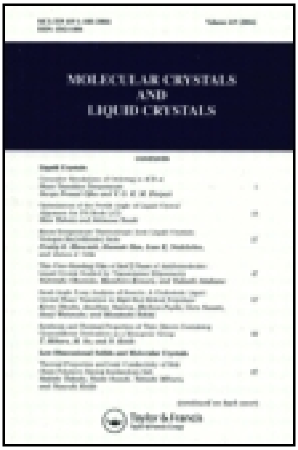

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

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Version of record first published: 24 Sep 2006

To cite this article: Hee-Gweon Woo, Sun-Jung Song, Bo-Hye Kim & Sock-Sung Yun (2000): Dehydrocoupling Synthesis and Optoelectronic Properties of Polysilole, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 349:1, 87-90

To link to this article: http://dx.doi.org/10.1080/10587250008024872

Mol. Cryst. Liq. Cryst., 2000, Vol. 349, pp. 87-90
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Dehydrocoupling Synthesis and Optoelectronic Properties of Polysilole

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Dehydrocoupling of 2,3,4,5-tetraphenylsilole dihydride **1** with various inorganic hydrides (such as Red-Al, N-Selectride, and super-hydride) produces polysiloles **2** in high yields. The polysiloles emit green light at 520 nm and are electroluminescent at 520 nm.

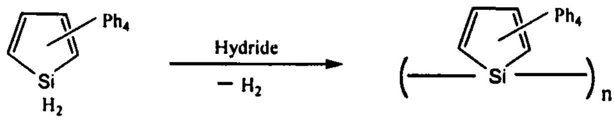
Keywords: dehydrocoupling; silole dihydride; polysilole; photoluminescence; electroluminescence; green light

INTRODUCTION

Silole is a silicon-containing five-membered cyclic diene, and it has attracted considerable attention because of its peculiar electronic properties [1] and potential application as electron-transporting materials in devices such as light-emitting diodes (LED's) [2]. The high electron-accepting ability of the silole ring attributed to the $\sigma^* - \pi^*$ conjugation arising from the interaction between the σ^*-orbital of the σ-bonded silicon atom and the π^*-orbital of the butadiene moiety of the ring [3-5]. Silicon-catenated polysiloles are regarded as a new class of polysilanes with $\sigma^* - \pi^*$ conjugation between the σ^*-orbital delocalized over the polysilane main chain and the π^*-orbital localized on the *cis*-butadiene moiety in every silole ring [6]. West *et al.* recently prepared polysiloles in about 30% yield from the reductive dehalocoupling of 1,1-dichlorotetraphenylsilole with lithium, sodium, and potassium [7]. In this paper we report the effective synthesis and optoelectronic properties of polysilole.

RESULTS AND DISCUSSION

Polysiloles **2** have been easily synthesized from the dehydrocoupling of **1** using various hydrides in high yields.



1 **2**

In a typical procedure, to a Schlenk flask containing **1** (0.50 g, 0.29 mmol) in THF (2.00 mL) was injected Red-Al (or Vitride; $Na[H_2Al(OCH_2CH_2OMe)_2]$) at 25 ℃. The reaction immediately turned burgundy with vigorous gas evolution and finally yielded clear orange solution. After 24 hour, the mixture was passed rapidly through a silica gel column (10 x 2 cm) using 100 mL THF as an eluent. Removal of the volatile materials under reduced pressure gave 0.42 g (84% yield) of **2** as light yellow powder. ^1H NMR ($CDCl_3$, 300 MHz, δ ppm): 4.46 (s, SiH), 6.80 - 7.40 (m br, Ph); ^{13}C NMR ($CDCl_3$, 300 MHz, δ ppm): 125.8 - 131.7, 137.0 - 140.0 (m br, Ph); IR (KBr pellet, cm^{-1}): 2130 (υ_{Si-H}); GPC M_w = 4100, M_n = 3900, M_w/M_n = 1.1; UV (THF, λ_{max}, nm): 300. Similarly, the dehydrocoupling reactions of **1** with N-selectride and super-hydride were also carried out. The results are summarized in Table 1.

TABLE 1. GPC characterizations for the dehydrocoupling reactions of **1** with hydrides[a]

Hydrides[b]	% Yield	Mol. wt.[c] M_w	M_n	M_w/M_n
Red-Al	84	4100	3900	1.1
N-Selectride	82	4800	4000	1.2
Super-Hydride	87	5800	4790	1.2

[a] Stirred at 25 ℃ for 24 h. [b] [Silole]/[Hydride] = 2.0.
[c] Determined by GPC in THF (*vs* polystyrene).

The weight average molecular weights of the obtained polysiloles are ranged from 4000 to 5000. These polysiloles have characteristic absorption around 300 nm, assigned to the σ - σ^*

transition of the Si-Si backbone chain in the UV absorption spectra, and are photoluminescent, emitting green light at 520 nm where the excitation was at 330 nm. Especially, these polymers are strongly electroluminescent around 520 nm. The LEDs (active area: 2.4 × 3 mm^2) were prepared by the spin-coating of **2** on a clean ITO glass plate (resistance: 300 hm/cm^{-2}) and the subsequent vacuum-depositon of an Mg:Ag layer as a cathode at a pressure of 1 × 10^{-6} torr. The LEDs were operated at 100 μA pulse current. The EL spectrum and the absorption/photoluminescence spectra of polysilole are shown in Figure 1 and Figure 2, respectively.

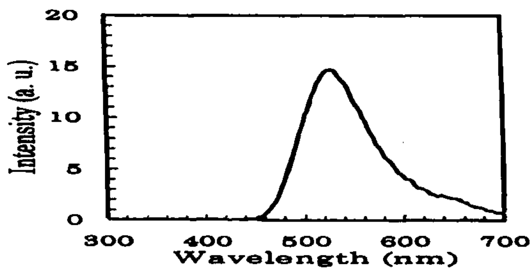


FIGURE 1. Electroluminescence spectrum of **2** at 25 ℃.

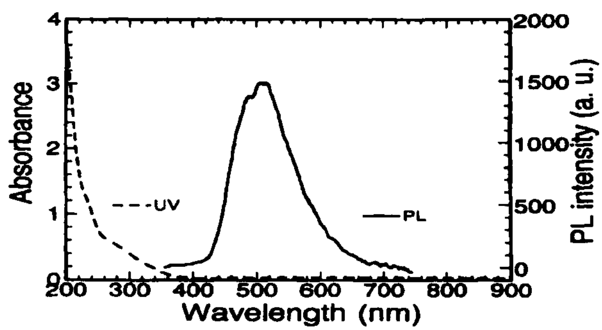


FIGURE 2. Absorption and photoluminescence spectra of **2** at 25 ℃.

Acknowledgments

This research was supported partly by the Korea Science & Engineering Foundation (1999) and partly by the Korea Research Foundation through the International Collaborative Research Program (1998). The authors greatly acknowledge the experimental assistance of Dr. Honglae Sohn in UC San Diego.

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