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SYNTHESIS OF 2-NAPHTHYL 2-CHLOROACETATE AND STUDY OF ITS NUCLEOPHILIC SUBSTITUTION REACTIONS WITH CITRIC ACID †

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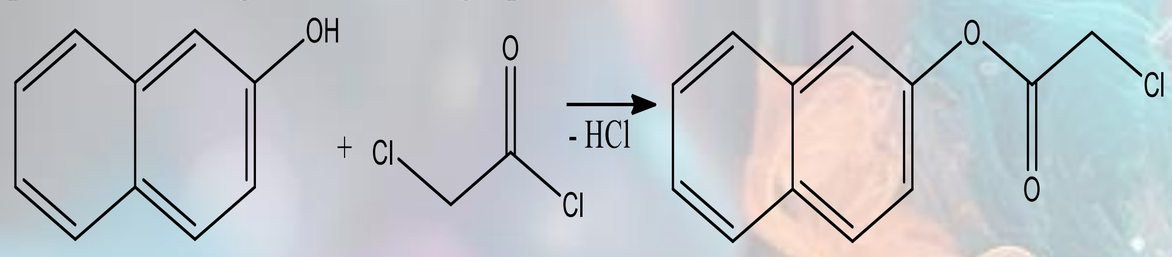
INTRODUCTION & AIM

Naphthol derivatives, particularly those modified via chloroacetylation, have garnered significant attention in pharmaceutical and agrochemical research due to their antibacterial, analgesic, and fungicidal properties. These compounds often serve as precursors to bioactive molecules and intermediates in drug and pesticide synthesis. Aromatic amines, halogenated phenols, and their esters are widely used in industries ranging from dye and pigment production to pharmaceutical formulation.

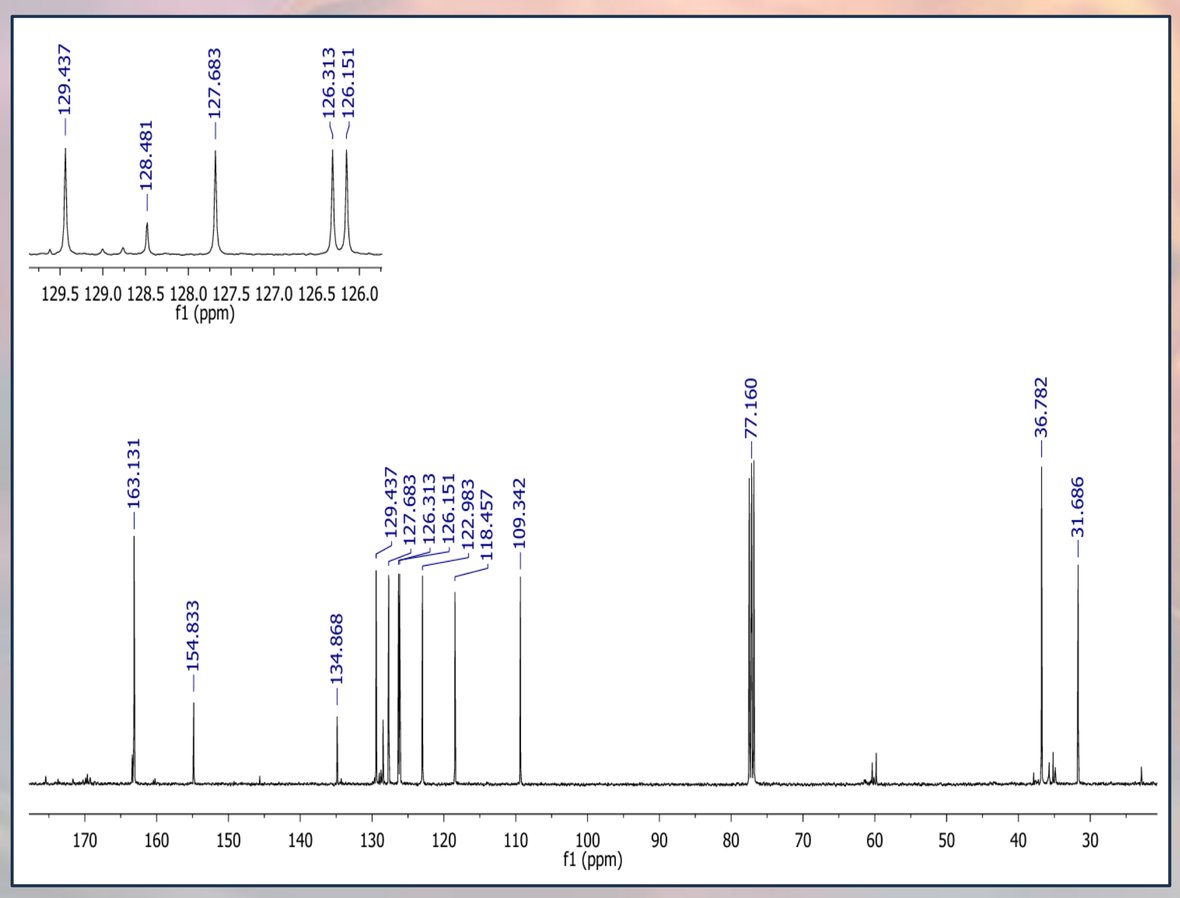
In this study, we synthesized 2-naphthyl 2-chloroacetate via electrophilic substitution using chloroacetyl chloride and investigated its nucleophilic substitution reaction with citric acid, a naturally occurring, non-toxic reagent. The product, 2-naphthylcarboxymethylene citrate *(3-hydroxy-3-((2-naphthalen-2-yloxy)-2-oxoethoxy)pentanedioic acid)*, was structurally characterized and evaluated for its analytical application in Fe(III) ion detection.

The influence of solvents on the course of the O-chloroacetylation reaction of 2-naphthol was investigated. The reagents were used in equimolar amounts, and the reactions were carried out at the boiling points of the respective solvents. The reactions proceed according to the following equation:



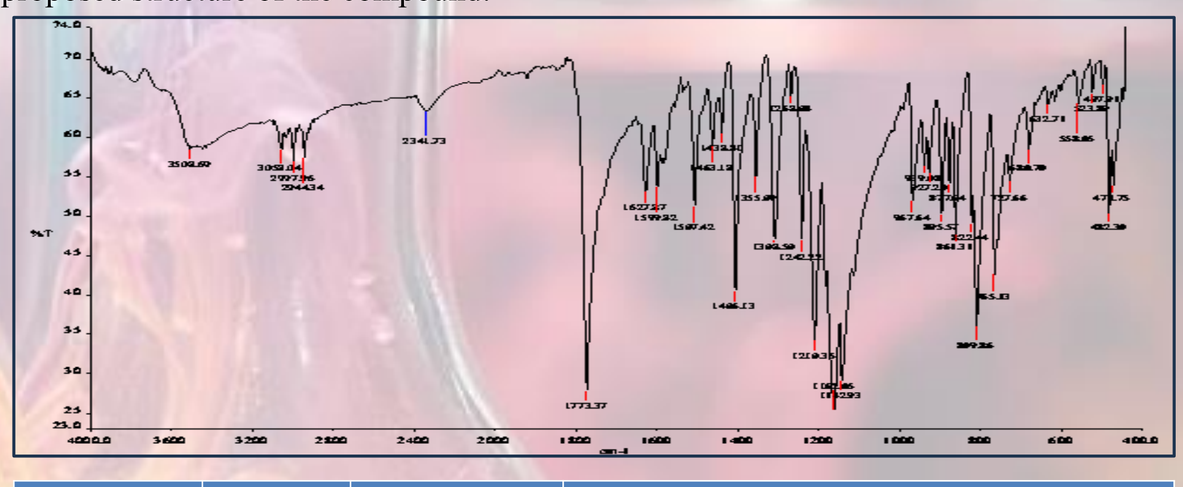
METHOD

The purity and identity of the synthesized compounds were evaluated by thin-layer chromatography (TLC) on Silufol-254 plates using a iso-octane : ethyl acetate (9:1) solvent system, with ultraviolet (UV) light as the visualization method.For the TLC stationary phase, silica gel-coated aluminum plates (silica gel 60 F254) bought from MERCK, India were utilized. The Fourier-transform infrared (FT-IR) spectra were recorded in the 400–4000 cm^{-1} range using the KBr pellet method on a Specord IR-71 spectrophotometer (Carl Sies, Germany). The nuclear magnetic resonance (^{1}H and ^{13}C NMR) spectra were obtained on a Bruker 400 MHz NMR spectrometer (Germany), using tetramethylsilane (TMS) as an internal standard. Chemical shift values were reported in parts per million (ppm). The uncorrected melting points of the synthesized compounds were determined using the open capillary method on an Mvtec melting point apparatus.



RESULTS & DISCUSSION

The mechanism of this reaction was proposed as follows: during the reaction between the –OH group of the 2-naphthol molecule and chloroacetyl chloride, the electron density in the chloroacetyl chloride molecule shifts toward the more electronegative oxygen atom, making the oxygen partially negatively charged. Due to the electronegative effects of both the chlorine and oxygen atoms, the carbon atom becomes partially positively charged and interacts with the lone electron pair of the hydroxyl group in the 2-naphthol molecule to form an intermediate complex. As the reaction proceeds, a covalent bond forms between the oxygen and carbon atoms, resulting in the formation of a new complex, from which the reaction product is released along with hydrogen chloride. The resulting reaction product was identified as naphthalen-2-yl 2-chloroacetate and was analyzed using IR and NMR spectroscopy. The IR spectrum confirms that the synthesized compound is indeed naphthalen-2-yl 2-chloroacetate. The positions and intensities of the observed functional groups correspond well with the proposed structure of the compound.



Wavenumber (cm^{-1})	Intensity	Nature	Comment
1741	Strong	C=O (ester)	Characteristic ester carbonyl peak — confirms the 2-chloroacetate group.
1602	Medium	C=C (aromatic)	Vibrational mode of the naphthalene ring
1506, 1456	Medium	C=C (aromatic)	Resonance peaks typical of aromatic systems
1272, 1224	Strong	C–O–C stretching (ester)	Stretching vibrations of the ester oxygen atoms
1061	Medium	C–Cl	Vibration of the C–Cl bond in the chloroacetate chain
840, 758	Strong	Ar–H out-of-plane	Out-of-plane bending of aromatic hydrogen atoms (distinct for naphthalene)

CONCLUSION

In this study, the synthesis of 3-hydroxy-3-((2-(naphthalen-2-yloxy)-2-oxoethoxy)carbonyl)pentanedioic acid was successfully achieved through the reaction of 2-naphthyl chloroacetate with the monosodium salt of citric acid under mild conditions. The influence of various reaction parameters, including molar ratios, temperature, and reaction time, was systematically investigated. It was found that a 2:1 molar ratio of 2-naphthyl chloroacetate to sodium citrate, combined with a reaction temperature of 70–80 °C and a duration of 6 hours, afforded the highest yield of 83%.

FUTURE WORK / REFERENCES

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