

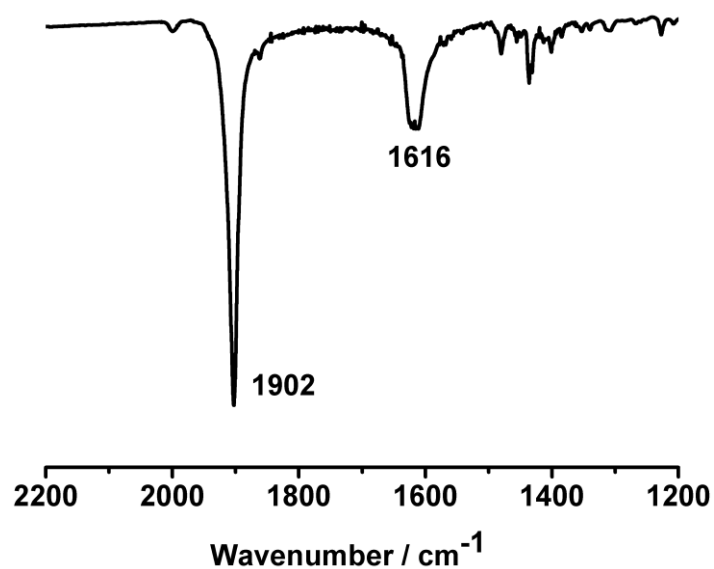
Supporting information for

**Solvent-Dependent Chain Conformation for Ring Closure of Metal Carbonyl  
Oligomers via Migration Insertion Polymerization (MIP) of  
 $\text{CpFe(CO)}_2(\text{CH}_2)_6\text{PPh}_2$**

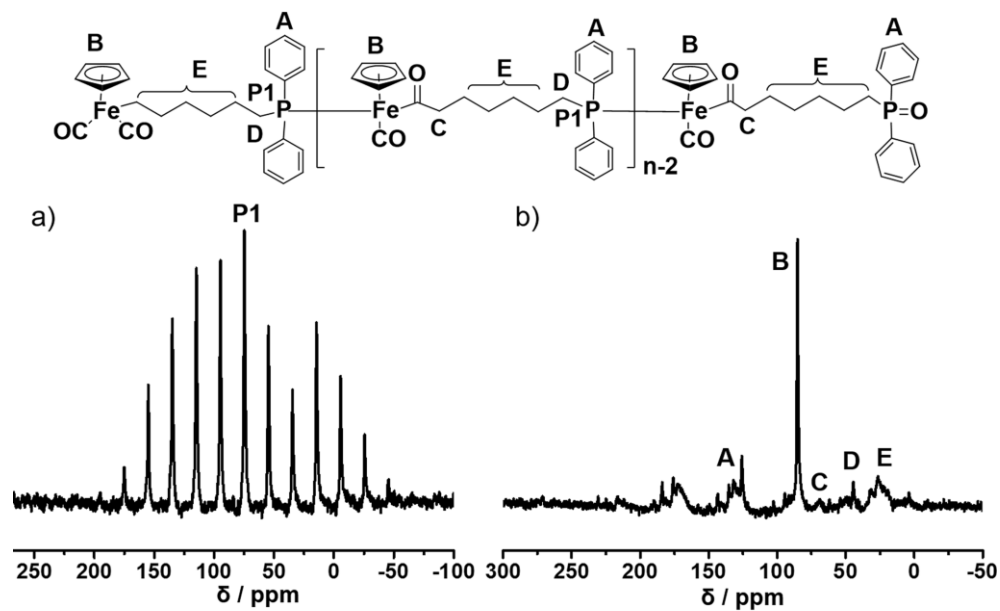
Jin Liu,<sup>‡ab</sup> Zhou Guan,<sup>‡a</sup> Xiaohui Tian,<sup>a</sup> Jiaping Lin,<sup>\*a</sup> and Xiaosong Wang<sup>\*b</sup>

<sup>a</sup> Shanghai Key Laboratory of Advanced Polymeric Materials, State Key Laboratory of Bioreactor Engineering, Key Laboratory for Ultrafine Materials of Ministry of Education, School of Materials Science and Engineering, East China University of Science and Technology, Shanghai, China, 200237

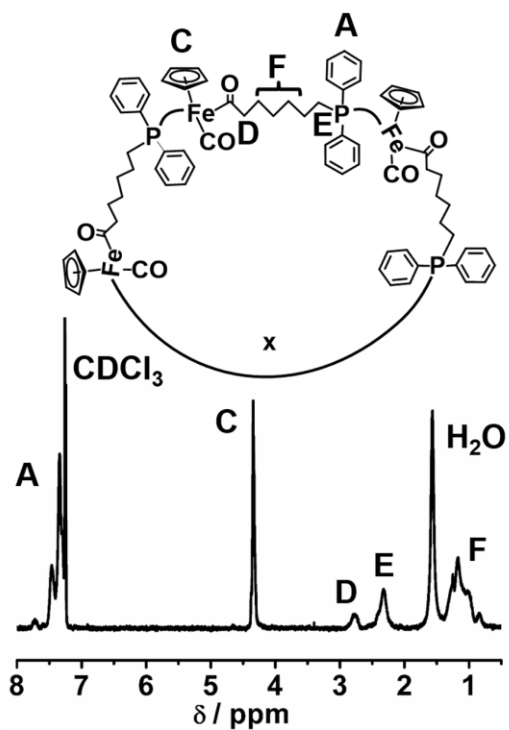
<sup>b</sup> Department of Chemistry and Waterloo Institute for Nanotechnology, University of Waterloo, Waterloo, ON, Canada, N2L 3G1



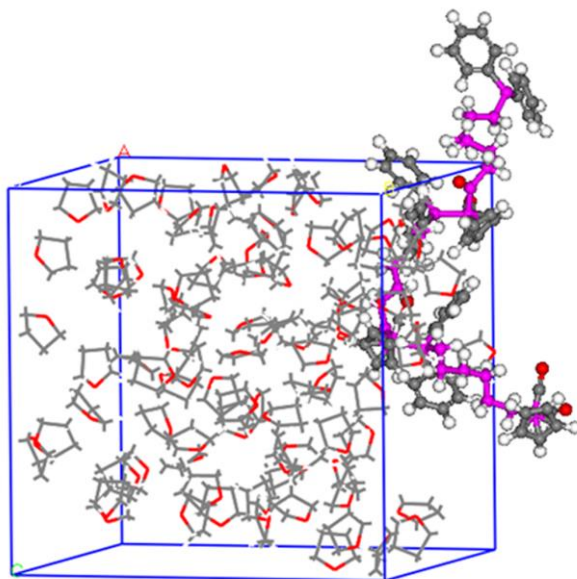
**Figure S1.** FTIR spectrum for THF-insoluble materials produced from solution migration insertion polymerization of PFpC6P in THF.



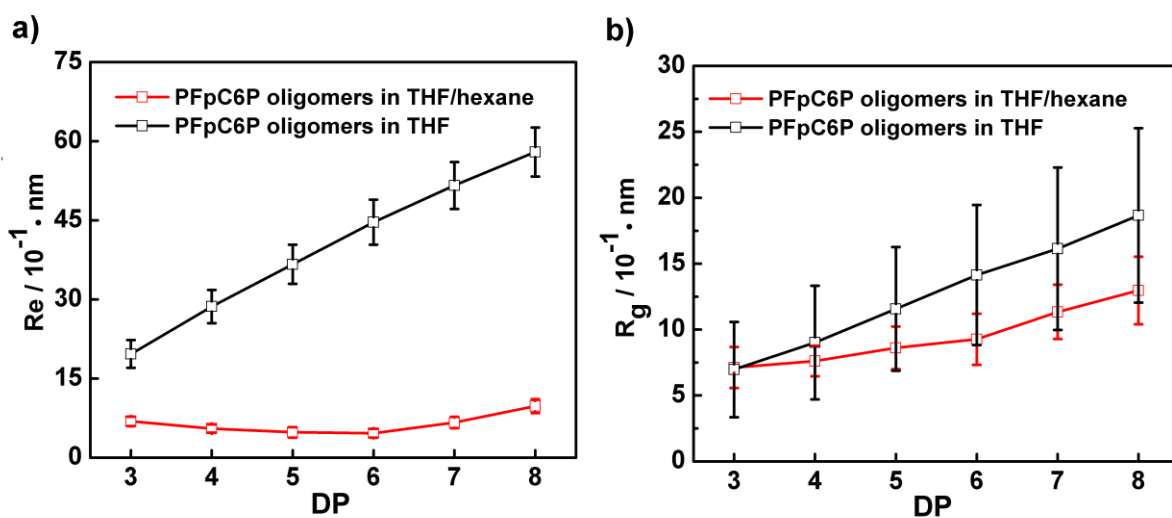
**Figure S2.** a) Solid-state  $^{31}\text{P}$  NMR and b) Solid-state  $^{13}\text{C}$  NMR spectra of THF-insoluble materials produced from solution migration insertion polymerization of  $\text{CpFe}(\text{CO})_2(\text{CH}_2)_6\text{PPh}_2$  in THF.



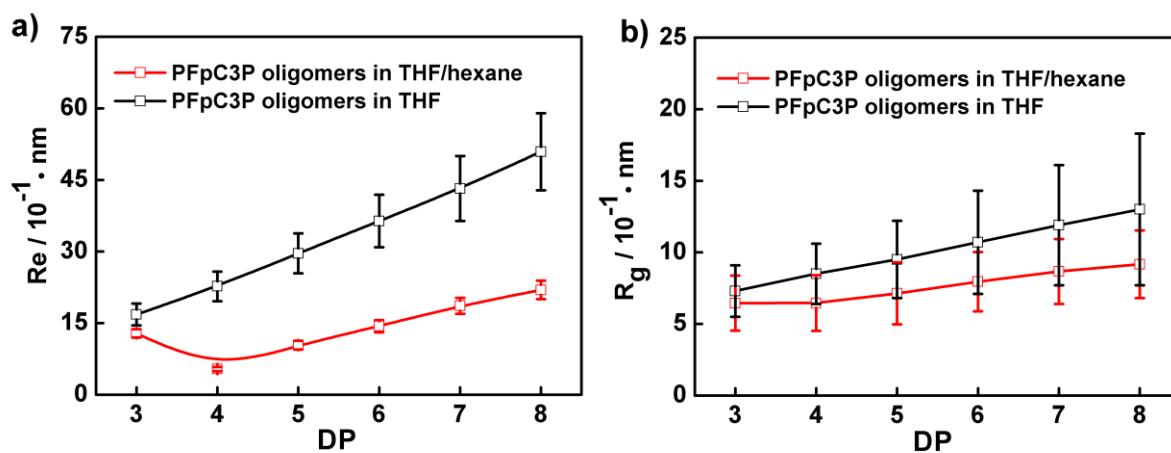
**Figure S3.**  $^1\text{H}$  NMR spectrum of THF-soluble product produced from solution migration insertion polymerization of  $\text{CpFe}(\text{CO})_2(\text{CH}_2)_6\text{PPh}_2$  in THF/hexane mixed solvents.



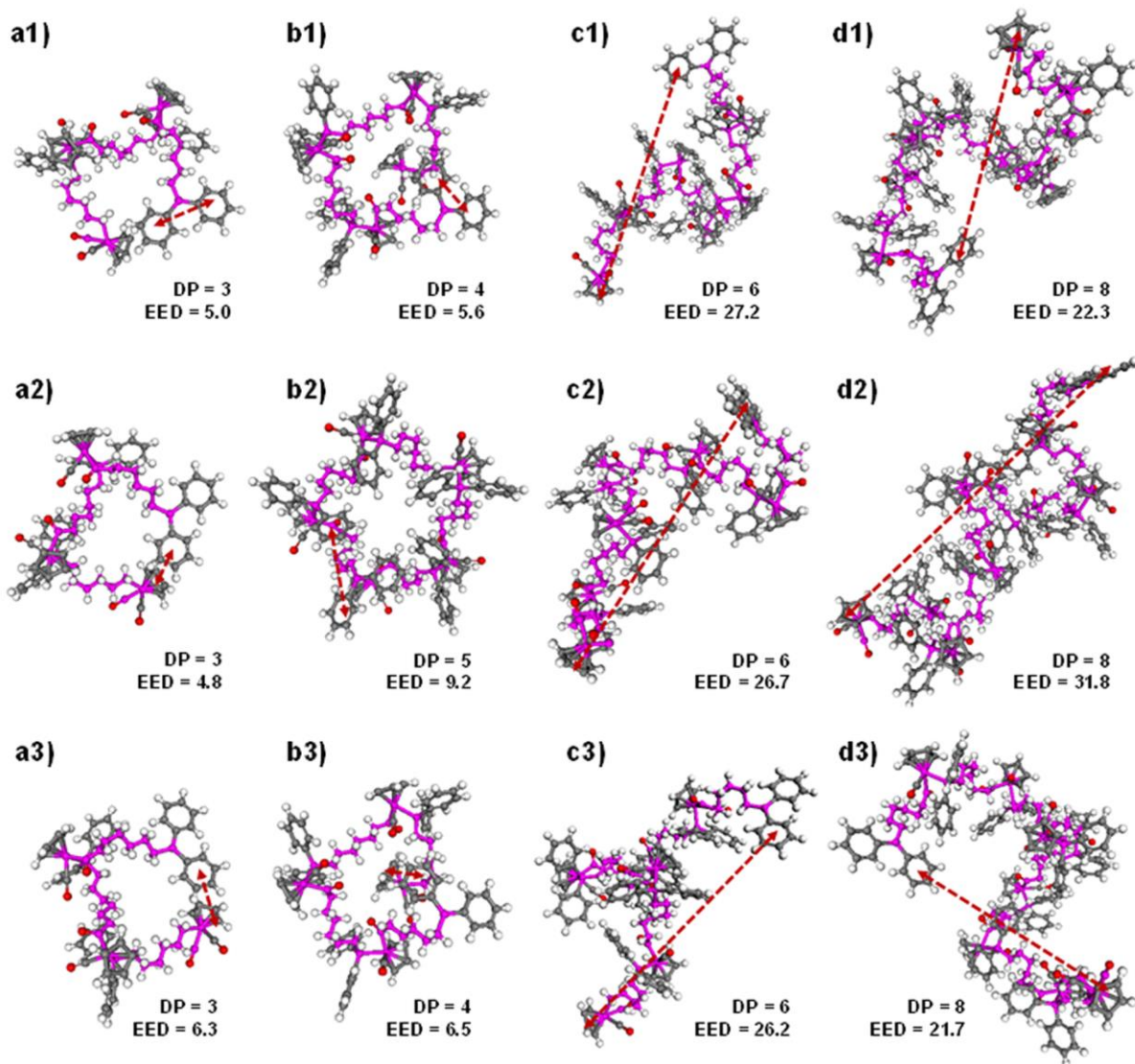
**Figure S4.** Initial morphology of the simulation system containing one PFpC6P oligomer with DP = 3 and 74 THF molecules. The box size is  $23.27 \times 23.27 \times 23.27 \text{ \AA}^3$ .



**Figure S5.** a) Root mean squared end-to-end distance ( $R_e$ ) and b) radius of gyration ( $R_g$ ) of FpC6P oligomers as a function of degree of polymerization (DP).



**Figure S6.** a) Root mean squared end-to-end distance ( $R_e$ ) and b) radius of gyration ( $R_g$ ) of FpC3P oligomers as a function of degrees of polymerization (DP).



**Figure S7.** Simulated structures of PFpC6P oligomers in THF/DMSO (a1-d1), THF/pyrrole (a2-d2) and THF/pyridine (a3-d3) mixed solvents. Purple lines denote PFpP backbones; Red arrows represent end-to-end distances ( $Re$ ). The unit of distance is Å.