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Composition of adipic esters used as lubricants

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Abstract

In this article, we determined the composition of adipic esters by nuclear magnetic resonance using a Bruker spectrophotometer. We synthesized the following adipic esters: isodecyl 2-(p-nonyl-phenoxy) ethyl adipate, isodecyl 2-(o-sec-butyl-phenoxy) ethyl adipate, and isodecyl 2-phenoxy ethyl adipate. These compounds have the following components: RCH_3, R_2CH_2, $C=C–CH_3$, HC–COOH, RCOO–CH, ArOH, and Ar-H.

Keywords: Ester, ^{1}H-NMR, structure, adipic ester

Introduction

Nuclear magnetic resonance (NMR) is one of the most advanced and most frequently used techniques in the study of matter in its three states of aggregation: solid, liquid and even gaseous. The main advantages of NMR techniques lie in their completely non-invasive nature and in the fact that most of the time no prior preparation of the samples to be studied is necessary. The most well-known NMR technique to the general public is NMR tomography, especially for its applications in medicine. Other NMR techniques such as spectroscopy, diffusometry and NMR relaxometry are generally known only to specialists in the field of physics or chemistry. Although NMR has multiple applications in the field of engineering, it seems that it is much less popular among engineers. This situation can also be explained by the fact that most NMR techniques are described within the formalism of quantum physics and are therefore accessible only to people who have specifically studied that chapter of physics. In order to support a wider category of readers, this book aims to approach nuclear magnetic resonance using the formalism of classical physics. Thus, both the principles and the main NMR techniques, together with their applications, will be explained in a formalism based on the evolution of the magnetization vector, which is much more accessible. Also, the techniques presented here do not require the acquisition of expensive NMR instruments with superconducting magnets [1, 6].

Nuclear magnetic resonance (NMR) is one of the most reliable techniques for investigating matter, being applied both in the study of liquids and solids and gases. Only plasma, the fourth state of matter, has escaped (so far) investigations by NMR. Unlike other techniques for investigating matter, nuclear magnetic resonance is completely non-perturbative and non-destructive. Samples investigated by NMR can then be used in other experiments. The most well-known application of the phenomenon of nuclear magnetic resonance is in medicine, namely MRI tomography (or MRI imaging), but nuclear magnetic resonance can be equally useful in chemistry, biology, materials science, soil science, and oil extraction. In chemistry, high-field MRI spectroscopy is most often known, but MRI diffusometry or relaxometry has also proven to be particularly useful. In oil extraction, the study of soils, porous media, and the migration of molecules through them often uses low-field MRI diffusometry and relaxometry techniques [7, 12].

Material and methods

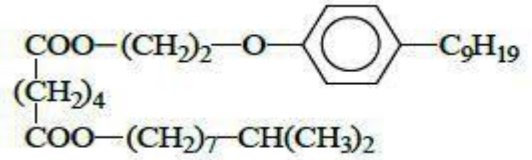
Structure determination

Nuclear magnetic resonance (^{1}H-NMR) spectra were recorded on a 200 MHz Bruker spectrometer. Deuterated chloroform $CDCl_3$ (99.8% atom. %D) + 0.05% TMS (v/v) or DMSO-d6 (99.9% atom. %D) + 0.05% TMS (v/v) was used [12, 17]. Chemical shift values (δ) in 1H-NMR spectra are expressed in ppm (for CDCl3 $\delta = 7.27$ ppm), and coupling constants (J) are expressed in Hz. The abbreviations used for the multiplicity of signals are: s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet) [13].

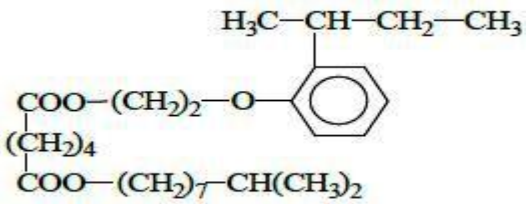
Fig 1: Bruker 200 MHz spectrometer

Synthesis of adipic esters

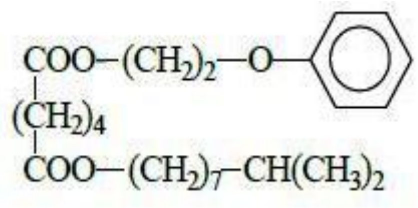
Isodecyl adipate and 2-(p-nonyl-phenoxy) ethyl is obtained by synthesizing 1,100 moles of adipic acid with 1,100 moles of 2-(p-nonyl-phenoxy) ethanol and 0.037 moles of p-toluene sulfonic acid. In stage I: temperature 115 - 145^{0}C, time 5 - 7 hours, toluene 175 ml. In the second stage, 1,100 moles of isodecanol are added at a temperature between 120^{0}C - 165^{0}C, time 5 - 7 hours.



Isodecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl is obtained by synthesizing 1.270 moles of adipic acid with 1.270 moles of 2-(o-sec-butyl-phenoxy) ethanol and 0.037 moles of p-toluene sulfonic acid. In stage I: temperature 115 - 145^{0}C, time 5 - 7 hours, toluene 175 ml. In the second stage, 1.270 of isodecanol is added at a temperature between 120^{0}C - 165^{0}C, time 5 - 7 hours.



Isodecyl adipate and 2-phenoxy ethyl are obtained in the first stage from 1.450 moles of adipic acid, 1.450 moles of 2-phenoxy ethanol and 0.037 moles of p-toluene sulfonic acid. In stage I: temperature 115 - 145^{0}C, time 5 - 7 hours, toluene 175 ml. In the second stage, 1.450 moles of isodecanol are added at a temperature between 120^{0}C - 165^{0}C, time 5 - 7 hours.



Results and discussion

Figure 2 shows the ^{1}H-NMR spectrum of isodecyl adipate and 2-(p-nonyl-phenoxy)ethyl.

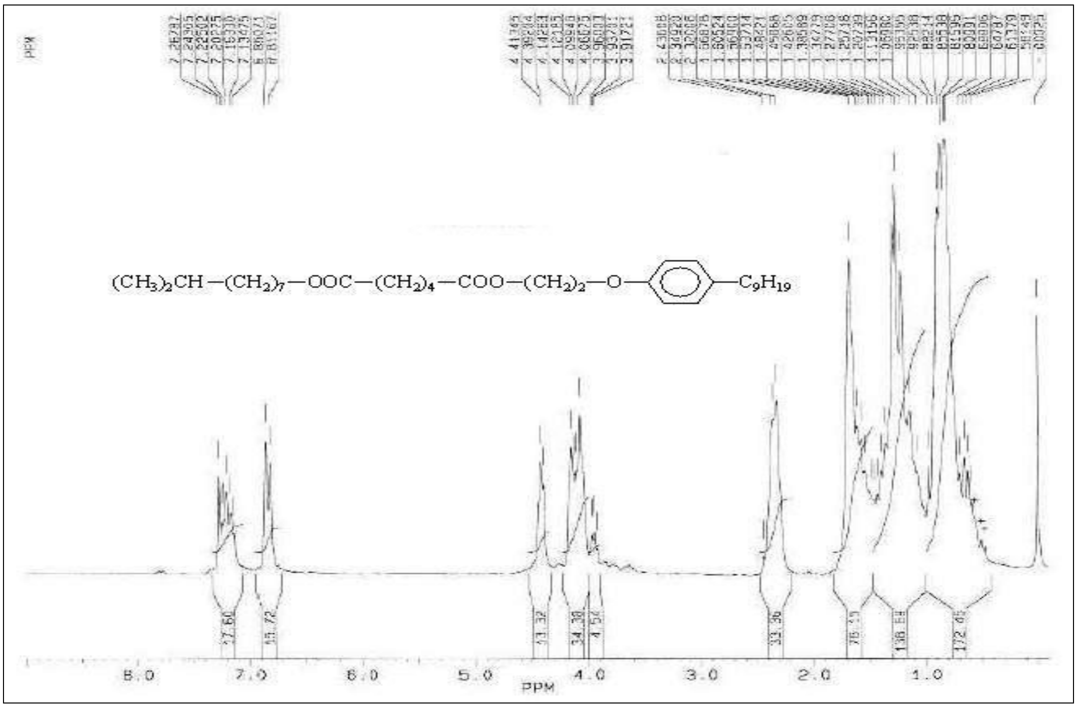


Fig 2: ^{1}H-NMR spectrum of isodecyl adipate and 2-(p-nonyl-phenoxy) ethyl

Table 1 shows the compound types of isodecyl adipate and 2-(p-nonyl-phenoxy) ethyl.

Table 1: Characteristic Proton NMR Shifts

Type of proton	Type of compound	Chemical shift range, ppm
RCH_3	1˚ aliphatic	0,81-0,96 (multiplet)
R2CH2	2˚ aliphatic	1,20-1,27 (multiplet)
C=C–CH3	allylic	1,66 (multiplet)
HC–COOH	acids	2,32-2,43 (multiplet)
RCOO–CH	esters	3,91-3,96 (multiplet)
ArOH	phenolic	4,06-4,14 (multiplet)
ArOH	phenolic	4,41 (multiplet)
Ar–H	aromatic	6,81-6,85 (dublet)
Ar–H	aromatic	7,13-7,26 (multiplet)

Figure 3 shows the ^{1}H-NMR spectrum of isodecyl adipate and 2-(o-sec-butyl-phenoxy)ethyl.

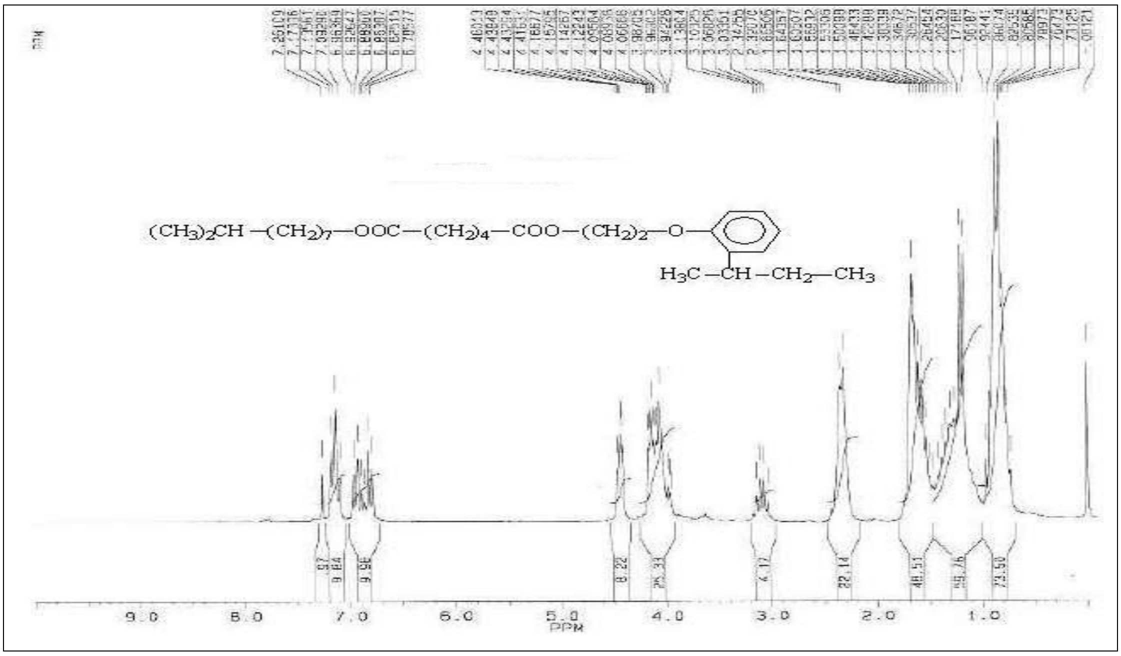


Fig 3: ^{1}H-NMR spectrum of isodecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl

Table 2 shows the compound types of isodecyl adipate and 2-(o-sec-butyl-phenoxy) ethyl.

Table 2: Characteristic Proton NMR Shifts

Type of proton	Type of compound	Chemical shift range, ppm
RCH_3	1˚ aliphatic	0,82-0,96 (multiplet)
R2CH2	2˚ aliphatic	1,17-1,26 (multiplet)
C=C–CH3	allylic	1,66 (multiplet)
HC–COOH	acids	2,32-2,34 (multiplet)
RCOO–CH	esters	3,03-3,13 (multiplet)
RCOO–CH	esters	3,94-3,98 (multiplet)
ArOH	phenolic	4,06-4,15 (multiplet)
ArOH	phenolic	4,41 (multiplet)
Ar–H	aromatic	6,78-6,96 (dublet)
Ar–H	aromatic	7,05-7,26 (multiplet)

Figure 4 shows the ^{1}H-NMR spectrum of isodecyl adipate and 2-phenoxy ethyl.

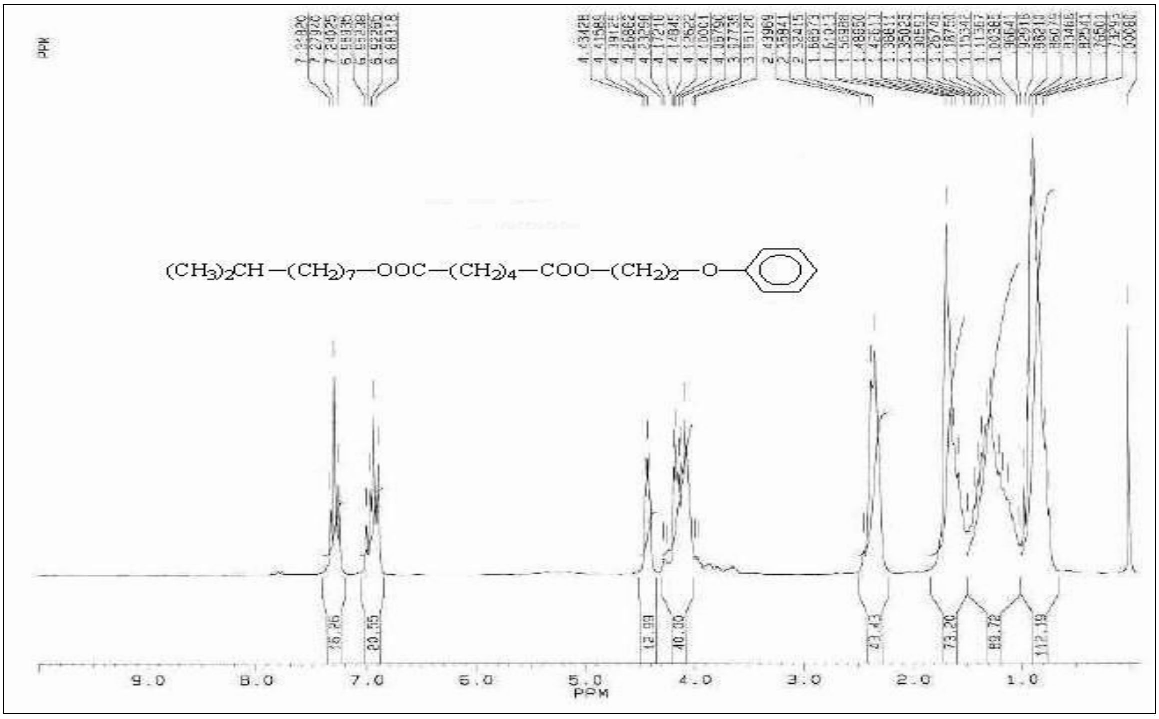


Fig 4: ^{1}H-NMR spectrum of isodecyl 2-phenoxy ethyl adipate

Table 3 shows the types of compounds that are part of isodecyl 2-phenoxy ethyl adipate.

Table 3: Characteristic Proton NMR Shifts

Type of proton	**Type of compound**	**Chemical shift range, ppm**
RCH_3	1˚ aliphatic	0,82-0,96 (multiplet)
R2CH2	2˚ aliphatic	1,15-1,26 (multiplet)
C=C–CH3	allylic	1,66 (multiplet)
HC–COOH	acids	2,32-2,43 (multiplet)
RCOO–CH	esters	3,95-4,06 (multiplet)
ArOH	phenolic	4,14 (multiplet)
ArOH	phenolic	4,39-4,43 (multiplet)
Ar–H	aromatic	6,88-6,98 (multiplet)
Ar–H	aromatic	7,24-7,31 (multiplet)

Conclusions

The ^{1}H-NMR spectra of adipic esters reflect the symmetry and flexibility of the aliphatic chain: the methylene protons in the central chain ($–(CH_2)_4–$) appear as distinct but close signals, due to the relatively homogeneous chemical environment. The methylene groups in the vicinity of the ester ($–O–CH_2–$ and $–CH_2–COO–$) give characteristic signals at higher chemical shifts (δ ~4.0–4.3 ppm for $–O–CH_2–$ and δ ~2.2–2.4 ppm for $–CH_2–COO–$), which confirms the formation of the ester. The internal methylene protons of the adipic chain ($–CH_2–CH_2–CH_2–CH_2–$) are found in the region δ ~1.2–1.6 ppm, showing multiplets due to spin-spin coupling. The terminal groups of the alcohol radicals (e.g. $–CH_3$, $–CH_2–$, –aryl) determine additional signals specific to the ester structure: $–CH_3$ at δ ~0.8–1.0 ppm, $–CH_2–O–$ at δ ~3.5–4.2 ppm, aromatic groups at δ ~7.0–8.0 ppm. The symmetry of the molecule influences the simplicity of the spectrum – in the case of identical diesters, the number of signals is reduced (equivalent groups), while in asymmetric esters a greater diversity of signals appears. In conclusion, ^{1}H-NMR spectroscopy is a reliable method for confirming the structure of adipic esters, allowing the identification of functional groups, verification of symmetry and differentiation of alcohol radicals.

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