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Chemical composition of aspirin determined by IR spectroscopy

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Abstract
Aspirin, also known under the pharmaceutical name acetylsalicylic acid, is one of the most widely used types of nonsteroidal anti-inflammatory drugs, being able to combat not only mild and moderate pain, found at several levels of the body, but also to reduce fever (antipyretic effect).
In this article, we determined the chemical composition of aspirin by IR spectroscopy using the SHIMADZU FT–IR spectrometer for wavelengths between 4000–400 cm^{-1}. The wavelength range in which absorption bands appear is between 4000cm-1 and 400 cm^{-1}. Aspirin contains the following functional groups: C-H, C-OH, CH_3, C=O, C=C, P-OH, CO_2.

Keywords: Composition, IR spectroscopy, aspirin

Introduction

Aspirin, also known under the pharmaceutical name acetylsalicylic acid, is one of the most widely used types of nonsteroidal anti-inflammatory drugs, being able to combat not only mild and moderate pain, found at several levels of the body, but also to reduce fever (antipyretic effect). In addition, it is used for its anticoagulant properties, reducing the risk of unwanted cardiovascular events, as well as for anti-inflammatory purposes.

Although there are a multitude of benefits that acetylsalicylic acid fulfills, it is important to know all its interactions with the body, in order to administer it effectively, safely and that leads to obtaining the desired effect, with minimal adverse reactions.

Aspirin (acetylsalicylic acid) is the first nonsteroidal anti-inflammatory drug discovered and put into practice, being a treatment that has continued its course to this day. This fact was possible due to its benefits of relieving pain, reducing fever and decreasing the risk of cardiovascular events.

Over time, it was discovered that different doses of acetylsalicylic acid have different effects. Thus, while higher doses of acetylsalicylic acid have analgesic and antipyretic benefits, as well as anti-inflammatory effects, lower doses are used for anticoagulant purposes, in order to maintain a low risk of acute coronary events [1, 5].

Aspirin represents, from several points of view, a revelation in the world of medicine. Not only was it the most widely used treatment during the 20th century, but it was also used as a model to highlight the mode of action of non-steroidal anti-inflammatory drugs in the body.

In order for acetylsalicylic acid to exert its therapeutic effects, it interferes with the action of the enzyme called cyclooxygenase (COX), inhibiting it. In this way, cyclooxygenase is no longer able to determine the formation of prostaglandins, mediators of inflammation, pain and fever.

Thus, by preventing the formation of prostaglandins, inflammation, pain and fever are, in turn, stopped.

However, it is important to remember that prostaglandins have an important protective role for the gastric mucosa. By inhibiting their formation, the mucosa is exposed to the aggression of hydrochloric acid and undergoes an irritation process, an adverse reaction often encountered in the case of the administration of acetylsalicylic acid.

Prostaglandins are also involved in the regulation of renal function and blood clotting, physiological processes that can undergo changes following the ingestion of acetylsalicylic acid.

Aspirin is a type of drug treatment widely used. Not only its low cost, but also the multitude of therapeutic effects it has make this drug one of the first choice in multiple conditions, from simple colds and fevers to cardiovascular and autoimmune diseases.

Thus, the roles performed by acetylsalicylic acid are extremely numerous and varied. Inhibition of cyclooxygenase and stopping the formation of prostaglandins have a clinical impact on several pathological conditions. This fact is translated into the effects exerted by acetylsalicylic acid [6, 11].

Among the main roles performed by acetylsalicylic acid are: pain relief - analgesic effect; inflammation relief - anti-inflammatory effect; reducing the risk of cardiovascular events (thrombotic) - anticoagulant effect, more precisely antiplatelet effect; improvement of the symptoms of autoimmune diseases (lupus, rheumatoid arthritis), as well as pericarditis.

Opting for a therapeutic regimen that includes acetylsalicylic acid is most often done in the following situations: in common colds, as well as in the case of flu-like conditions - it improves the symptoms; in most isolated headaches (including migraines), toothaches, rheumatic joint and periarticular pain, neuralgia, etc.; in order to reduce the intensity of menstrual pain; in the case of sprains and dislocations - it relieves pain and inflammation; in inflammatory conditions in rheumatoid arthritis, lupus and other diseases associated with a prolonged inflammatory status.

Both in the case of people who have suffered a thrombotic cardiovascular event (myocardial infarction or stroke), and in the case of those at high risk of developing such an event, the administration of low doses of acetylsalicylic acid for longer periods of time is a treatment of choice.

Aspirin prevents the adhesion and aggregation of blood platelets (thrombocytes) in the blood, preventing the formation of blood clots (vascular thrombi), associated with myocardial infarction, stroke, pulmonary thromboembolism, etc. after vascular surgery or surgical interventions or other situations that favor blood stasis (stagnation) and blood hypercoagulability.

Aspirin is used for prophylactic purposes against cardiovascular events, in the following situations: the patient suffers from vascular pathologies that increase the risk of thrombosis; there is a vascular distribution that prevents the supply of oxygen to the brain; hypertension is present; blood tests reveal dyslipidemia and/or atherosclerotic plaques are identified in the blood vessels; there are other associated pathologies (e.g. diabetes).

Treatment with acetylsalicylic acid for anticoagulant purposes can also be administered in acute situations, immediately following the onset of a thrombotic event, for example acute myocardial infarction, in order to reduce the risk of mortality. Subsequently, it is also maintained in the long-term therapeutic regimen, for prophylactic purposes [12, 17].

Materials and methods

The FT–IR spectrum of the aspirin crystal was recorded using SHIMADZU FT–IR spectrometer in the range 4000–400 cm^{-1}. The sample for this measurement was finely ground and mixed with KBr.

Fig 1: SHIMADZU FT–IR spectrometer

Results and discussions

Figure 2 shows the FTIR spectrum of aspirin.

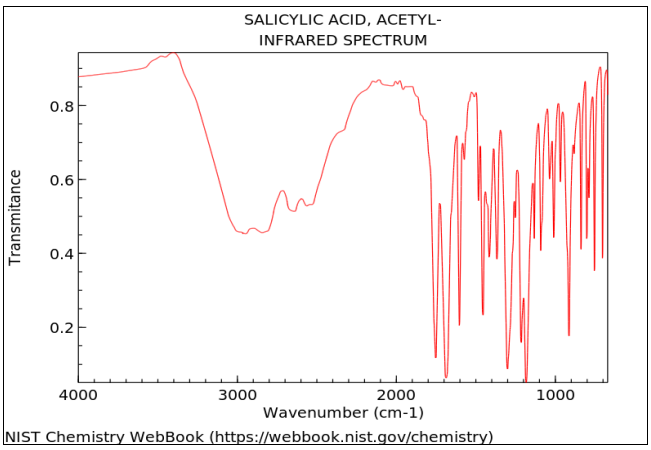

Fig 2: FT-IR spectrum of aspirin crystal

Table 1 shows the assignment of peaks in the FTIR spectrum of aspirin.

Table 1: Observed wavenumbers and their assignments for aspirin crystal in FT-IR

FT – IR ($\bar{\upsilon}$ / cm^{-1})	Assignment
3080 (s, br)	υ C–H; υ C–OH
2999 (s, br)	υ_{as} –CH3; υ C–OH
2833 (s, br)	υ_{s} –CH3 ; υ C–OH
2696 (m) 2587 (m) 2599 (m) 2546 (m)	υ P–O–H
1757 (vvs)	υ C=O (ester)
1690 (vvs)	υ C=O (acid)
1605 (m)	υ C=C
1576 (w)	υ C–C
1483 (w)	δas–CH3
1418 (s)	β O–H
1369 (m)	δs–CH3
1306 (vs)	υ C–O (acid)
1256 (m)	β P–O–H
1219 (s)	β C–H; υ C–O (acid); υ P =O
1186 (vvs)	β C–H
1092 (m)	β C–H; υ C–O (ester)
1038 (w)	β C–H; Ring breathing
1011 (m)	β C–H ; υ C–O (ester)
970 (s)	δas P(OH)2
918 (s)	γ O–H
884 (sh)	δs P(OH)2
839 (m)	γ C–H; ν P–OH
799 (m)	γ C–H
754 (m)	γ C–H
704 (m)	γ C–H
563 (m)	ρ CO2
542 (m)	ρ CO2

s– strong; vvs- very very strong; vs- very strong: m–medium; w–weak; vw- very weak: sh– shoulder; υ – stretching;

υ *s– sym. stretching;* υ *as– asym. stretching; ρ– rocking;* γ– out–of–plane bending; β– in–plane bending; δas– asym. bending; δs– sym. bending

Conclusions

The wavelength range in which absorption bands appear is between 4000 cm^{-1} and 400 cm^{-1}. Aspirin contains the following functional groups: C-H, C-OH, CH_3, C=O, C=C, P-OH, CO_2 determined by IR spectroscopy.

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