

**Electronic supplementary information for**

**Electron-deficient Acene-based Liquid Crystals:  
Dialkoxydicyanopyrazinoquinoxalines**

Takashi Takeda,<sup>a\*</sup> Jun'ya Tsutsumi,<sup>b</sup> Tatsuo Hasegawa,<sup>b</sup> Shin-ichiro Noro,<sup>c</sup> Takayoshi Nakamura<sup>c</sup> and Tomoyuki Akutagawa<sup>a\*</sup>

<sup>a</sup> Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Miyagi 980-8577, Japan

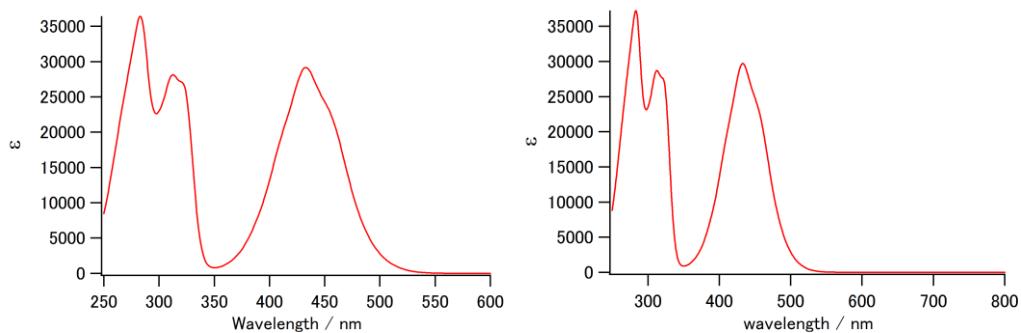
<sup>b</sup> National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8562, Japan

<sup>c</sup> Research Institute for Electronic Science, Hokkaido University, Sapporo, Hokkaido 001-0020, Japan

**CONTENTS**

	Page
1. UV-Vis spectra of 1a and 1c .....	S2
2. Redox potentials of 1 and cyclic voltammogram of 1b .....	S2
3. XRD patterns and schematic representation of molecular arrangements of 1b .....	S3
4. Polarized optical microscope images of 1c in heating and cooling process .....	S3
5. <sup>1</sup> H and <sup>13</sup> C NMR spectra of 1a-c .....	S4
6. References .....	S7

## 1. UV-Vis spectra of **1a** and **1c**



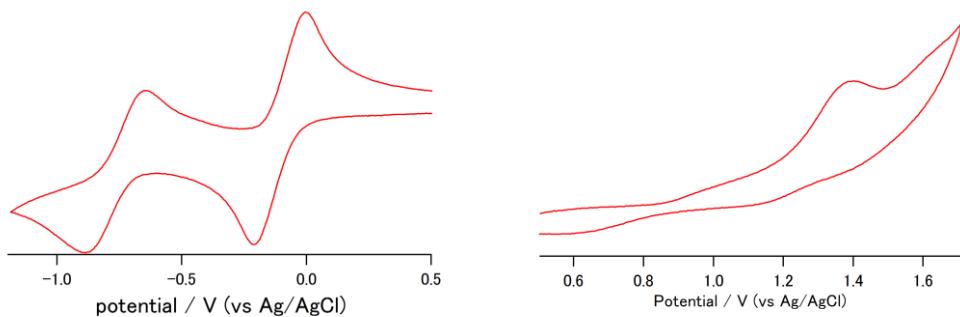
**Figure S1** UV-Vis spectra of **1a**(left) and **1c** (right) in  $\text{CH}_2\text{Cl}_2$ .

## 2. Redox potentials of **1** and cyclic voltammogram of **1b**

**Table S1** Redox potential of **1a-e<sup>a</sup>**

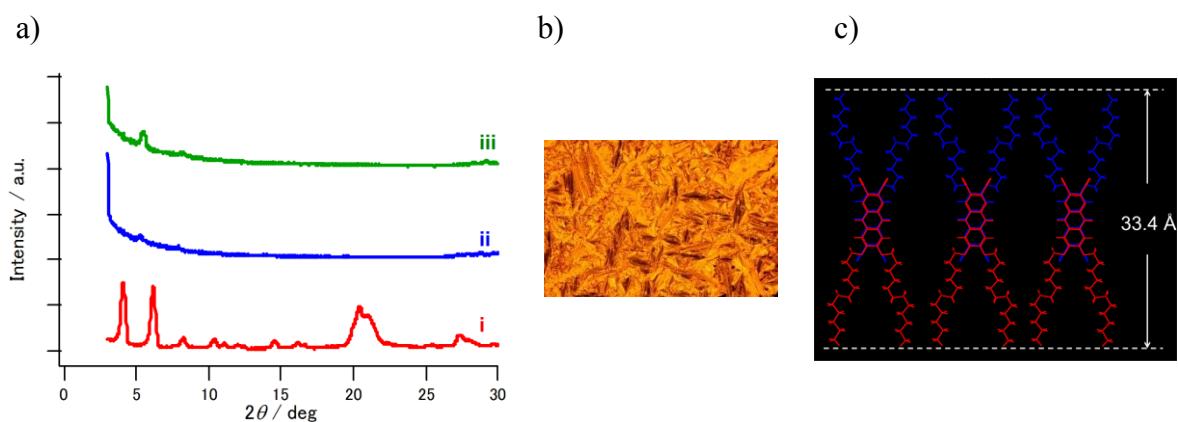
Compd	$E_{\text{red}1}, \text{V}^{-1}$	$E_{\text{red}2}, \text{V}^{-1}$	$E_{\text{ox}}, \text{V}^{-1}$	LUMO <sup>b</sup> , eV <sup>-1</sup>	HOMO <sup>c</sup> , eV <sup>-1</sup>
<b>1a<sup>d</sup></b>	-0.11	-0.87	1.39	-4.12	-5.26
<b>1b<sup>d</sup></b>	-0.11	-0.76	1.40	-4.12	-5.36
<b>1c<sup>d</sup></b>	-0.10	-0.87	1.41	-4.15	-5.27
<b>1d<sup>e, S1</sup></b>	-0.03	-0.87			
<b>1e<sup>e, S1</sup></b>	-0.27	-0.98			

a: Measured in  $\text{CH}_2\text{Cl}_2$  containing 0.1M  $\text{Bu}_4\text{NBF}_4$ . b:  $E_{\text{LUMO}} = -[4.8 - E_{1/2, \text{Fc/Fc+}} + E_{\text{red, onset}}]^{S2}$ ; c:  $E_{\text{HOMO}} = -(4.8 - E_{1/2, \text{Fc/Fc+}} + E_{\text{ox, onset}})$ ; d: vs Ag/AgCl ; e: vs SCE



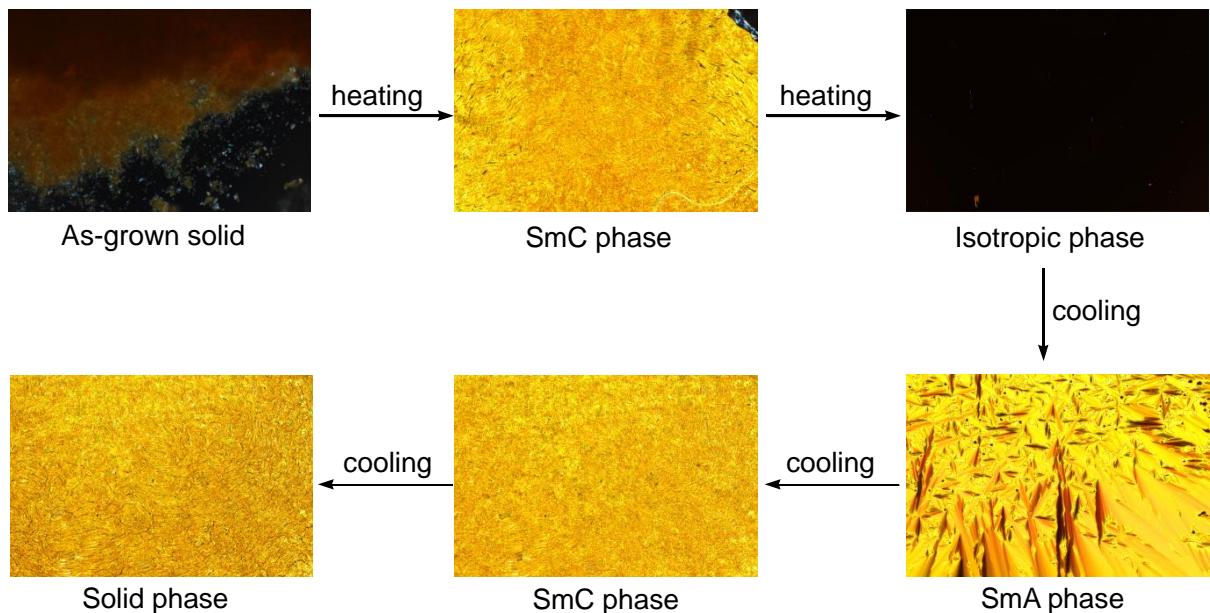
**Figure S2** Cyclic voltammograms of **1b**.

### 3. XRD patterns and schematic representation of molecular arrangements of **1b**



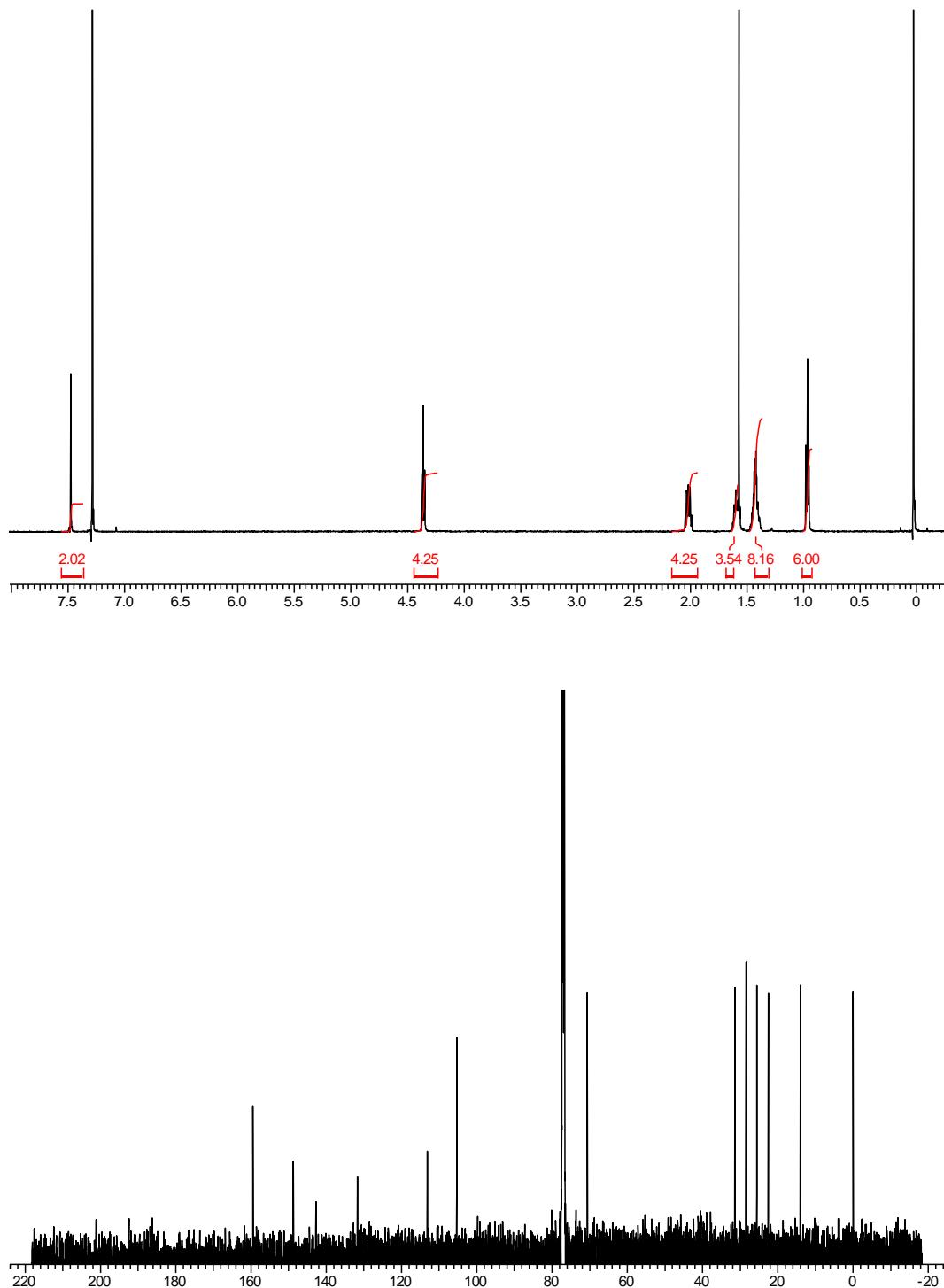
**Figure S3** Molecular orientations of **1b** in solid and SmA phases. a) Temperature dependent XRD patterns of as-grown solid at 303 K (i), SmA phase at 438 K (ii), and solid phase after the SmA phase at 303 K (iii). b) Polarized optical microscope image of SmA phase of molecule **1b**. c) Schematic representation of possible molecular arrangements SmA phase of **1b**.

### 4. Polarized optical microscope images of **1c** in heating and cooling process

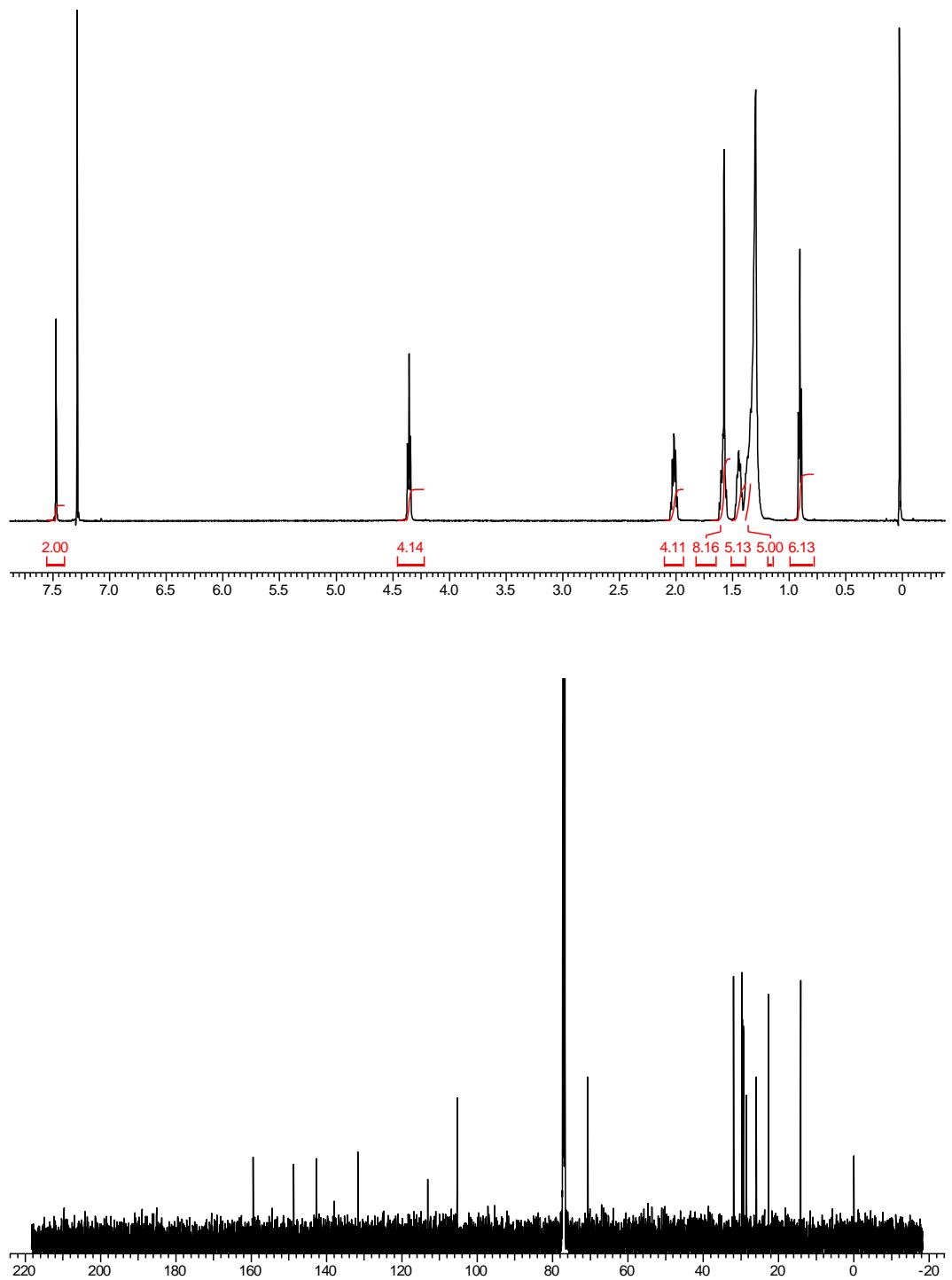


**Figure S4** Polarized optical microscope images of **1c** in heating and cooling process.

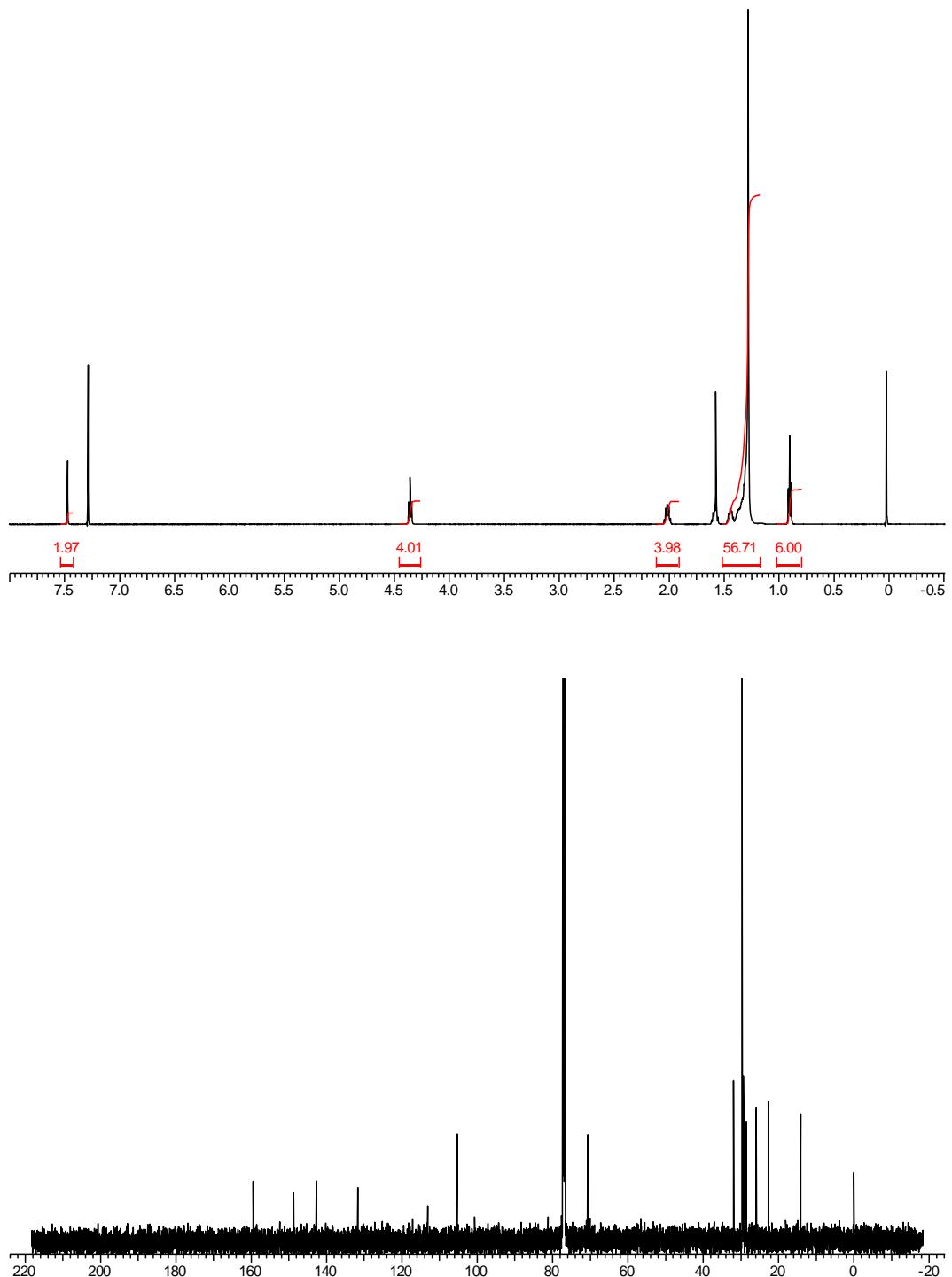
**5.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of 1a-c**



**Figure S5**  $^1\text{H}$  (top) and  $^{13}\text{C}$  (bottom) NMR spectra of **1a**.



**Figure S6**  $^1\text{H}$  (top) and  $^{13}\text{C}$  (bottom) NMR spectra of **1b**.



**Figure S7**  $^1\text{H}$  (top) and  $^{13}\text{C}$  (bottom) NMR spectra of **1c**.

## **6. References**

- S1. J. Nishida, S. Murai, E. Fujiwara, H. Tada, M. Tomura, Y. Yamashita *Org. Lett.* **2004**, *6*, 2007–2010.
- S2. Y. Liu, M. S. Liu and A. K.-Y. Jen *Acta Polym.* **1999**, *50*, 105–108.