

Synthesis, characterisation and thermal stability of 2-ferrocenylidene (1-tetralone), 2-ferrocenylideneindan-1,3-dione, diferrocenylidenecyclohexanone and diferrocenylidenecyclopentanone

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Abstract

Purpose – To discuss synthesis and evaluation of organo-metallic chalcones as second-order nonlinear optical (SONLO) materials.

Design/methodology/approach – The new chalcones have been synthesised via Knoevenagel reactions of ferrocen carboxaldehyde with two active methylene compounds.

Findings – The ferrocenyl chalcones prepared have shown bathochromic shift and thermal stability in polymeric film. On heating the dye films up to 80°C the extent of degradation reached up to 12 per cent and very small amount of degradation was observed at 43 and 60°C.

Originality/value – The paper shows that these compounds have UV-Vis bathochromic shift, enabling them to be used as SONLO materials in the blue domain as well as dyes.

Keywords Thermal stability, Optical properties of materials, Organometallic compounds

Paper type Research paper

Introduction

Mankind has been interested in light and its interaction with matter since ancient times. In our modern society, light is not limited to the scientific society but has grown immensely to encompass many kinds of application, such as optical communication, medical surgery and diagnostics using optical tools and techniques. With the advent of lasers, the search for new nonlinear materials took on a great momentum. The ability to manipulate frequency, phase, polarization or path of light has an important utilisation such as production of tuneable laser light, data storage and solar protection. Currently, research being devoted to organic and organometallic materials that exhibits nonlinear optical (NLO) effects, especially second harmonic generation (SHG) which causes doubling the frequency of light. (Burland, 1994; Chemla and Zyss, 1987; Williams, 1985; Zyss, 1994; Asiri *et al.*, 2005; Long, 1995). The criteria for constructing an SHG device with large (β) hyperpolarizability, the molecule needs to be a noncentrosymmetric so that their NLO properties do not cancel out and small energy gap (Long, 1995).

During the last two decades, organometallic compounds have shown to be good candidates for NLO especially SHG (Green *et al.*, 1987). For example, compound **A** (Figure 1) with 3-dicyanomethylidene-2,3-dihydrobenzothiophene-1,1-dioxide as acceptor has a $\mu\beta$ value of $(11,200 \times 10^{-48}$ esu) (Alain *et al.*, 1996a, b) and compound **B** (Figure 1) with 1,3-bis(dicyanomethylidene)indane as acceptor has a $\mu\beta$ value of $(8,720 \times 10^{-48}$ esu) (Janowska *et al.*, 2006) as determined with electric field induced second harmonic (EFISH) technique. In these types of compounds, one expects additional behaviour to mixing with the metal states, thus a methyl substituted at the cyclopentadienyl ring should increase the dipole moment as well as nonlinearity by making the donor component electron rich.

“Push-pull” compounds with ferrocenyl (Fc) donor group linked to a conjugated polyenic chain capped by an acceptor moiety **A**, (Fc- π -**A**), have shown to be good candidates as second-order nonlinear optical (SONLO) chromophores (Di Bella, 2001). We have recently synthesised and characterised NLO materials containing Fc as a donor and barbituric and thiobarbituric acids as acceptor with conjugated moieties and with moderate solubility in polar organic solvents (Asiri, 2001; Asiri and Al-Amoudi, 2006). In this paper, we report our study of “push-pull” compounds containing Fc donor group bound to a conjugated chain capped by an acceptor ketone moiety **A**, of the form (Fc- π -**A**) and (Fc- π -**A**- π -Fc) (Figure 2).

Experimental

Melting points were recorded on a Thomas-Hoover capillary melting apparatus without correction. IR spectra were taken as

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