

## Adipic acid composition determined by IR spectroscopy

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### Abstract

In this article, we determined the composition of adipic acid using IR spectroscopy and the Nicolet-Magna 550 IR spectrometer as the instrument. Adipic acid has the formula  $(\text{CH}_2)_4(\text{COOH})_2$  and contains the following functional groups: C=O, C-H,  $\text{CH}_2$ . Adipic acid (also called hexanedioic acid) is a dicarboxylic organic compound, characterized by the molecular formula  $\text{C}_6\text{H}_{10}\text{O}_4$  and the linear structure of the aliphatic chain. The molecule contains two carboxyl groups (-COOH) located at the ends of a chain of six carbon atoms, separated by four methylene units (- $\text{CH}_2$ -). This architecture gives adipic acid moderate acidic properties, high thermal stability and versatility in polycondensation reactions. Due to its symmetry and chain flexibility, adipic acid is an essential precursor in the synthesis of polymers, especially nylon-6,6 polyamides, as well as in various industrial applications where a well-defined dicarboxylation is required.

**Keywords:** Composite, adipic acid, IR spectroscopy

### Introduction

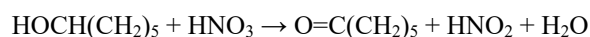
Adipic acid or hexanedioic acid is the organic compound with the formula  $(\text{CH}_2)_4(\text{COOH})_2$ . From an industrial perspective, it is the most important dicarboxylic acid: about 2.5 billion kilograms of this white crystalline powder are produced annually, mainly as a precursor for the production of nylon [1, 5]. Adipic acid otherwise rarely occurs in nature, but it is known as manufactured E number food additive E355. Salts and esters of adipic acid are known as adipates. About 60% of the 2.5 billion kg of adipic acid produced annually is used as monomer for the production of nylon by a polycondensation reaction with hexamethylene diamine forming nylon 66. Other major applications also involve polymers; it is a monomer for the production of polyurethane and its esters are plasticizers, especially in PVC. Adipic acid has been incorporated into controlled-release formulation matrix tablets to obtain pH-independent release for both weakly basic and weakly acidic drugs. It has also been incorporated into the polymeric coating of hydrophilic monolithic systems to modulate the intragel pH, resulting in zero-order release of a hydrophilic drug. The disintegration at intestinal pH of the enteric polymer shellac has been reported to improve when adipic acid was used as a pore-forming agent without affecting release in the acidic media. Other controlled-release formulations have included adipic acid with the intention of obtaining a late-burst release profile. Small but significant amounts of adipic acid are used as a food ingredient as a flavorant and gelling aid. It is used in some calcium carbonate antacids to make them tart. As an acidulant in baking powders, it avoids the undesirable hygroscopic properties of tartaric acid. Adipic acid, rare in nature, does occur naturally in beets, but this is not an economic source for commerce compared to industrial synthesis.

Adipic acid, like most carboxylic acids, is a mild skin irritant. It is mildly toxic, with a median lethal dose of 3600 mg/kg for oral ingestion by rats. The production of adipic acid is linked to emissions of  $\text{N}_2\text{O}$ , a potent greenhouse gas and cause of stratospheric ozone depletion. At adipic acid producers DuPont and Rhodia (now Invista and Solvay, respectively), processes have been implemented to catalytically convert the nitrous oxide to innocuous products [6, 12].

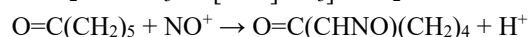
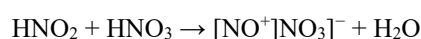
### Materials and methods

#### Synthesis

Adipic acid is produced by oxidation of a mixture of cyclohexanone and cyclohexanol, which is called KA oil, an abbreviation of ketone-alcohol oil. Nitric acid is the oxidant. The pathway is multistep. Early in the reaction, the cyclohexanol is converted to the ketone, releasing nitrous acid:



The cyclohexanone is then nitrosated, setting the stage for the scission of the C-C bond:



Side products of the method include glutaric and succinic acids. Nitrous oxide is produced in about one to one mole ratio to the adipic acid, [5] as well, via the intermediacy of a nitrolic acid. Related processes start from cyclohexanol, which is obtained from the hydrogenation of phenol.

The FT-IR spectra recording of salts was carried out on a Fourier Transform Nicolet-Magna 550 IR spectrometer. The samples are ground in the KBr (2 mg of sample per 200 mg of KBr) and then pressed in the form of pellets. The spectra were treated by Omnic 8.1 software [13, 17].



Fig 1: Transform Nicolet-Magna 550 IR spectrometer

## Results and discussions

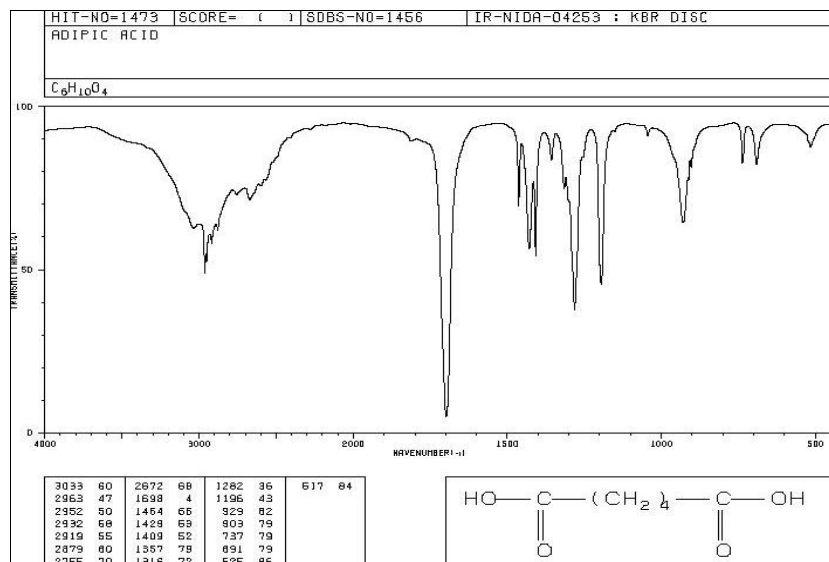


Fig 2: Spectrul IR al acidului adipic

## Conclusions

In conclusion, adipic acid is a dicarboxylic compound with a linear aliphatic structure, defined by the molecular formula C<sub>6</sub>H<sub>10</sub>O<sub>4</sub> and by the presence of two carboxyl groups at the ends of the carbon chain. This symmetrical structure gives the molecule stability and specific reactivity, making it an essential precursor in the synthesis of polyamides and in industrial processes based on polycondensation reactions. Therefore, the well-defined chemical composition of adipic acid is the basis for its wide use in the polymer materials industry and in numerous technological applications. Adipic acid has the formula (CH<sub>2</sub>)<sub>4</sub>(COOH)<sub>2</sub> and contains the following functional groups determined by IR spectroscopy: C=O, CH<sub>2</sub> and C-H.

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