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Non-linear optical properties of arylfuranylpropenones

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Abstract

A series of arylfuranylpropenones 3a-i were synthesized by the reaction of 5-(2-nitro-4-methoxyphenyl)-2-furfural 1 with various acetophenones 2 by Claisen–Schmidt condensation. All the newly synthesized chalcones were characterized by elemental analysis and spectral studies. Most of them showed SHG conversion efficiency in powder form.

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Keywords: A2. Claisen–Schmidt condensation; B1. Arylfuranylpropenones; B2. Non-linear optical materials

1. Introduction

Non-linear optical materials are expected to be active materials for optical communications and optical electronic devices. The most commonly used non-linear optical crystals in bulk form are inorganic crystals such as ADP, KDP, ADA, LiNbO₃, etc. Several organic molecular crystalline materials have also been identified as high performance, second-order, optically non-linear crystals [1–3]. The second-order NLO effects in organic molecules originate from a strong donor–acceptor intramolecular interaction. Organic crystals hold promise because of the large variety of such materials and the potential to synthesize molecules according to some design principles. As a result, there have been extensive efforts at developing such materials for application in non-

linear optics [4,5]. The second-order non-linear optical property of an organic compound is derived from conjugated delocalized π electrons. Among many organic compounds reported for their second harmonic generation [6–15], propenone derivatives are noticeable materials for their excellent blue light transmittance and good crystallizability [16–19].

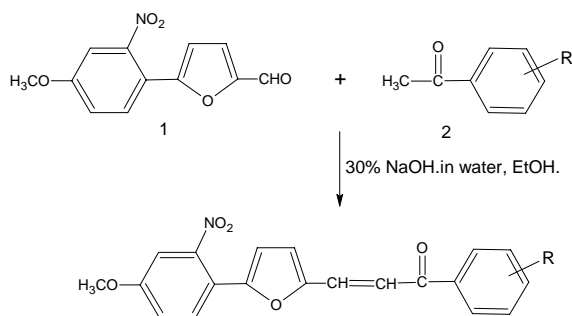
The required 1-aryl-3-[5-(2'-nitro-4'-methoxyphenyl)-2-furyl]-2-propen-1-ones 3a-i were synthesized by the reaction of 2-nitro-4-methoxyphenylfurfural 1 with various acetophenones 2 by Claisen–Schmidt condensation, as shown in Scheme 1. 2-Nitro-4-methoxyphenylfurfural was synthesized by Meerwein reaction.

2. Experimental procedure

Melting points were determined by capillary method and are uncorrected. The IR spectra (in

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Scheme 1.

KBr pellets) were recorded on a Shimadzu FT-IR 157 spectrophotometer. ^1H NMR spectra were recorded either on a Perkin–Elmer EM-300 MHz or on a Bruker WH-200 MHz NMR spectrometer using TMS as an internal standard. The purity of the compounds was checked by thin layer chromatography (TLC) on silica gel plates.

2.1. Synthesis and characterization of chalcones

2.1.1. General procedure

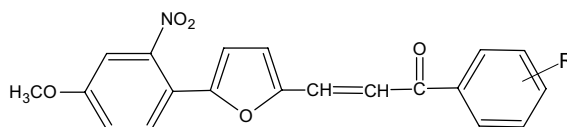
To a mixture of suitably substituted acetophenone (10 mmol) and 5-(2-nitro-4-methoxyphenyl)-2-furfural solution, sodium hydroxide (5 ml, 30%) was added with continuous stirring. The clear solution so obtained was left for 4 h at room temperature with stirring and was allowed to stand overnight. The solid which separated on standing out was filtered off, dried and recrystallized from a suitable solvent.

The IR spectrum of compound 3c showed prominent absorption bands at 3100 cm^{-1} (C–H

str.) $1529\text{ (NO}_2\text{ asym)}$, $1473\text{ (NO}_2\text{ sym)}$, 1646 (C=O str.) , 1603 (C=O) .

In the 300 MHz ^1H NMR of compound 3b, a sharp singlet was observed at δ 3.9 integrating for three protons which corresponds to of the *p*-methoxy protons. Two doublets appeared in the region δ 6.6–6.7 ($J = 3\text{ Hz}$) and 6.8–6.9 ($J = 3\text{ Hz}$) corresponding to the two β -protons of furan ring. The olefinic protons resonated as two doublets at δ 7.05 and δ 7.1, respectively, integrating for two protons. The *p*-chlorophenyl proton signals appeared as two distinct doublets at δ 7.25 and δ 7.45, respectively, each integrating for two protons. The remaining aromatic protons of the phenyl ring appeared as multiplets in the region δ 7.5–8.0, respectively.

2.1.2. General structure



2.1.3. NLO property studies

The arylfuranylpropenone derivatives absorb light in the UV region and transmit in the remaining region. The SHG conversion efficiency of the compounds was measured by powder technique using Nd:YAG laser. The laser power was 13 mJ/s and the wavelength was $1.064\text{ }\mu\text{m}$. The SHG conversion efficiency and the wavelength for the maximum absorption (λ_{max}) of the compounds are given in Table 1.

Table 1
Characterization data of 1-aryl-3-[5-(2'-nitro-4'-methoxyphenyl)-2-furyl]-2-propene-1-ones (3)

Comp no	R	% yield	m.p. ($^{\circ}\text{C}$)	SHG (\times urea)	λ_{max} (nm)	Nature of compound	Molecular formula
3a	H	84	115	Weak	390	White micro crystals	$\text{C}_{20}\text{H}_{15}\text{NO}_5$
3b	4-Cl	90	138	0.739	439	Yellow micro crystals	$\text{C}_{20}\text{H}_{14}\text{ClNO}_5$
3c	4-OCH ₃	80	140	Weak	421	Pale yellow micro crystals	$\text{C}_{21}\text{H}_{17}\text{NO}_6$
3d	2,4-Cl ₂	72	200	Weak	407	White micro crystals	$\text{C}_{20}\text{H}_{13}\text{Cl}_2\text{NO}_5$
3e	4-NO ₂	78	163	Weak	413	Pale yellow micro crystals	$\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_7$
3f	4-Br	86	155	0.623	423	White micro needles	$\text{C}_{20}\text{H}_{14}\text{BrNO}_5$
3g	3Cl, 4F	74	158	Weak	401	Yellow micro crystals	$\text{C}_{20}\text{H}_{13}\text{ClFNO}_5$
3h	4-OH	65	132	0.98	430	Pale yellow micro crystals	$\text{C}_{20}\text{H}_{15}\text{NO}_6$
3i	2-OH	58	143	Weak	398	Pale yellow micro crystals	$\text{C}_{20}\text{H}_{15}\text{NO}_6$

3. Conclusion

Nine newly synthesized arylfuranylpropenones (3a-i) were subjected to NLO property studies. The compounds showed good crystalline property and absorb light in the UV region. Among the tested compounds three propenones showed SHG conversion efficiency in powder form. All the three active propenones possessed only a para substituent at aryl moiety. Other propenones possessing disubstituted aryl ring and ortho substituted aryl rings exhibited only weak SHG conversion efficiency.

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