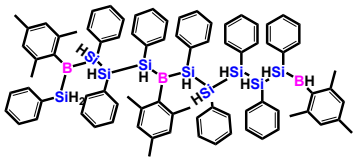
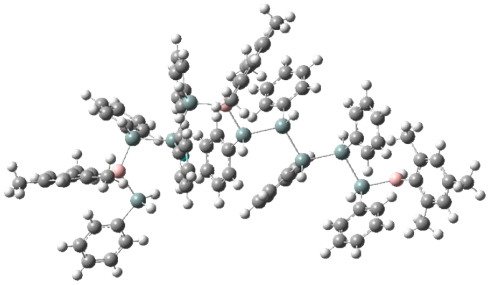
Electronic Supplementary Material (ESI) for Polymer Chemistry.

σ-p Conjugated Copolymers via Dehydrocoupling Polymerization of Phenylsilane and Mesitylborane

Puhup Puneet[a,b], Raman Vedarajan[a] and Noriyoshi Matsumi[a,*]

The peaks at 3.2 and 4-5 ppm have been assigned to Si-H protons. In order to assign various kinds of Si-H protons in ^{1}H-NMR, a polymer mimic model structure was calculated (**Table S1**) and the ^{1}H-NMR spectrum was predicted (**Figure S1**) using DFT calculations (DFT, DMSO-solvation, B3LYP-6-311G (d,p), NMR-GIAO method, Gaussian 09). The model was decided considering random nature of the polymer sequence. The predicted ^{1}H-NMR spectrum of polymer mimic model (Table 1) was closely matching with the experimental spectra. The peaks at 3.17 and 4.01-4.60 were also present in the experimental spectrum.

Table S1: Chemical Structure, Optimized Structure and Chemical Shift Values Predicted by DFT Calculations.

S. No.	Chemical Structure	Optimized Structure	^{1}H-NMR Signals /ppm Due to Si-H
1			3.17, 4.05, 4.07, 4.10, 4.19, 4.30, 4.40, 4.60, 4.92, 5.26

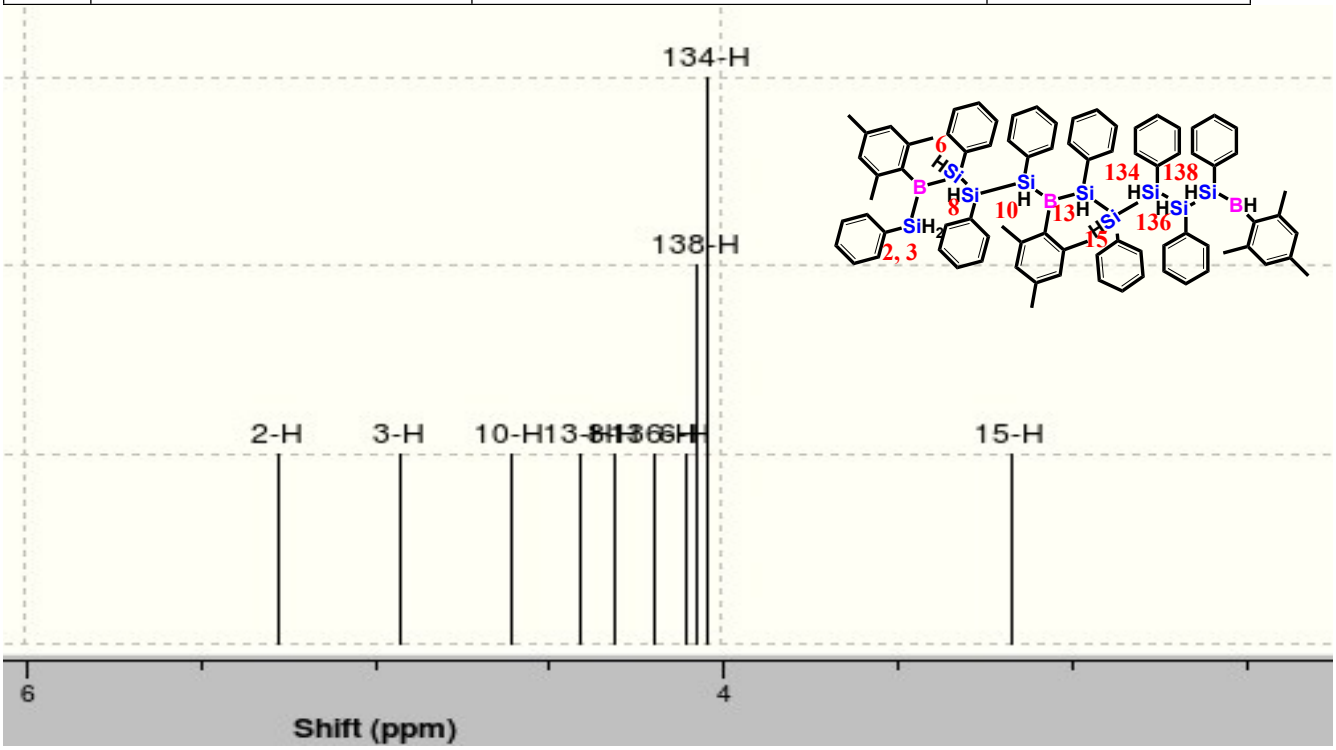


Figure S1: Predicted ^{1}H-NMR spectrum of polymer mimic model (Table S1). (Labelling is according to Gaussian 09).