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Chemical composition of methyl orange determined by IR spectroscopy

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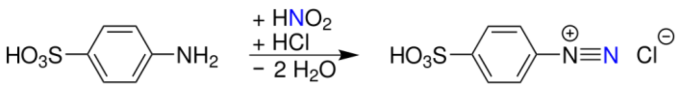
Abstract
Methyl orange (also known as helianthine or acid Orange 52) is a synthetic azo dye, commonly used as a pH indicator in titrations. Its chemical formula is $C_{14}H_{14}N_3NaO_3S$, with a molecular weight of 327.33 g/mol. Its structure includes an azo group (-N=N-) linking two benzene rings, one of which is substituted with a sulfonic group ($-SO_3Na$) and the other with a dimethylamino group ($-N(CH_3)_2$).

Methyl orange is soluble in water and exhibits a significant color change depending on pH: it turns red in acidic medium (pH < 3.1) and yellow in basic medium (pH > 4.4), with a color transition between these values. This property makes it useful in acid-base analysis, especially in titrations of weak acids with strong bases.

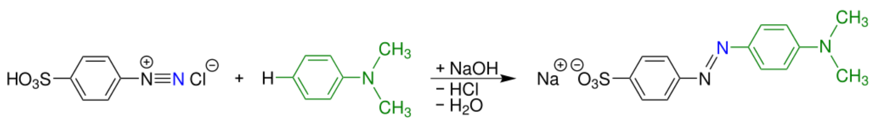
Keywords: Composition, Methyl Orange, Spectroscopy, FTIR

Introduction

Methyl orange (helianthine or orange-III) is an orange-colored pH indicator, often used in titrations due to its easily observable color change. It has the molecular formula $C_{14}H_{14}N_3NaO_3S$ and a molecular mass of 327.33 g/mol. It is an azo dye, being the sodium salt of 4-[4-(dimethylamino)phenylazo]benzenesulfonic acid. Because it changes color under the action of a medium-strength acid, it is used especially for the purpose of titrating acids. Unlike a universal indicator, methyl orange does not show the full color spectrum when changing color. Methyl orange is red in acidic medium and yellow in basic medium. To obtain methyl orange, sulfanilic acid is diazotized with nitric acid and thus converted into 4-benzene diazonium sulfonic acid [1-7].



Subsequently, 4-benzene diazonium sulfonic acid is coupled with N,N-dimethylaniline and treated with sodium hydroxide, transforming into the sodium salt.



Methyl orange is used primarily as an indicator because of the visible color change that occurs. Thus, when used in a solution that is increasingly acidic, the color will change from yellow to orange and finally to red in the most acidic solution. If the process is reversed, the color will change again, from red to orange and finally to yellow in the alkaline solution. Methyl orange has a pKa in water of 3.47 at 25 °C [8-12].

Materials and methods

Measurements were carried out using Bruker Alpha Spectrophotometer, utilizing the ATR (Attenuated Total Reflection) FT-IR sampling technique.

Fig 1: Bruker Alpha Spectrophotometer

Results and discussions

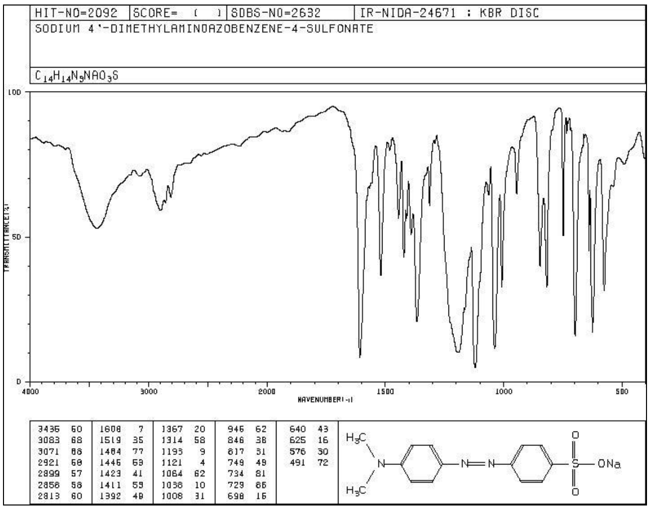


Fig 2: Spectrul indicatorului metil orage

The FTIR spectra of control Methyl orange (Fig 2), displays peak at 2,924.06 cm^{-1} for asymmetric CH_3 stretching vibrations; peaks at 1,519.78 and 1,421.71 cm^{-1} for the C = C–H in plane C–H bend; peaks at 1,040.00, 1,007.29, and 846.66 cm^{-1} for ring vibrations; and a peak at 816.67 cm^{-1} for the1, 4 disubstituted (Para) benzene ring [13-17].

Conclusions

Methyl orange is a synthetic azo dye, with the chemical formula $C_{14}H_{14}N_3NaO_3S$, which contains an azo group (-N=N-) linking two benzene rings.

Its structure includes functional groups important for its properties: sulfonic group (-SO_3Na) and dimethylamino group (-$N(CH_3)_2$).

It is soluble in water and acts as a pH indicator, changing color from red in acidic medium to yellow in basic medium.

Its color change property makes it a useful tool in acid-base titrations and chemical analysis.

Its chemical stability and reactivity make it valuable in laboratories and various industrial applications, but it must be used with caution due to its synthetic chemical nature.

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