

# Infrared Spectrum Processing and Interpretation

Infrared spectrum analysis is a data method for obtaining sample molecular structure information through a series of analysis and calibration of the original spectrum. Through the analysis of infrared spectrum, we can infer the molecular structure information and functional group information of organic and inorganic substances, which can provide a basis for studying the reaction mechanism and identifying the types of compounds. At present, the commonly used software for infrared spectrum analysis is OMNIC 8.2.

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### Infrared spectroscopy applications

Infrared absorption spectroscopy is mainly used for qualitative analysis of functional groups in molecules, and can also be used for quantitative analysis. The applicability of infrared spectroscopy to samples is quite wide, solid, liquid or gaseous samples can be applied, and inorganic, organic, and polymer compounds can be detected.

Commonly, when analyzing unknown products, infrared spectroscopy can give information about functional groups, combined with other methods such as mass spectrometry, nuclear magnetism, single crystal diffraction, etc., to help confirm the structure of the product;

Infrared spectroscopy, especially in-situ infrared plays an important role in the catalytic reaction, which can be used to determine the intermediate products of the reaction and the adsorption of the species on the surface of the catalyst during the reaction;

The properties of the material can also be known through the adsorption of specific substances, such as pyridine adsorption infrared can test the acid type and acid amount of the material, and the infrared adsorption of CO can judge the adsorption state of CO on the material according to its peak, and then know whether the metal atom in the catalyst exists in the form of single atom and so on.

### Steps of infrared spectrum interpretation

According to the molecular formula, calculate the unsaturation:  $f = 1 + n_4 + 1/2 (n_3 - n_1)$

Whether there are double bonds, triple bonds or aromatic rings in the molecular structure formula can be estimated by calculating the degree of unsaturation, and whether the spectral analysis is reasonable can be verified.

The main strong absorption peaks are found according to the infrared spectra of unknown substances. According to the order from simple to complex, it is customary to divide the infrared region into five regions to analyze:

4000~2500cm<sup>-1</sup>. This is the stretching vibration region of X-H (X includes C, N, O, S, etc.). The main absorbing groups are hydroxyl group, amino group, alkyl group and so on.

2500~2000cm<sup>-1</sup>. This is the stretching vibration region of triple bond and cumulative double bond (-C≡C-, -C≡N-, -C=C=C-, -N=C=O-, -N=C=S-).

2000~1500cm<sup>-1</sup>. This is a double bond stretching vibration region, which mainly includes carbonyl group absorption, carbon carbon double bond absorption, skeleton vibration of benzene ring and absorption of C=N, N=O groups.

2000~1500cm<sup>-1</sup>. This is the bending vibration absorption peak of C-H.

1300~400cm<sup>-1</sup>. In this region, there are some absorption, such as the stretching vibration frequency of single bond, the vibration frequency of molecular skeleton and the bending vibration frequency of benzene ring and olefin, which reflect the substitution type.

The correctness of the analytical results was verified by the standard spectrum.

#### **Important infrared spectrum database**

Sadtler Database of Infrared Spectra

Spectral Database for Organic Compounds (SDBS)

Chemistry Database of SIOC

Chemexper Chemical Directory (CCD)

FTIRsearch

NIST Chemistry WebBook

Spectral Databases - The Coblenz Society

American Petroleum Insearch Project 44, Infrared

Spectral Data

Documentation Of Molecular Spectroscopy

#### **T,C&A Lab**

The processing of IR data has become the task of experts, who can understand the data and its format, as well as software, programs and databases. With the support of the most advanced IR platform and expert team, T,C&A Lab is committed to helping customers with IR experiment design, data collection and interpretation. Welcome to contact our experts for consultation.

#### Reference

James Ashenhurst. Infrared Spectroscopy: A Quick Primer On Interpreting Spectra. February 19th, 2020.

<https://tcalab.alfa-chemistry.com/data-interpretation-simulation/infrared-spectrum-processing-and-interpretation.html>