

## Study of the composition of diclofenac sodium determined by IR spectroscopy

Ioana Stanciu\*

Faculty of Chemistry, Department of Physical Chemistry, University of Bucharest, Bucharest, Romania

### Abstract

Summary of typical FTIR peaks for diclofenac sodium are around 3000–3100  $\text{cm}^{-1}$  is C-H stretch (aromatic), around 1600  $\text{cm}^{-1}$  is C=C stretch (aromatic), around 3300–3400  $\text{cm}^{-1}$  is N-H stretch (amine group), around 1700–1725  $\text{cm}^{-1}$  is C=O stretch (carboxylate group), around 1200–1300  $\text{cm}^{-1}$  is C-N stretch (amine), around 700–800  $\text{cm}^{-1}$  is C-Cl bending vibrations (chlorophenyl) and around 1200–1400  $\text{cm}^{-1}$  is sodium ion interaction (if salt form is present).

**Keywords:** Spectroscopy, ftir, diclofenac sodium

### Introduction

Diclofenac sodium is a widely used nonsteroidal anti-inflammatory drug (NSAID) that belongs to the class of arylacetic acid derivatives. Its primary mechanism of action involves the inhibition of cyclooxygenase (COX) enzymes, which play a critical role in the biosynthesis of prostaglandins, compounds responsible for pain, inflammation, and fever. Clinically, diclofenac sodium is employed to manage conditions such as rheumatoid arthritis, osteoarthritis, ankylosing spondylitis, and acute musculoskeletal pain. Given its widespread pharmaceutical use, understanding the chemical composition and structural characteristics of diclofenac sodium is essential for quality control, drug formulation, and pharmacological research.

Chemically, diclofenac sodium is the sodium salt of 2-[(2,6-dichlorophenyl) amino]phenylacetic acid. The presence of the dichlorophenyl group, amine linkage, and carboxylate functional group contributes to its pharmacological activity and influences its physicochemical properties, such as solubility, stability, and bioavailability. The purity of diclofenac sodium in pharmaceutical preparations is critical, as impurities or structural alterations may affect its therapeutic efficacy or induce adverse effects. Therefore, precise analytical techniques are employed to characterize its molecular composition and confirm its identity.

Infrared (IR) spectroscopy is a powerful analytical technique for identifying organic compounds and elucidating their structural features. The technique is based on the absorption of infrared radiation by molecular bonds, leading to vibrational transitions specific to different functional groups. Each chemical bond in a molecule absorbs IR radiation at characteristic frequencies, producing a spectrum that can be interpreted as a molecular fingerprint. This makes IR spectroscopy a valuable tool for confirming the presence of functional groups in diclofenac sodium, such as carboxylates ( $\text{COO}^-$ ), amine (NH), and aromatic rings. The technique also allows for the detection of potential impurities or structural modifications that may occur during synthesis or storage.

The IR spectrum of diclofenac sodium typically displays distinctive absorption bands corresponding to its functional groups. The carboxylate group exhibits strong asymmetric and symmetric stretching vibrations, usually observed in the region of 1600–1400  $\text{cm}^{-1}$ . The NH stretching vibration of the secondary amine appears in the region of 3300–3400

$\text{cm}^{-1}$ , while the aromatic C–H stretching vibrations are observed around 3000–3100  $\text{cm}^{-1}$ . Additionally, the aromatic C=C stretching vibrations produce bands in the region of 1500–1600  $\text{cm}^{-1}$ . By analyzing these characteristic absorption bands, researchers can confirm the molecular structure and ensure the authenticity of diclofenac sodium.

IR spectroscopy offers several advantages in the study of pharmaceutical compounds. It is rapid, non-destructive, and requires minimal sample preparation. This makes it particularly suitable for routine quality control and verification of raw materials and finished products. Furthermore, the combination of IR spectroscopy with other complementary techniques, such as nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry (MS), provides a comprehensive approach to structural characterization. While NMR and MS offer detailed information on molecular connectivity and molecular weight, IR spectroscopy provides direct evidence of functional groups and chemical bonds, which is crucial for confirming chemical identity<sup>[1, 5]</sup>.

The study of diclofenac sodium using IR spectroscopy not only ensures the integrity and quality of pharmaceutical formulations but also contributes to regulatory compliance. Pharmacopoeial standards often specify IR spectroscopy as a confirmatory test for the identification of active pharmaceutical ingredients (APIs). This ensures that the drug meets required specifications before being released to the market, protecting patient safety and therapeutic outcomes. Additionally, understanding the vibrational behavior of diclofenac sodium molecules under IR radiation provides insights into intermolecular interactions, hydrogen bonding, and solvation effects, which are important in formulation development and drug delivery systems.

Moreover, the application of IR spectroscopy in diclofenac sodium analysis extends to detecting degradation products and studying drug-excipient interactions. During storage, diclofenac sodium may undergo hydrolysis, oxidation, or other chemical transformations that alter its functional groups. IR spectroscopy can detect these changes by observing shifts in characteristic absorption bands, allowing researchers to assess the stability of the drug under various conditions. Similarly, interactions with excipients in solid dosage forms can influence drug performance. IR spectral analysis can reveal such interactions, guiding the design of stable and effective pharmaceutical formulations.

The study of diclofenac sodium composition through IR spectroscopy is a vital aspect of pharmaceutical research and quality assurance. By providing precise information on functional groups, molecular structure, and potential impurities, IR spectroscopy ensures that diclofenac sodium formulations are safe, effective, and compliant with regulatory standards. The insights gained from this analytical technique also support the development of improved formulations, understanding of stability profiles, and investigation of drug-excipient interactions. As a non-destructive and highly informative method, IR spectroscopy remains an indispensable tool in the characterization and quality control of diclofenac sodium and other pharmaceutical compounds [6, 12].

## Materials and methods

Fourier transform infrared (FTIR) spectra of the diclofenac sodium were obtained in the range of 400 to 4000  $\text{cm}^{-1}$  using a FTIR Spectrophotometer (Shimadzu Corp.) (Fig.1) by the diffuse reflectance method.



Fig 1: Spectrophotometer Shimadzu

## Results and discussions

Figure 2 shows the IR spectrum of diclofenac sodium.

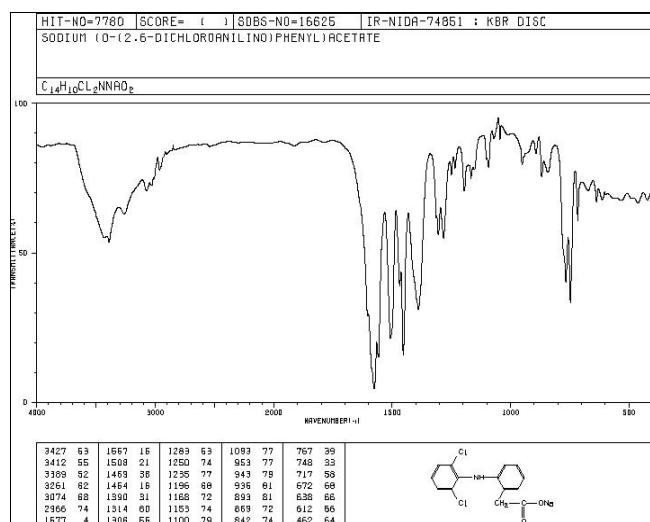


Fig 2: Spectrum IR of diclofenac sodium

Aromatic C-H Stretch (around 3000  $\text{cm}^{-1}$ ) has wavenumber range is 3000–3100  $\text{cm}^{-1}$ . This region corresponds to the stretching vibrations of the C-H bonds in the aromatic (benzene) ring. Diclofenac sodium contains two aromatic rings (one being a dichlorophenyl group), so the absorption peak here is due to these C-H stretches.

Aromatic C=C stretch (around 1600  $\text{cm}^{-1}$ ) has wavenumber range is 1600–1650  $\text{cm}^{-1}$ . This is a characteristic absorption due to the stretching of the carbon-carbon double bonds in the aromatic rings. The peak is sharp and is typically observed in the range of 1600  $\text{cm}^{-1}$ , indicative of the aromatic structure of the molecule.

Amine (N-H) stretch (around 3300–3400  $\text{cm}^{-1}$ ) has wavenumber range is 3300–3400  $\text{cm}^{-1}$ . The presence of an amino group (NH) in diclofenac sodium leads to a broad, medium-intensity absorption band in this region. It may be slightly broad due to hydrogen bonding.

C=O stretch (around 1700  $\text{cm}^{-1}$ ) has wavenumber range is 1700–1725  $\text{cm}^{-1}$ . Diclofenac sodium contains a carboxylate group ( $\text{COO}^-$ ), and the stretching vibration of the carbonyl group (C=O) is observed in this region.

C-N stretch (around 1200  $\text{cm}^{-1}$ ) has wavenumber range is 1200–1300  $\text{cm}^{-1}$ . This corresponds to the stretching vibration of the C-N bond in the amine group attached to the aromatic ring.

Chlorine (Cl) absorption (around 700–800  $\text{cm}^{-1}$ ) has wavenumber range is 700–800  $\text{cm}^{-1}$ . The presence of chlorine atoms (in the dichlorophenyl group) can cause absorption in this region. It results in a peak due to the bending vibrations of C-Cl bonds.

Sodium ion interaction (around 1200–1400  $\text{cm}^{-1}$ ) has wavenumber range is 1200–1400  $\text{cm}^{-1}$ . The sodium ion ( $\text{Na}^+$ ) component in diclofenac sodium may show subtle influences on the spectrum, especially if the compound is in a salt form (sodium salt).

These peaks and the specific shape of the spectrum help confirm the presence of diclofenac sodium and can be used to verify its identity in a sample. The FTIR spectrum of diclofenac sodium will reflect its molecular structure and the key functional groups present in the compound [13, 19].

## Conclusions

The composition of diclofenac is an essential element in understanding its therapeutic efficacy and safety. Both the active substance – diclofenac in different chemical forms – and the excipients included in the pharmaceutical formulations contribute to the way the drug is absorbed, distributed and metabolized in the body. The differences between the presentation forms, be they tablets, capsules, injectable solutions, gels or patches, are closely related to the variability of the composition, each variant being adapted to specific clinical needs. Overall, the analysis of the composition of diclofenac highlights the importance of choosing the right form to optimize treatment and minimize the risk of adverse reactions.

## References

1. Subagio A, Morita N. Food Chemistry, 2003;81:97–102.
2. Dupont J, White PJ, Carpenter MP, Schaefer EJ, Meydani SN, Elson CE, et al. Journal of the American College of Nutrition, 1990;9(5):438–470.
3. Veljković VB, Biberdžić MO, Banković-Ilić IB, Djalović IG, Tasi MB, Nježić ZB, et al. Renewable and Sustainable Energy Reviews, 2018;91:531–548.

4. Beadle JB, Just DE, Morgan RE, Reiners RA. Journal of the American Oil Chemists' Society, 1965;42(2):90-95.
5. Strocchi A. Journal of Food Science, 1982;47(1):36-39.
6. Stanciu I. Rheological behaviour of biodegradable lubricant. Journal of Science and Arts, 2019;3(48):703-708.
7. Stanciu I. Rheological investigation of soybean oil from soya beans. Journal of Science and Arts, 2019;4(49):938-988.
8. Stanciu I. Modeling the temperature dependence of dynamic viscosity for rapeseed oil. Journal of Science and Arts, 2011;1:55-58.
9. Meneghetti SMP, Meneghetti MR, Wolf CR, Silva EC, Lima GE, Coimbra MDA, et al. Journal of the American oil chemists' society, 2006;83(9):819-822.
10. Stanciu I. Journal of Science and Arts, 2018;18(2):453-458.
11. Sheibani A, Ghotbaddini-Bahraman NASER, Sadeghi FATEMEH. Oriental Journal of Chemistry, 2014;30(3):1205-1209.
12. Stanciu I. Some methods for determining the viscosity index of hydraulic oil. Indian Journal of Science & Technology, 2023;16(4):254-258.
13. Stanciu I. Rheological behavior of corn oil at different viscosity and shear rate. Oriental Journal of Chemistry, 2023;39(2):335-339.
14. Stanciu I. Rheological characteristics of corn oil used in biodegradable lubricant. Oriental Journal of Chemistry, 2023;39(3):592-595.
15. Stanciu I. Effect of temperature on rheology of corn (*Zea mays*) oil. Oriental Journal of Chemistry, 2023;39(4):1068-1070.
16. Stanciu I. Study Rheological Behavior of Rapeseed oils Compared to Mineral oil. Oriental Journal of Chemistry, 2021;37(1):247-249.
17. Stanciu I. Influence of Temperature on the Rheological Behavior of Orange Honey. Oriental Journal of Chemistry, 2021;37(2):440-443.
18. Ribot F, Toledano P, Sanchez C. Inorg Chim Acta, 1991;185(2):239-245.
19. Catterick J, Thornton P. Adv Inorg Chem and Radio Chem H.J. Emeleus and A.G. Sharpe (eds.) Vol. 20 (Academic), 1977.