

Supporting Information for

Alkyne [2 + 2 + 2] Cyclotrimerization Catalyzed by a Low-Valent Titanium Reagent Derived from CpTiX₃ (X = Cl, O-*i*-Pr), Me₃SiCl, and Mg or Zn

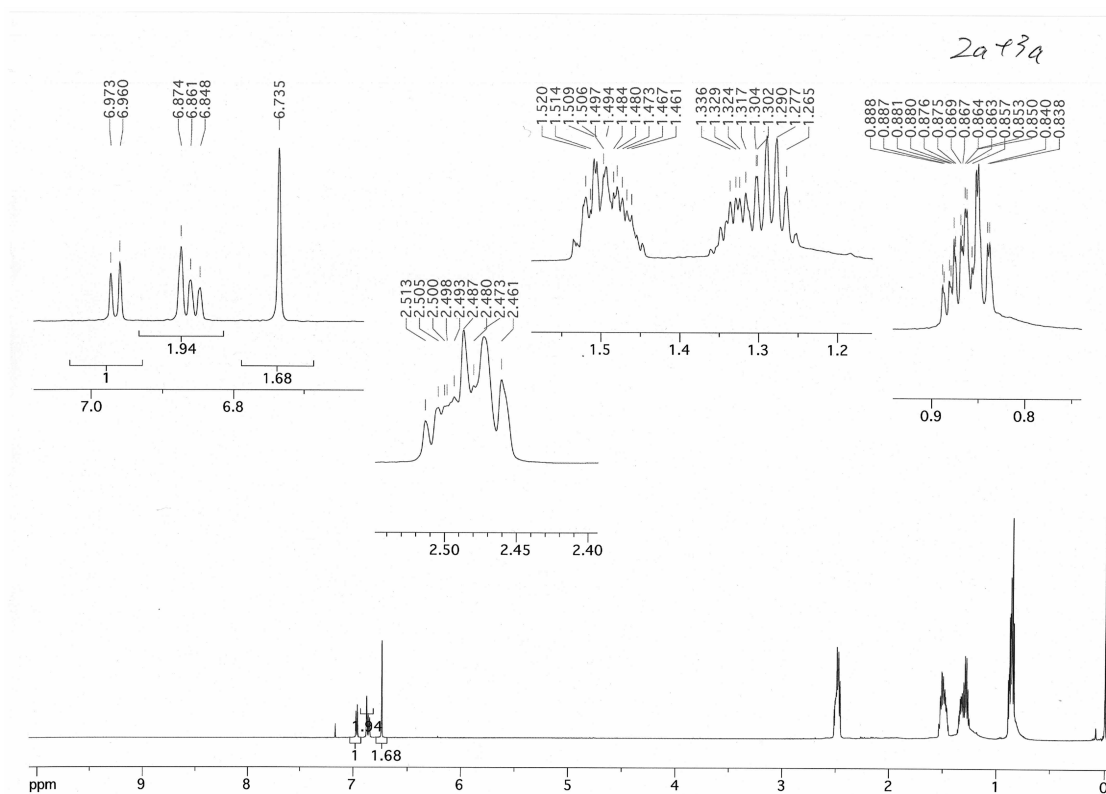
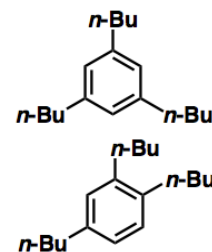
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3-27-1 Rokkakubashi, Kanagawa-ku, Yokohama 221-8686, Japan.

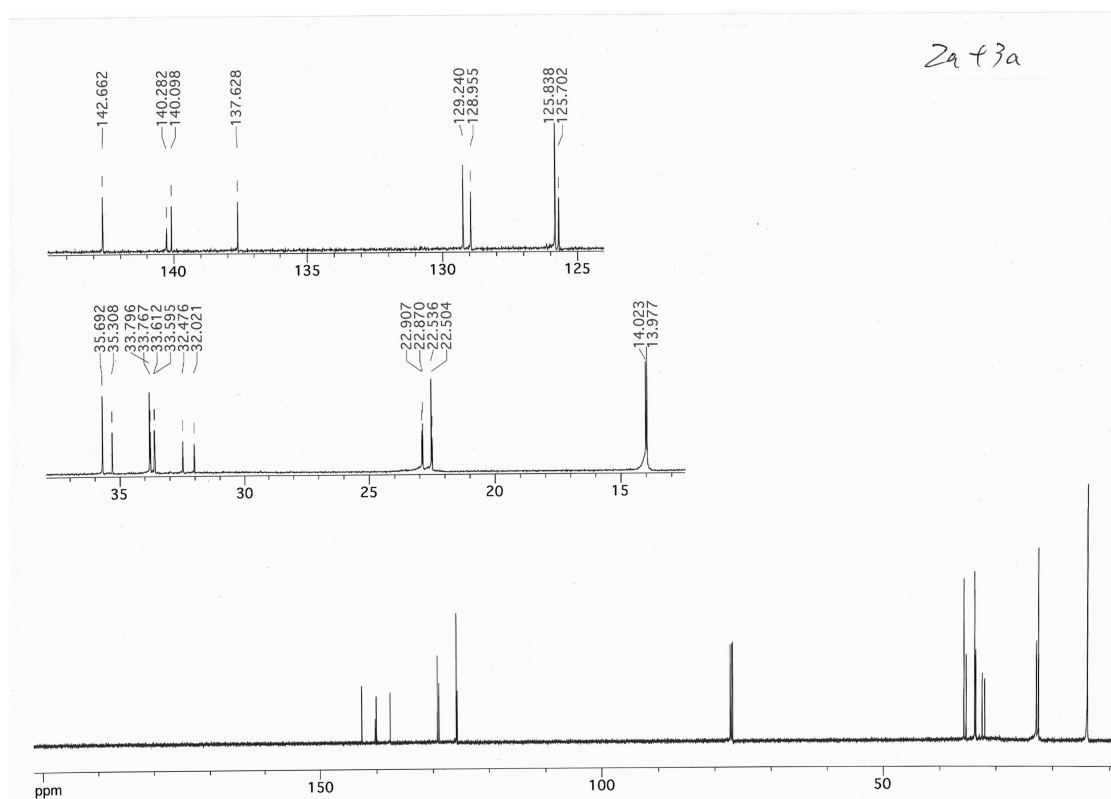
Fax: (+81)-45-413-9770; e-mail: okamos10@kanagawa-u.ac.jp

S1 NMR spectra of a mixture of compounds 2a and 3a

S1-1 ^1H NMR Compounds 2a and 3a (CDCl_3)

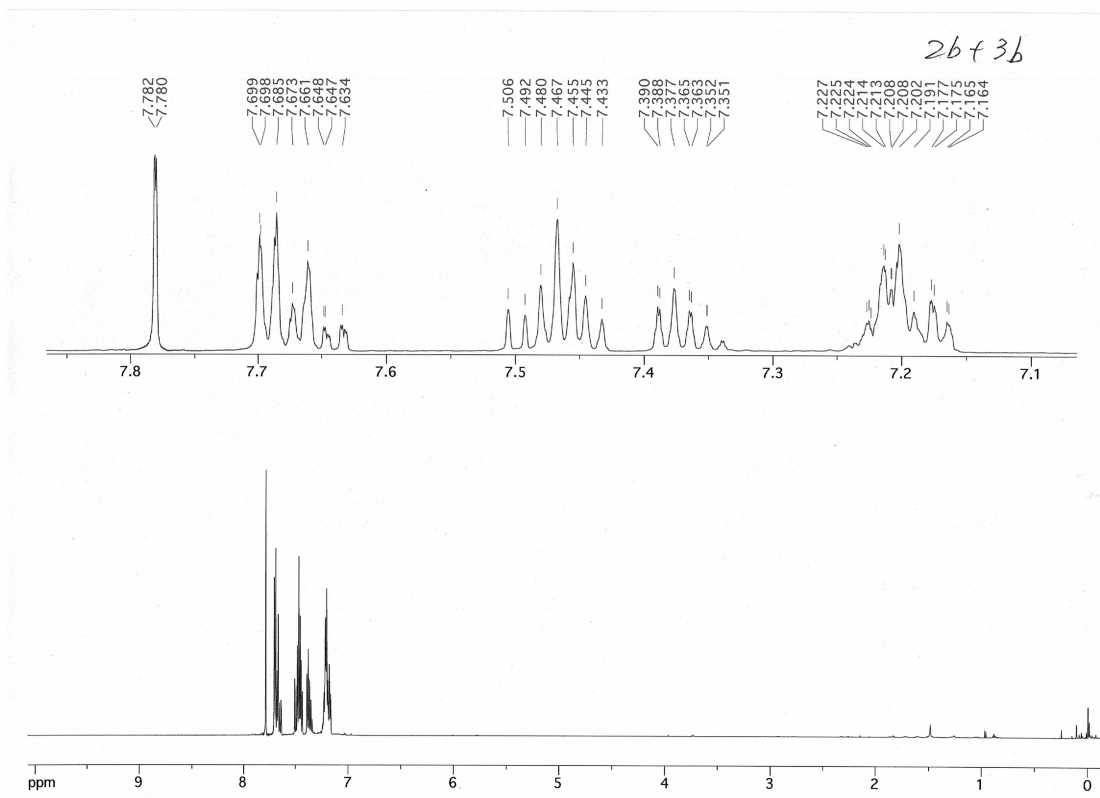
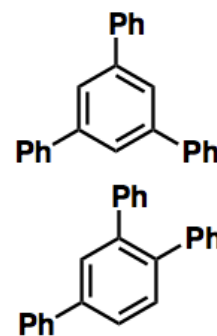


S1-2 ^{13}C NMR Compounds 2a and 3a (CDCl_3)

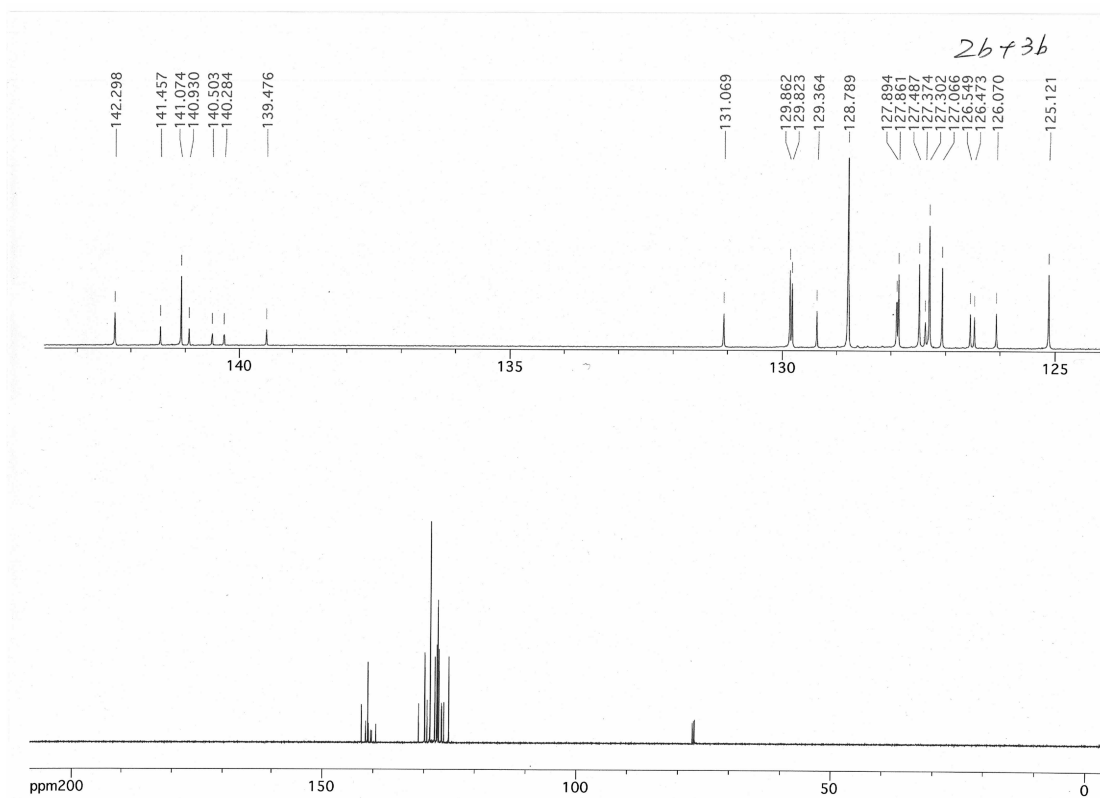


S2 NMR spectra of a mixture of compounds 2b and 3b

S2-1 ^1H NMR Compounds **2b** and **3b** (CDCl_3)

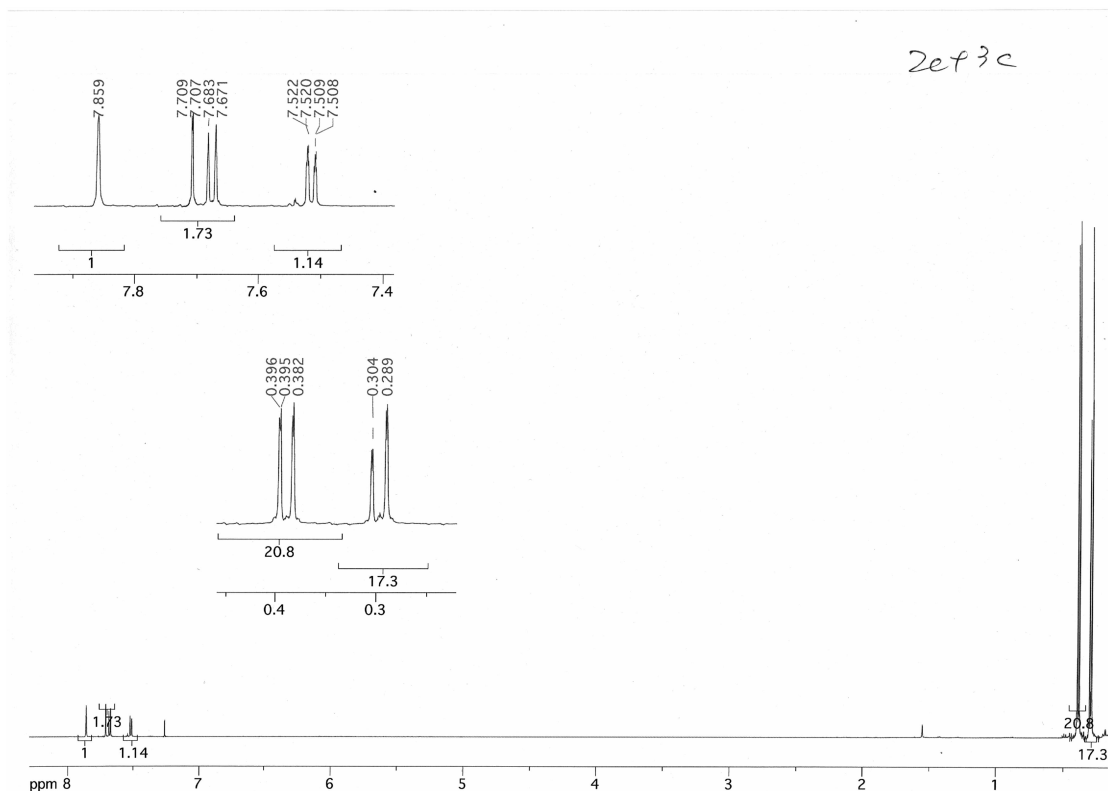


S2-2 ^{13}C NMR Compounds **2b** and **3b** (CDCl_3)

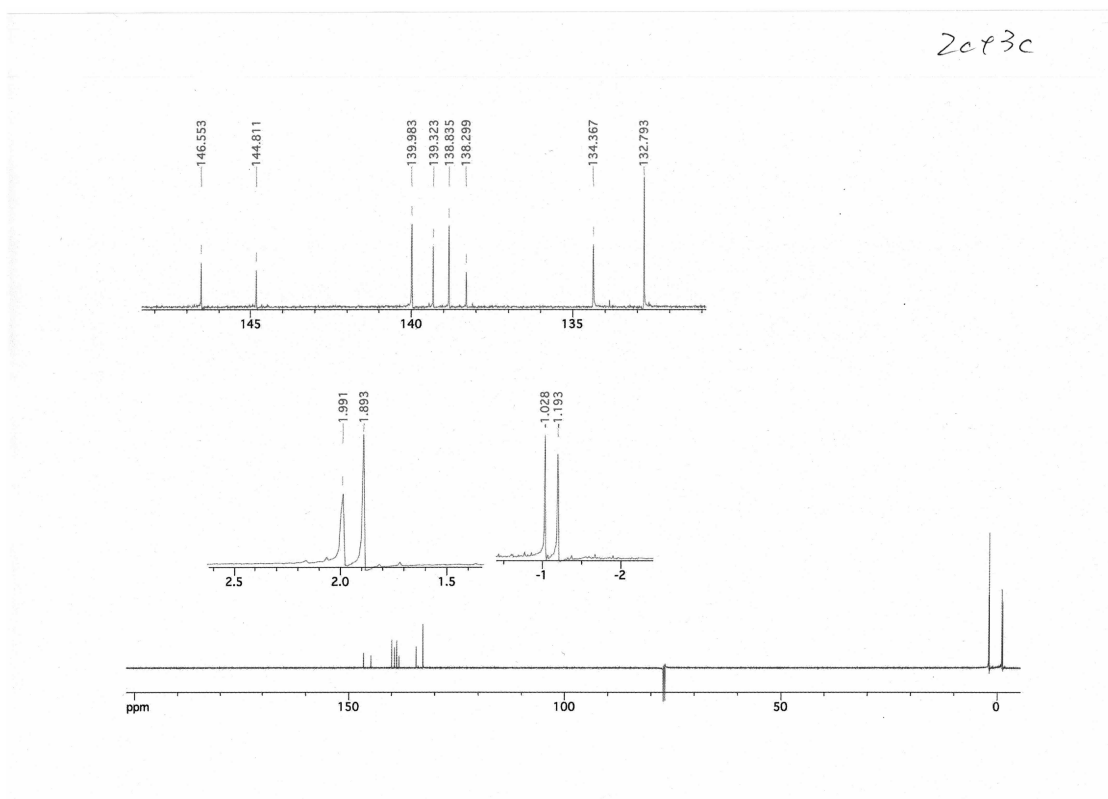


S3 NMR spectra of a mixture of compounds 2c and 3c

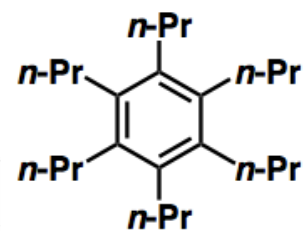
S3-1 ^1H NMR Compounds **2c** and **3c** (CDCl_3)



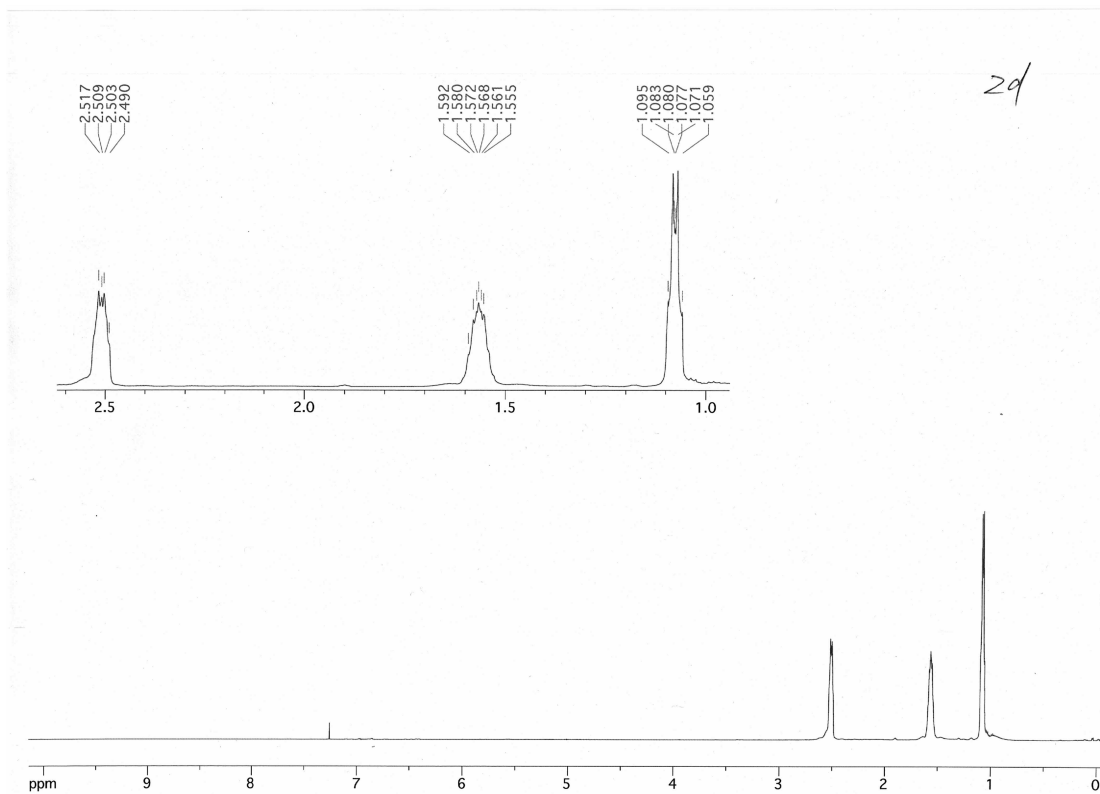
S3-2 ^{13}C NMR Compounds **2c** and **3c** (CDCl_3)



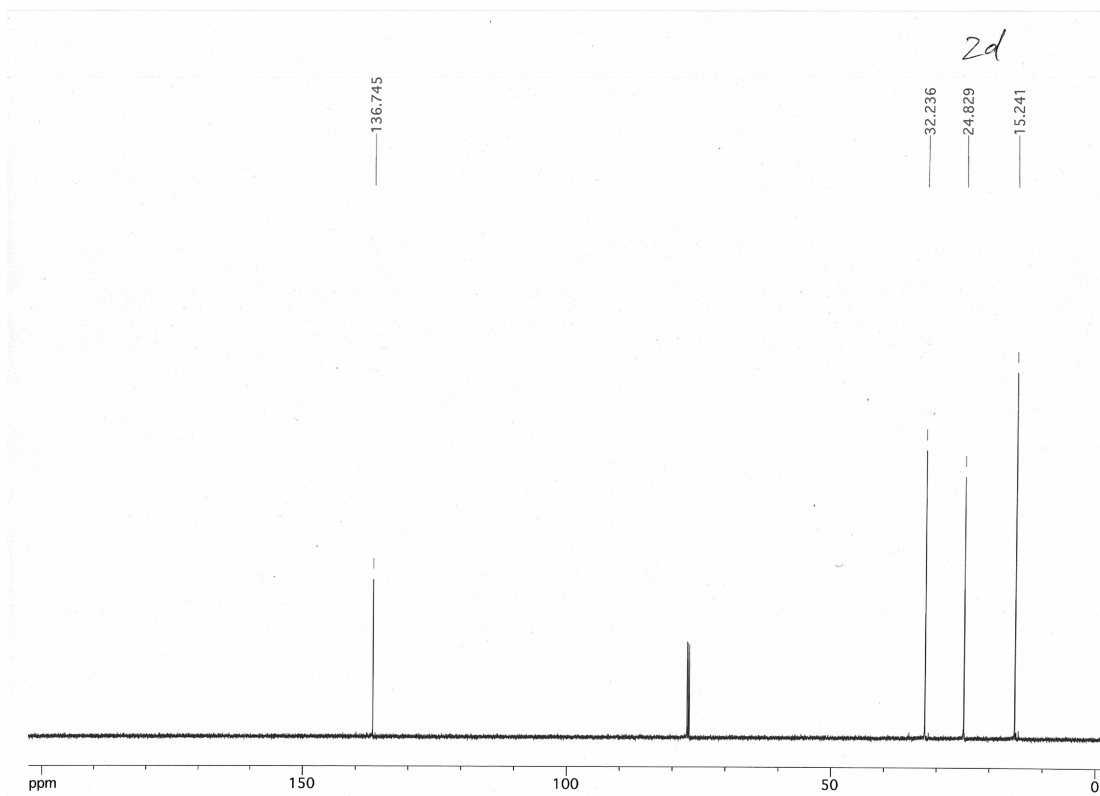
S4 NMR spectra of compound 2d



S4-1 ^1H NMR Compounds **2d** (CDCl_3)

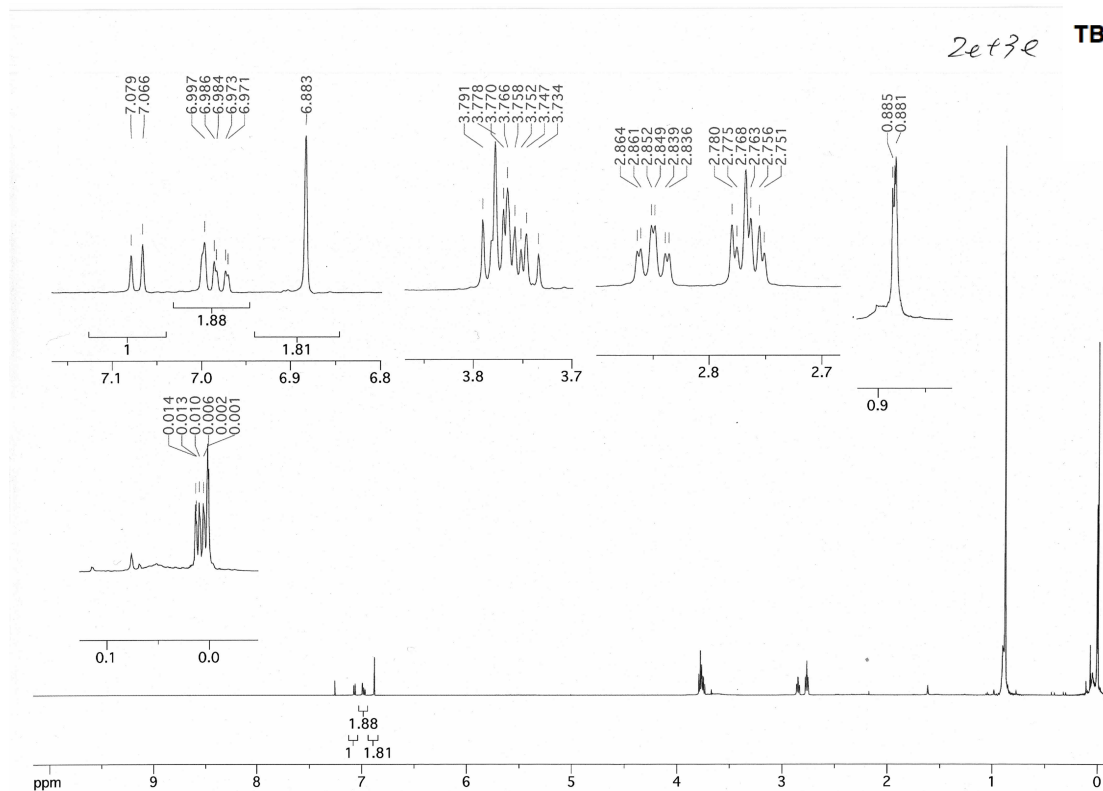


S4-2 ^{13}C NMR Compounds **2d** (CDCl_3)

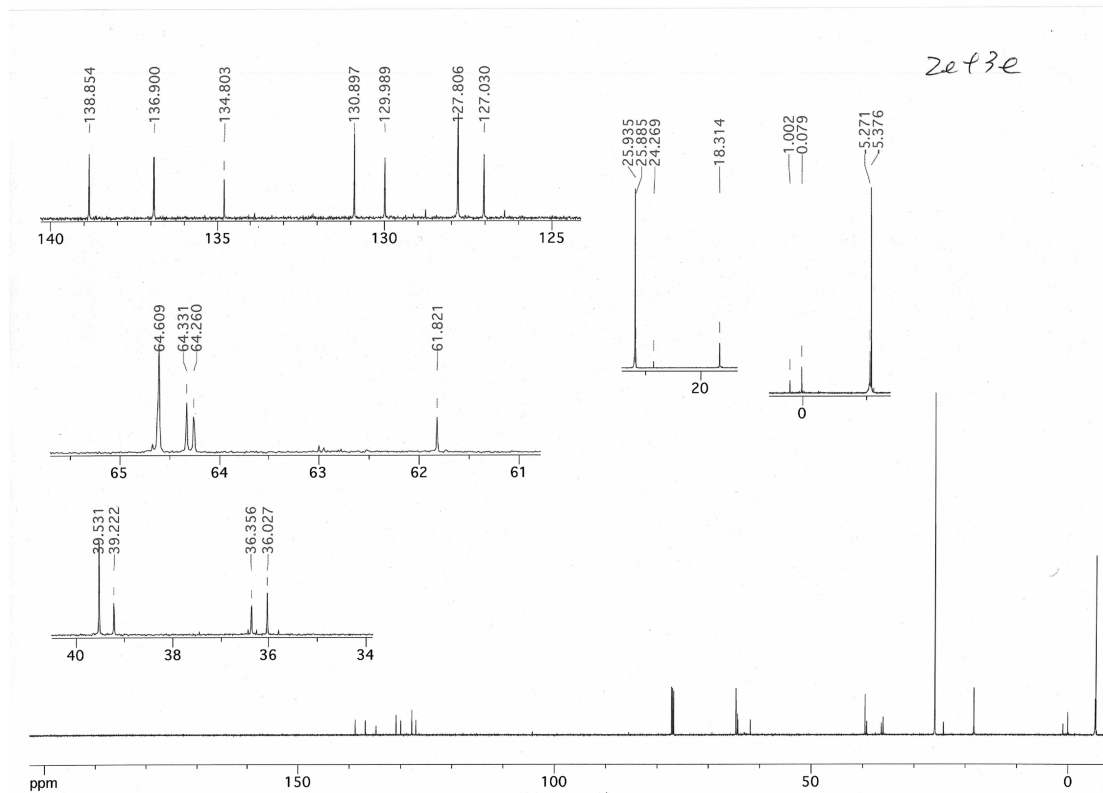


S5 NMR spectra of a mixture of compounds 2e and 3e

S5-1 ^1H NMR Compounds **2e** and **3e** (CDCl_3)

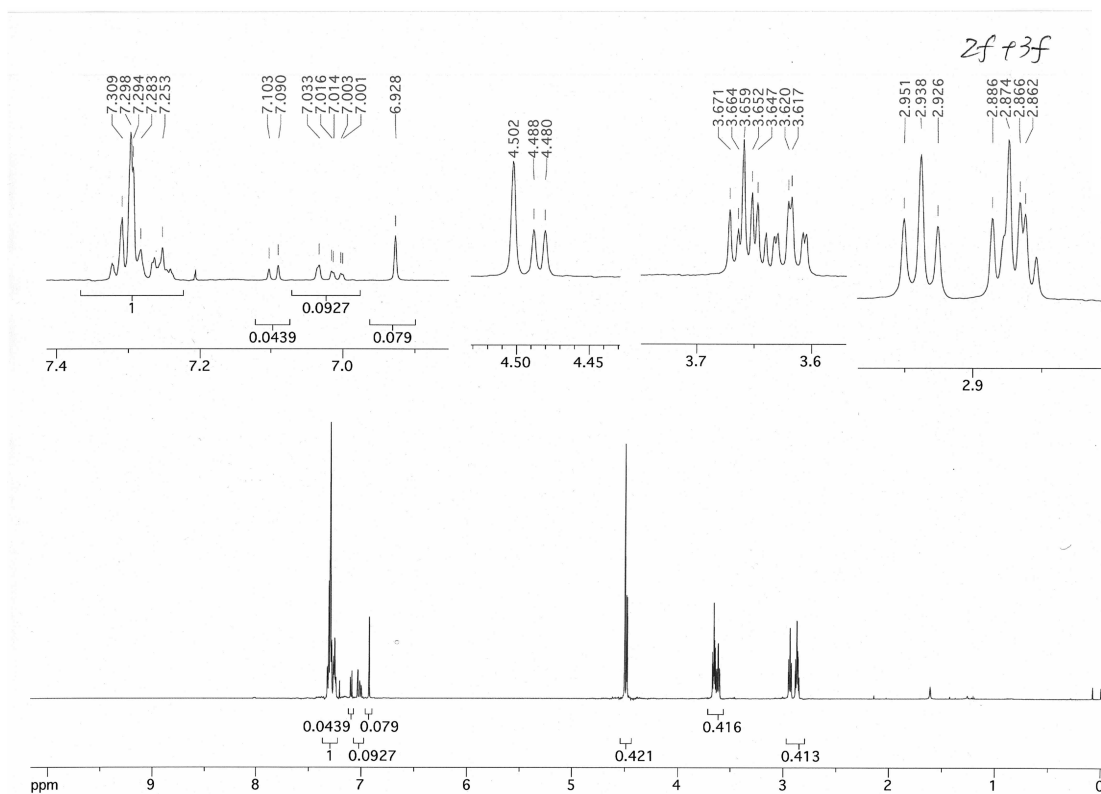


S5-2 ^{13}C NMR Compounds **2e** and **3e** (CDCl_3)

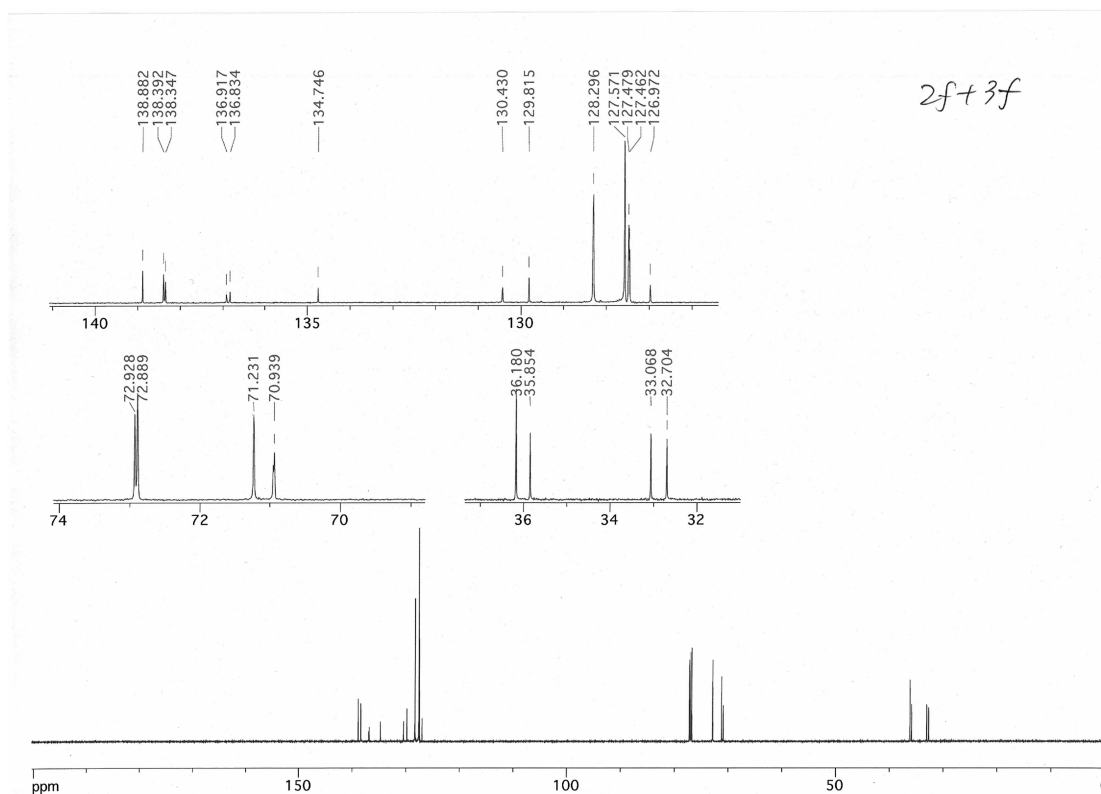


S6 NMR spectra of a mixture of compounds 2f and 3f

S6-1 ^1H NMR Compounds 2f and 3f (CDCl_3)

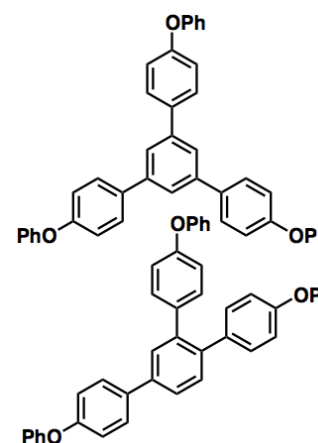


S6-2 ^{13}C NMR Compounds 2f and 3f (CDCl_3)



S7

S7-1

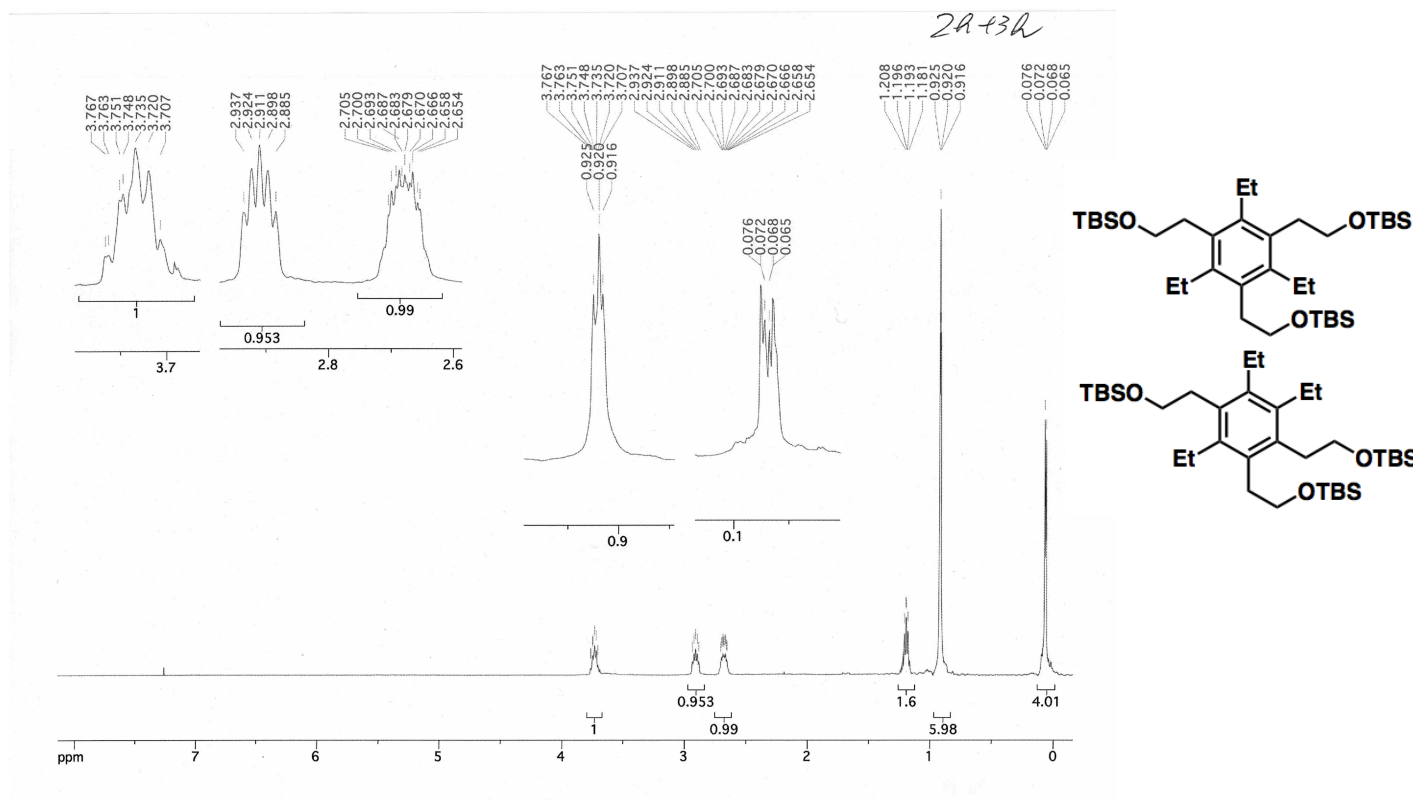


S7-2

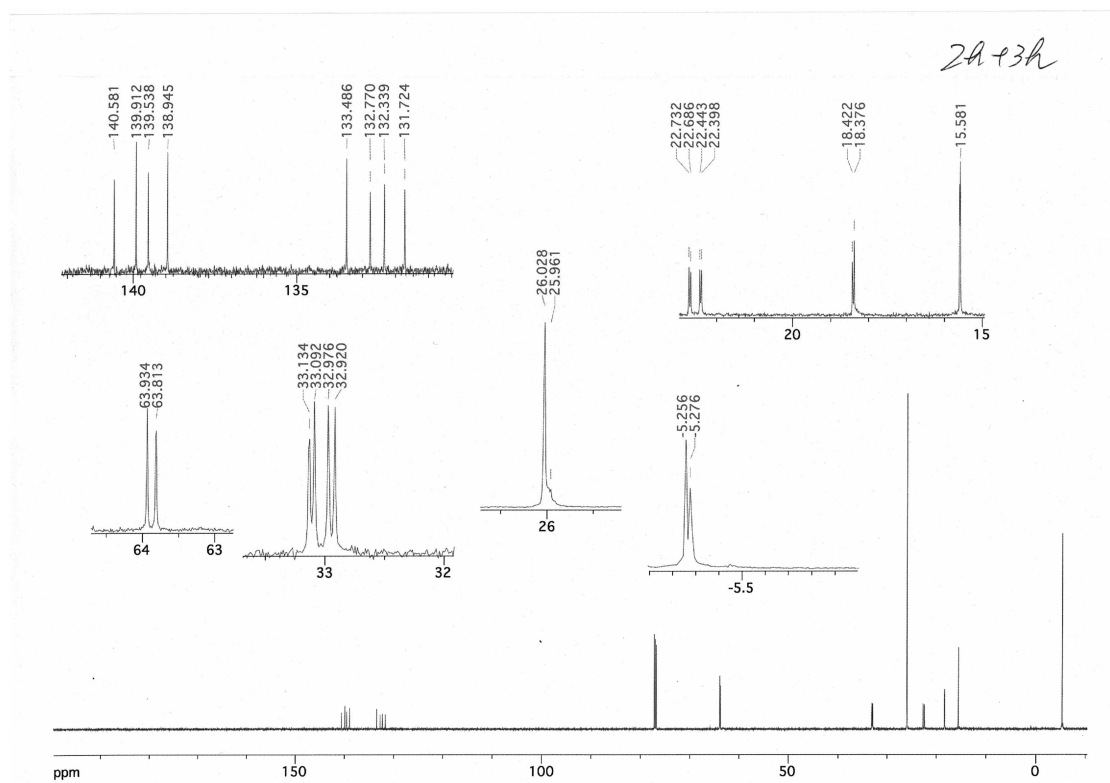


S8 NMR spectra of a mixture of compounds 2h and 3h

S8-1 ^1H NMR Compounds 2h and 3h (CDCl_3)

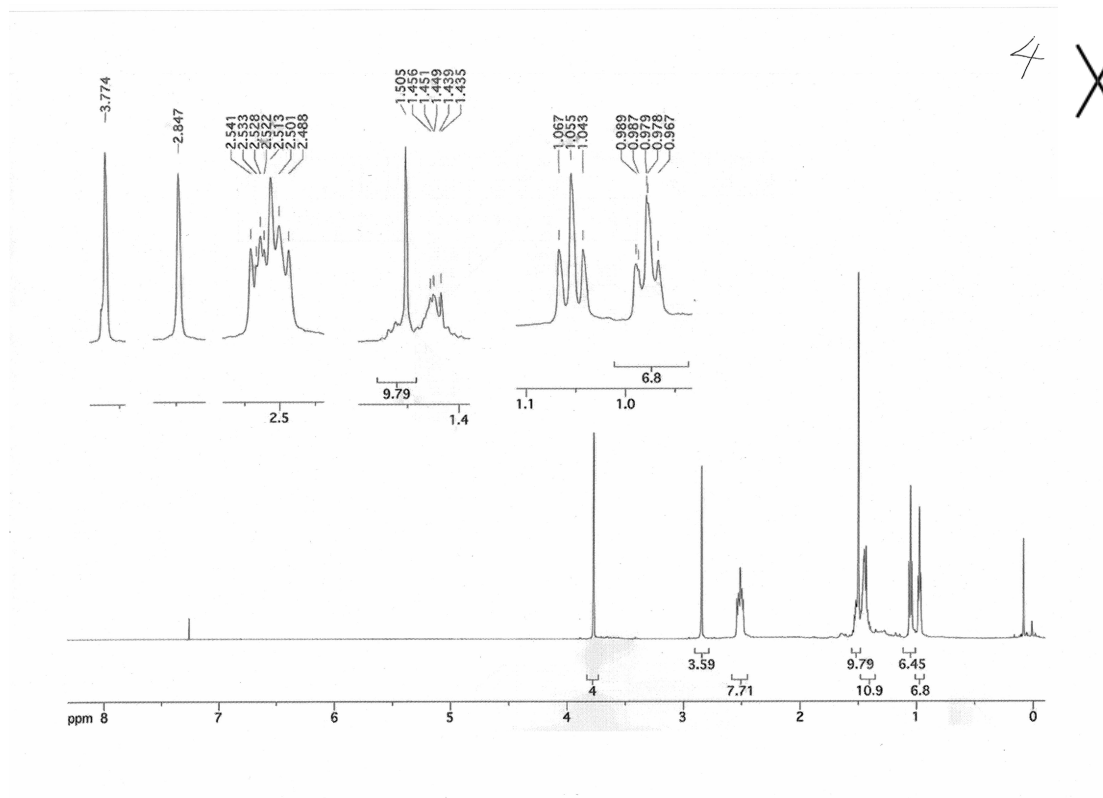


S8-2 ^{13}C NMR Compounds 2h and 3h (CDCl_3)

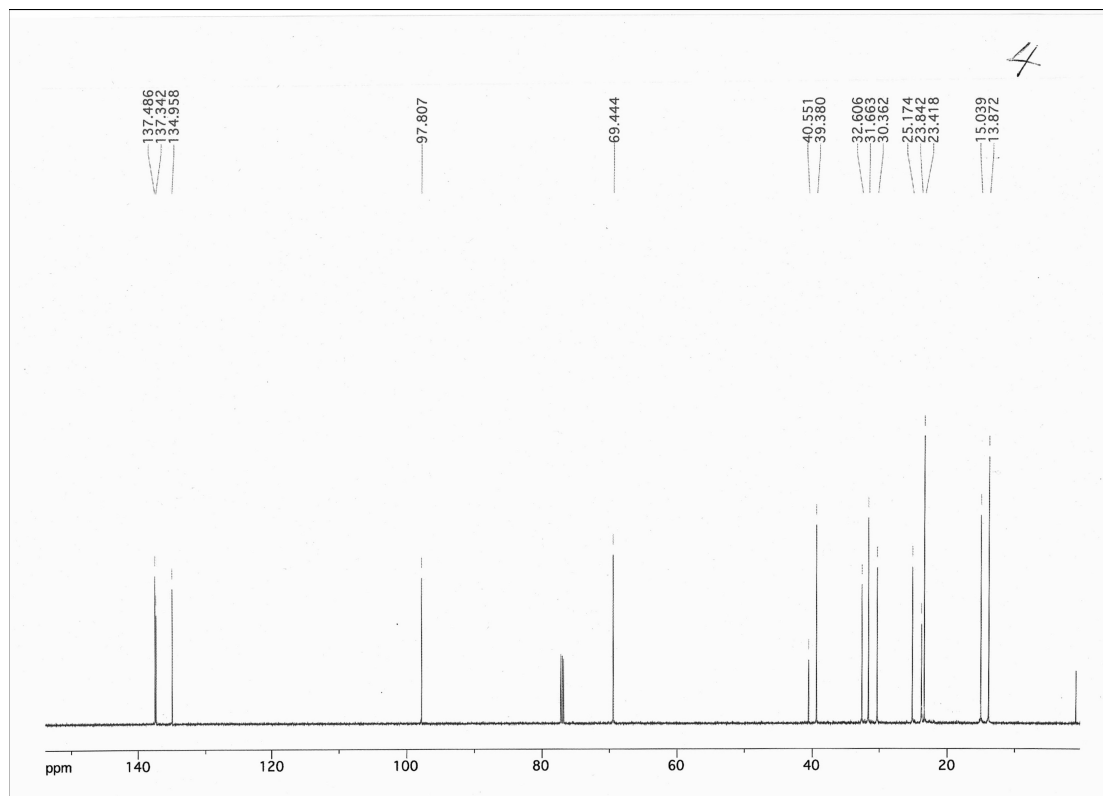


S9 NMR spectra of compound 4

S9-1 ^1H NMR Compounds 4 (CDCl_3)



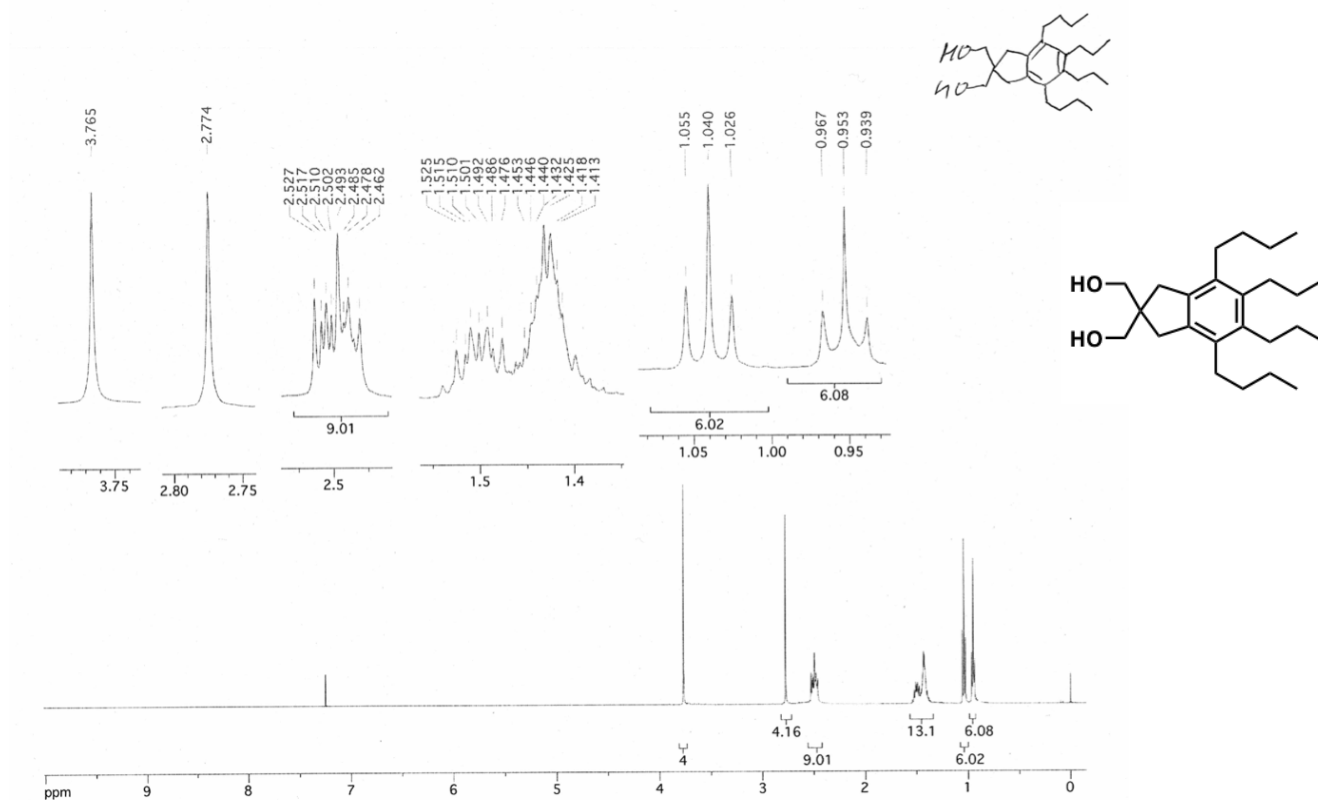
S9-1 ^{13}C NMR Compounds 4 (CDCl_3)



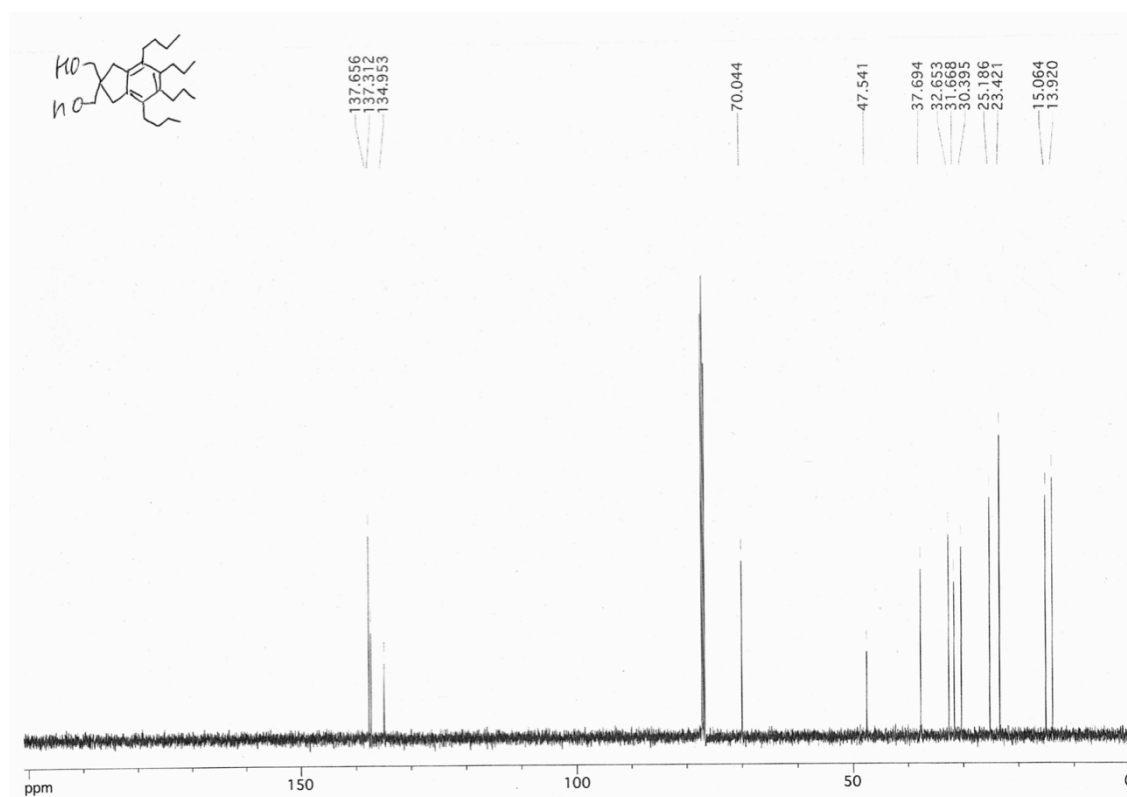
NMR spectra of (4,7-Dibutyl-5,6-dipropyl-2,3-dihydro-1H-indene-2,2-diyl)dimethanol

S10

S10-1 ^1H NMR (500 MHz, CDCl_3)

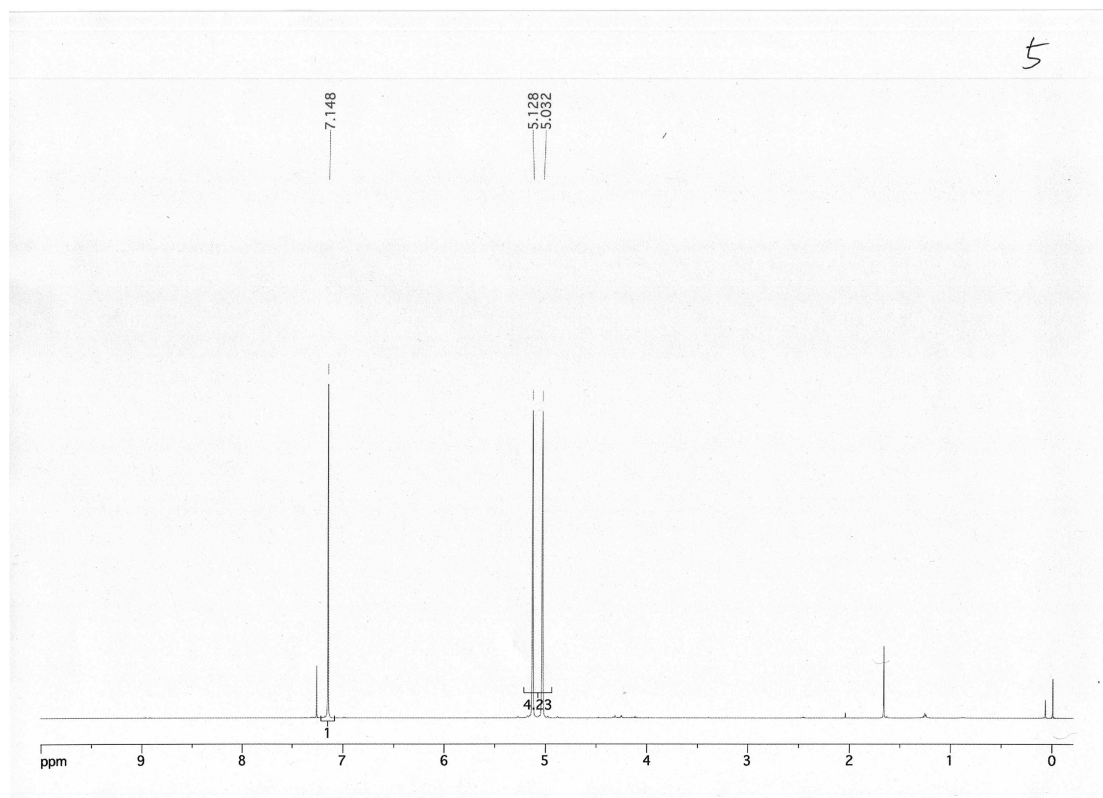
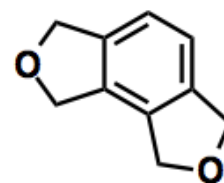


S10-2 ^{13}C NMR (125 MHz, CDCl_3)

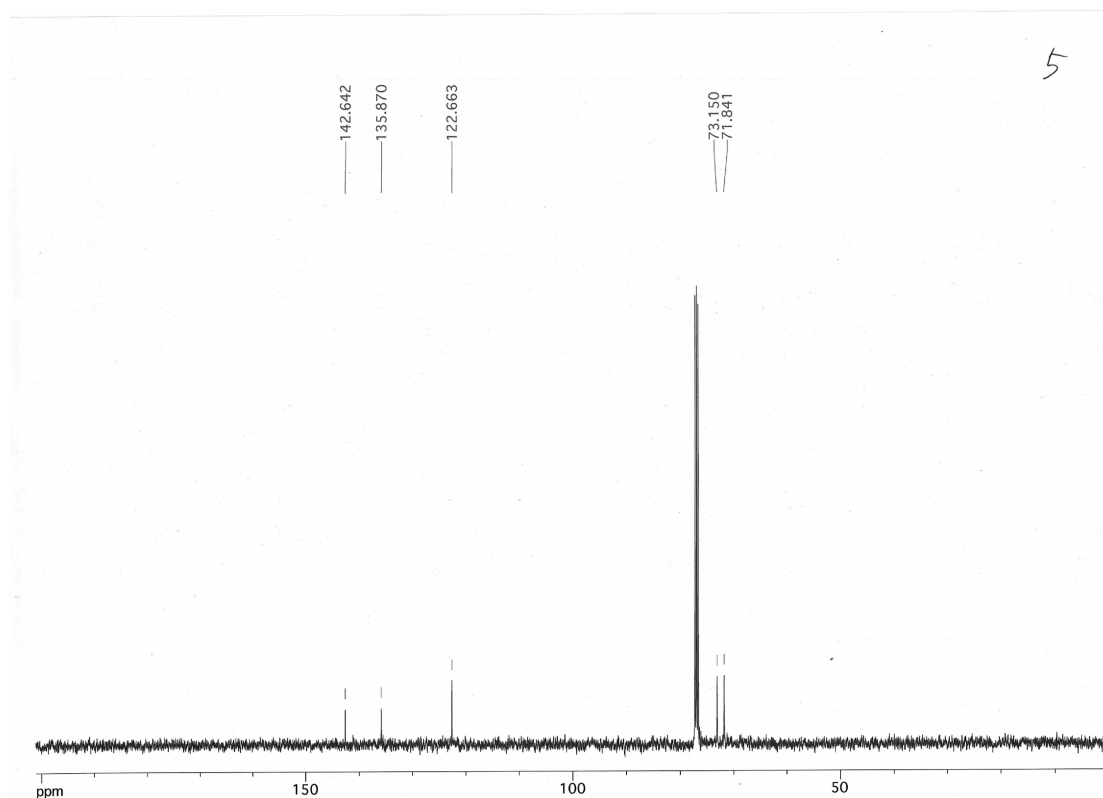


S11 NMR spectra of compound 5

S11-1 ^1H NMR Compounds 5 (CDCl_3)

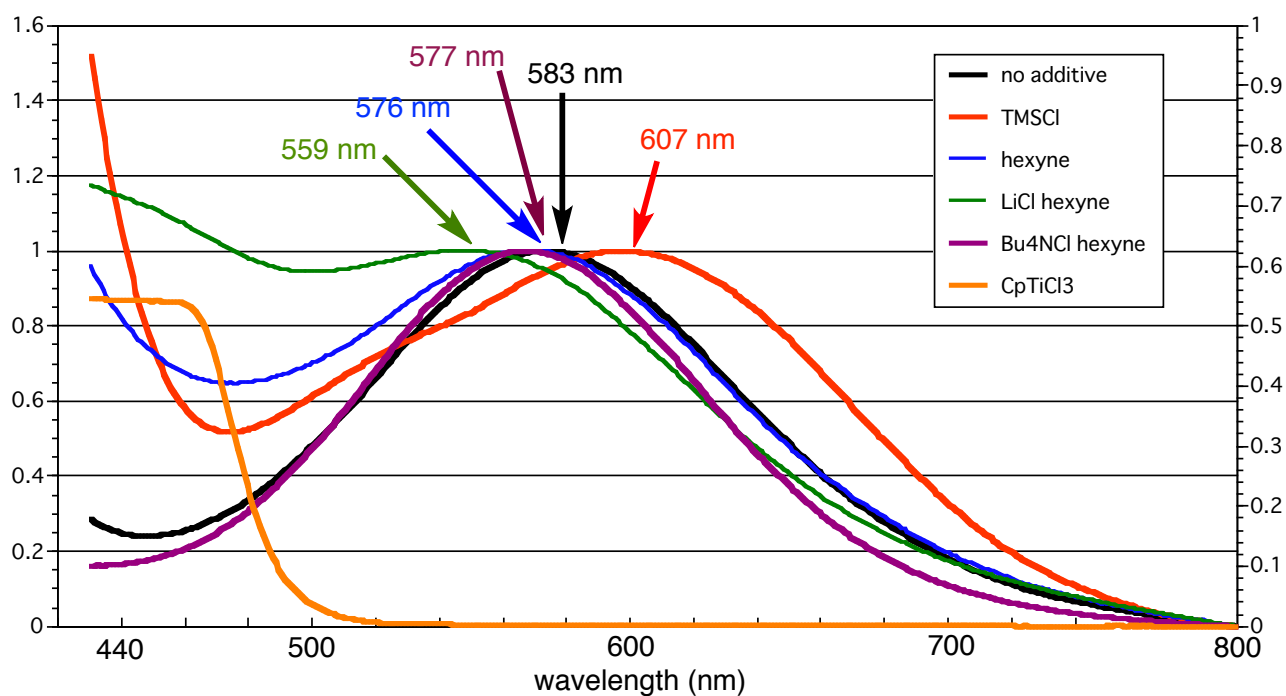


S11-2 ^{13}C NMR Compounds 5 (CDCl_3)

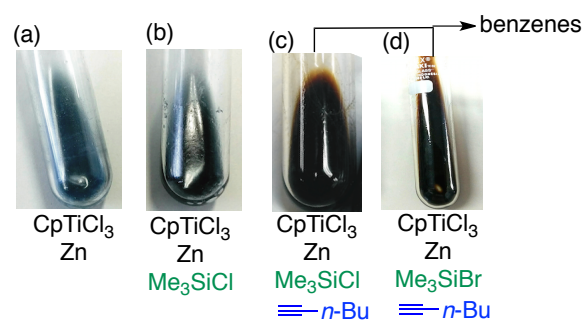


S-12 Visible-Light Absorption Spectra

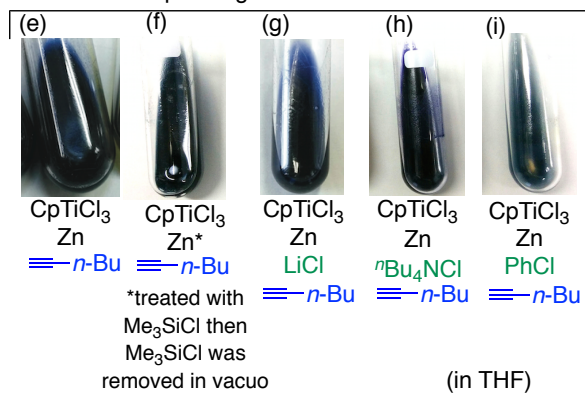
S-12 Vis.-Light Absorption Spectra



— no additive	$\text{CpTiCl}_3 + \text{Zn}$ in THF
— TMSCl	$\text{CpTiCl}_3 + \text{Zn} + \text{Me}_3\text{SiCl}$ in THF
— hexyne	$\text{CpTiCl}_3 + \text{Zn} + 1\text{-hexyne}$ in THF
— LiCl hexyne	$\text{CpTiCl}_3 + \text{Zn} + \text{LiCl} + 1\text{-hexyne}$ in THF
— Bu ₄ NCl hexyne	$\text{CpTiCl}_3 + \text{Zn} + n\text{-Bu}_4\text{NCl} + 1\text{-hexyne}$ in THF
— CpTiCl ₃	CpTiCl_3 in THF



The corresponding benzenes were not obtained.



S-13

S-13 **Figure.** Pictures of a reacting mixture of $\text{CpTiCl}_3/\text{Zn}$ with or without an additive