production.

Nonessential amino acids that are not necessarily essential are:

Alanine contributes to the production of proteins. It is used to break down tryptophan and vitamin B6. It is a source of energy for both the muscles and the central nervous system. It helps strengthen the immune system and helps the body use sugars properly.

Asparagine has a structural function in proteins and is used for their biosynthesis. It is necessary for brain growth and development. In addition, it helps with recovery and protein synthesis during the replication of poxviruses.

Aspartic acid helps with the production and release of hormones and contributes to the optimal functioning of the nervous system.

Glutamic acid is an amino acid that the human body uses to form proteins. In the body, glutamic acid is converted into glutamate. This helps nerve cells in the brain to send and receive information from other cells. Glutamic acid therefore plays an important role in cognitive functions of memory and learning. In addition, it can improve the specific symptoms of diseases that manifest themselves with reduced or absent gastric acidity.

This category is included in that of non-essential amino acids. Dietary supplements with such amino acids may be necessary in certain health conditions that prevent their natural production by the body. Here are some of them:

Glutamine is important for the efficiency of the immune system, plays an important role in intestinal health, increases physical performance and contributes to the growth of muscle mass.

Glycine helps the body produce glutathione, an antioxidant that protects against cell degeneration. It is also a component of creatine, the compound that provides energy to muscles and has been associated with a number of benefits, from bone health to optimal brain function. Glycine is an amino acid that is part of the structure of collagen, the structural protein of the skin, joints and bones. Glycine also has a calming effect and can improve sleep quality.

Proline is an amino acid produced by the body, but also found in foods and dietary supplements. Because it plays an important role in the formation of collagen, it has a number of benefits for the skin, joints and bones and helps heal superficial injuries and wounds.

Serine contributes to the biosynthesis of proteins and has a catalytic role in the functioning of several enzymes. Serine contributes to improving cognitive functions of memory and learning, so it is often used as a complementary treatment for the symptoms of conditions such as schizophrenia and Parkinson's disease. Serine contributes to improving sleep quality and also has the role of transmitting chemical signals to the brain.

Tyrosine is an essential component in the production of several chemicals in the brain, called neurotransmitters, including dopamine, epinephrine, norepinephrine.

Ornithine is metabolized into arginine, which stimulates the release of growth hormones. It has the property of contributing to the faster healing of superficial injuries and wounds and an immunomodulatory role.

Arginine is an amino acid with a vasodilating effect, often used as a complementary food supplement in the treatment of certain heart conditions, but also for the treatment of

erectile dysfunction. Arginine can contribute to reducing blood pressure and improving the symptoms of certain circulatory system conditions.
Cysteine contributes to the formation of proteins and has an important role in several metabolic functions. It is the main protein in hair, skin and nails and contributes to the formation of collagen. Cysteine has antioxidant properties and contributes to the growth of muscle mass [13, 17].

**Materials and methods**

Vibrational spectroscopy (FT-IR) is an extremely useful tool for examination of molecular structure of chemical compounds. All chemical compounds have their own typical IR spectrum. The grown $\gamma$ -glycine was subjected to FT-IR analysis to confirm the presence of functional groups by employing PERKIN-ELMER spectrometer in the range of 4000 $cm^{-1}$ to 400 $cm^{-1}$ using the KBr pellet technique with a resolution of 1.0 $cm^{-1}$ (fig.1).

**Fig 1:** PERKIN-ELMER Spectrometer

The FT-IR spectra of L-valine were obtained from potassium bromide pellets using a MAKE-BRUKER Optic Gmbh MODEL No-TENSOR 27 SOFTWARE-OPUS version 6.5 Spectrophotometer in the range of 4,000–400 $cm^{-1}$ (fig. 2).

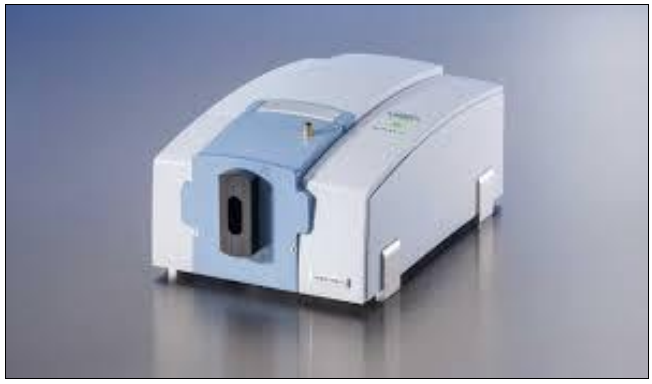

**Fig 2:** MAKE-BRUKER Optic

The IR study was carried out in Nicolas IS-5 model IR for L-leucine (fig.3).

**Fig 3:** Nicolas **IS**-5 model IR

**Results and discussions**

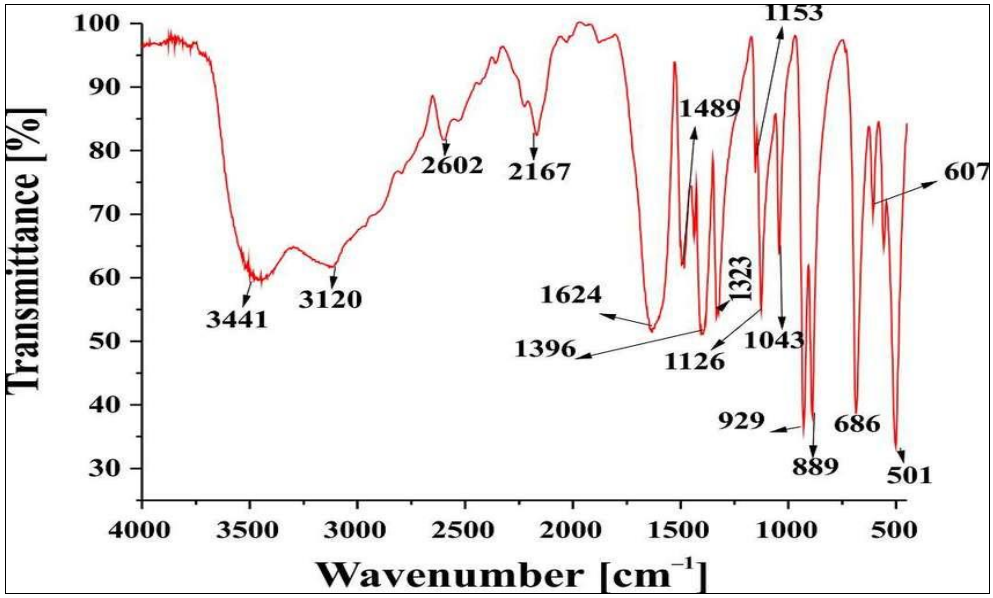


**Fig 4:** Spectrul IR al $\gamma$ -glicinei

The FT-IR spectrum of $\gamma$ -glycine is shown in Fig. 4. The bands arising due to $CH_2$ and $NH_3^+$
stretching vibrations are found to occur at high wave number region of 2167 $cm^{-1}$ to 2598 $cm^{-1}$ and 2794 $cm^{-1}$ to 3441 $cm^{-1}$, respectively. The peak around 1489 $cm^{-1}$ is attributed to symmetric stretching mode of $COO^-$ group. The peak at 1323 $cm^{-1}$ is assigned to CH2 wagging vibrations [8]. The peak at 929 $cm^{-1}$ is due to the bending vibration of C–H group. The peaks due to C–N stretching vibrations and C–C stretching vibrations are found to occur at 1043 $cm^{-1}$ and 889 $cm^{-1}$, respectively. The bands arising as a result of carboxylate group are observed at 501 $cm^{-1}$, 607 $cm^{-1}$ and 686 $cm^{-1}$, while the peak observed at 1126 $cm^{-1}$ is attributed to $NH_3^+$ group. The presence of both the vibrations of carboxylate and ammonium ion clearly indicates that the glycine molecule exists in zwitterionic form in $\gamma$ -glycine.

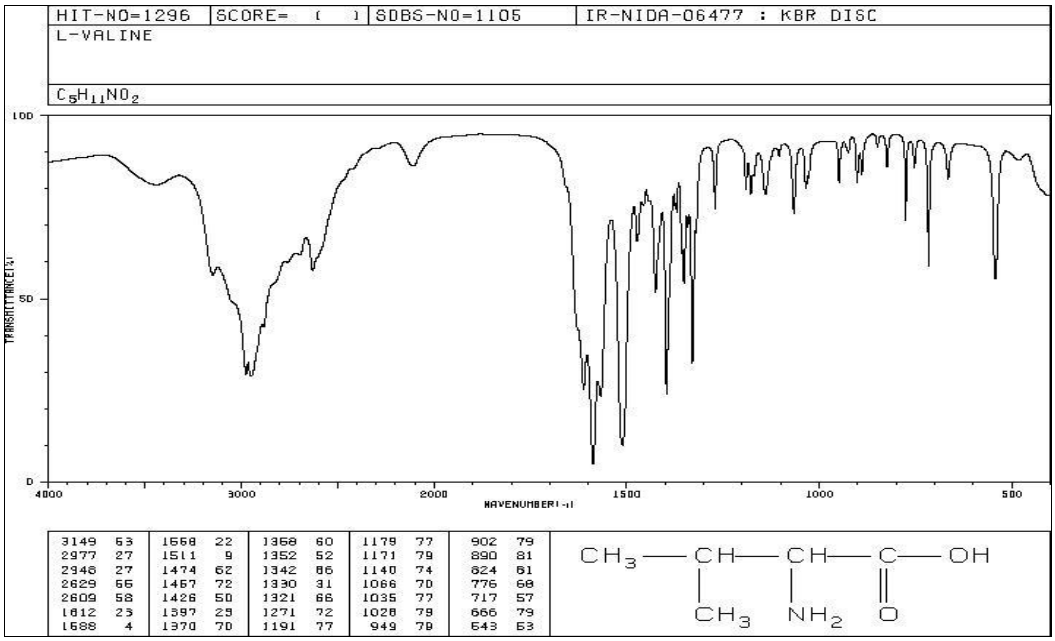


**Fig 5:** Spectrul IR al L valinei

The FT-IR spectra of L-valine are shown in Fig. 3, respectively. The FT-IR spectra ofmainly arise due to internal vibration of functional groups $NH_3$, CH, $CH_3$, and COOH. The absorptions of have been compared with those of the parent compound L-valine. The broad peak at 2,968 $cm^{-1}$ is due to the methylene symmetric stretching. The N–H–O valance stretching combination observed at 2,627 $cm^{-1}$. The sharp peaks at 1,615 $cm^{-1}$ are due to $NH_2$ bending vibration. The C–C stretching mode is observed at 1,181.7 $cm^{-1}$. The sharp peak at 1,077 $cm^{-1}$ is due to C– C–N stretching mode. The C=S stretching vibration is observed at 629.15 $cm^{-1}$.

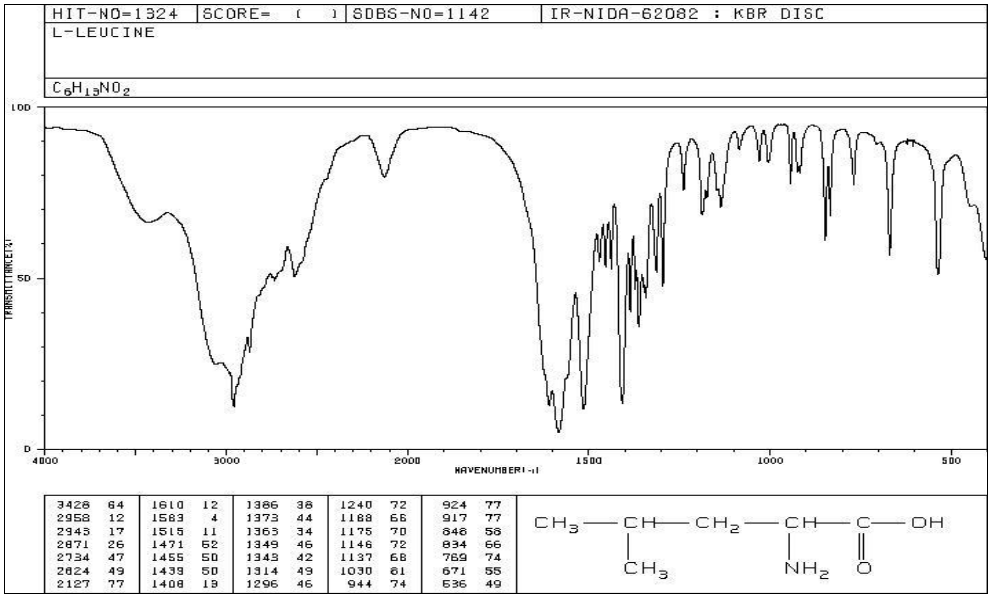


**Fig 6:** Spectrul IR al L leucinei

The characteristic band at 2957 $cm^{-1}$ corresponds to $\nu_{NH2}$ as present in L-leucine. The stretching vibration at 1406 $cm^{-1}$ and 1581 $cm^{-1}$ correspond to asymmetric ($\nu_{asy(C\text{-}O\text{-}C)}$) and symmetric ($\nu_{sym(C\text{-}O\text{-}C)}$).

**Conclusions**

IR spectroscopic analysis confirms the chemical composition characteristic of α-amino acids through the presence of the absorption band specific to the fundamental functional groups:

- Amino group ($–NH_2$/$–NH_3^+$), highlighted by the bands in the area 3200–3500 $cm^{-1}$;
- Carboxyl group (–COOH/$–COO^-$), recognized by the intense bands around 1700 $cm^{-1}$ (C=O) and 1400–1600 $cm^{-1}$ (asym. /sym. $COO^-$);
- The –C–N and C–H bonds specific to the structure of amino acids, observed in the regions 1000–1300 $cm^{-1}$ and 2800–3000 $cm^{-1}$.

The spectra obtained thus confirm the presence of both the amino group and the carboxyl group linked to the same carbon atom, demonstrating the characteristic structure of α-amino acids and the possibility of the existence of the zwitterionic form. Overall, IR spectroscopy allows for the rapid and reliable identification of the defining structural components for this class of compounds.

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