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FTIR study of L-Histidine

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Abstract
In this article, we determined the composition of L-histidine using a Perkin-Elmer Corp. spectrometer. L-histidine contains absorption bands between 2273 and 491cm^{-1}. L-histidine contains the following functional groups: NH_2-symmetric and asymmetric stretching, CH_2 asymmetric stretching, C=O stretching, asymmetric bending of NH^{+3} and C=N, NH_2 bending, C=S stretching, C-C stretching, C-N stretching, C-H in plane bending, C-N deformation, C-N deformation, C= O deformation and N-C-N stretching.

Keywords: Histidine, composition, spectroscopy, FTIR

Introduction

Histidine (symbol His or H) is an essential amino acid that is used in the biosynthesis of proteins. It contains an α-amino group (which is in the protonated –NH3+ form under biological conditions), a carboxylic acid group (which is in the deprotonated –COO− form under biological conditions), and an imidazole side chain (which is partially protonated), classifying it as a positively charged amino acid at physiological pH. Initially thought essential only for infants, it has now been shown in longer-term studies to be essential for adults also. It is encoded by the codons CAU and CAC [1-5].

Histidine was first isolated by Albrecht Kossel and Sven Gustaf Hedin in 1896. The name stems from its discovery in tissue, from ἱστός histós "tissue". It is also a precursor to histamine, a vital inflammatory agent in immune responses. The acyl radical is histidyl.

The conjugate acid (protonated form) of the imidazole side chain in histidine has a pKa of approximately 6.0. Thus, below a pH of 6, the imidazole ring is mostly protonated (as described by the Henderson–Hasselbalch equation). The resulting imidazolium ring bears two NH bonds and has a positive charge. The positive charge is equally distributed between both nitrogens and can be represented with two equally important resonance structures. Sometimes, the symbol Hip is used for this protonated form instead of the usual His. Above pH 6, one of the two protons is lost. The remaining proton of the imidazole ring can reside on either nitrogen, giving rise to what are known as the N3-H or N1-H tautomers. The N3-H tautomer is shown in the figure above. In the N1-H tautomer, the NH is nearer the backbone. These neutral tautomers, also referred to as Nε and Nδ, are sometimes referred to with symbols Hie and Hid, respectively. The imidazole/imidazolium ring of histidine is aromatic at all pH values. Under certain conditions, all three ion-forming groups of histidine can be charged forming the histidinium cation.

The acid-base properties of the imidazole side chain are relevant to the catalytic mechanism of many enzymes. In catalytic triads, the basic nitrogen of histidine abstracts a proton from serine, threonine, or cysteine to activate it as a nucleophile. In a histidine proton shuttle, histidine is used to quickly shuttle protons. It can do this by abstracting a proton with its basic nitrogen to make a positively charged intermediate and then use another molecule, a buffer, to extract the proton from its acidic nitrogen. In carbonic anhydrases, a histidine proton shuttle is utilized to rapidly shuttle protons away from a zinc-bound water molecule to quickly regenerate the active form of the enzyme. In helices E and F of hemoglobin, histidine influences binding of dioxygen as well as carbon monoxide. This interaction enhances the affinity of Fe(II) for O2 but destabilizes the binding of CO, which binds only 200 times stronger in hemoglobin, compared to 20,000 times stronger in free heme [6-12].

The tautomerism and acid-base properties of the imidazole side chain has been characterized by 15N NMR spectroscopy. The two 15N chemical shifts are similar (about 200 ppm, relative to nitric acid on the sigma scale, on which increased shielding corresponds to increased chemical shift). NMR spectral measurements shows that the chemical shift of N1-H drops slightly, whereas the chemical shift of N3-H drops considerably (about 190 vs. 145 ppm). This change indicates that the N1-H tautomer is preferred, possibly due to hydrogen bonding to the neighboring ammonium. The shielding at N3 is substantially reduced due to the second-order paramagnetic effect, which involves a symmetry-allowed interaction between the nitrogen lone pair and the excited π* states of the aromatic ring. At pH > 9, the chemical shifts of N1 and N3 are approximately 185 and 170 ppm.

Materials and methods

L-histidine was characterized using vibrational spectroscopy in the Fourier Transform Infrared Region (FT-IR), conducted with a spectrophotometer (Spectrum Frontier; Perkin-Elmer Corp.). This equipment has an attenuated total reflectance accessory (ATR) featuring a zinc selenide (ZnSe) crystal surface. The spectra were obtained with 32 scans spanning from 4000 to 550 cm-1, employing a resolution of 4 cm-1 in a transmittance model [13-20].

Fig 1: Spectrum Frontier; Perkin-Elmer Corp

Results and Discussions

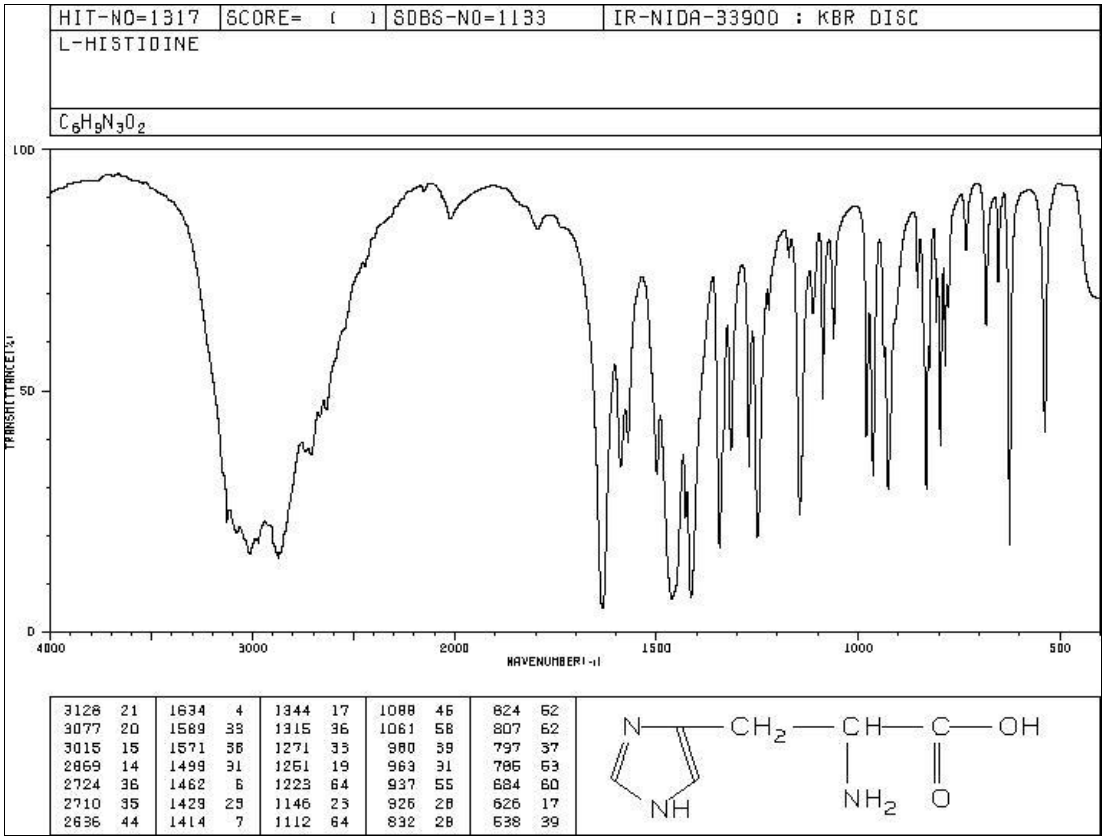

Fig 2: Spectre IR L-histidine

The FTIR spectra of L-Hisditine are shown in figure 2 respectively. The broad envelope positioned in 2773 cm^{-1} corresponds to the symmetric and asymmetric stretching modes of NH_2 group. The peak at 1606 cm-1 with medium intensity refers C-H Asymmetric bending of NH^{+3} and C=N stretching. The peak at 1498 cm^{-1} is due to NH_2 bending vibration. CH_2 deformation vibrations. The peaks at 1415 cm^{-1} corresponds to the C=S stretching. The C-C stretching mode of vibration occurs in 1336 cm^{-1} peak. The peak at 1186 cm^{-1} gives rise to C-N stretching mode of vibration. The spectra show absorption bands in the region of 1168 cm-1 and 1068 cm^{-1} which are due to in-plane C-H bending vibration. The band 1128 cm^{-1} signifies the N-H symmetric bending. C-C-N stretching vibration obtained at 1078 cm^{-1}. The bands at 867 cm^{-1} and 805 cm^{-1} revealed that C-N deformation mode. The ring deformation occurs the peak at 822 cm^{-1}. C=O deformation is identified by the band at 696 cm^{-1}.

Table 1: The infrared absorption frequencies (cm^{-1}) of L-Histidine

Frequencies (cm^{-1})	Assignments
2773	NH_2-symmetric and asymmetric stretching
2712	CH_2 asymmetric stretching
2364	C-H Combinational overtone
1638	C=O stretching
1606	Asymmetric bending of NH^{+3} and C=N
1498	NH2 bending
1415	C=S stretching
1336	C-C stretching
1186	C-N stretching
1168	C-H in plane bending
1128	N-H bending
1078	C-C -N stretching
1068	C-H in plane bending
867	C-N deformation
822	Ring deformation
805	C-N deformation
696	C= O deformation
630	C-C deformation
491	N-C-N stretching

Conclusions

L-histidine contains the following functional groups: NH_2-symmetric and asymmetric stretching, CH_2 asymmetric stretching, C=O stretching, asymmetric bending of NH^{+3} and C=N, NH_2 bending, C=S stretching, C-C stretching, C-N stretching, C-H in plane bending, C-N deformation, C-N deformation, C= O deformation and N-C-N stretching.

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