Supporting information

for

Syntheses of quaternary ammonium containing trithiocarbonate RAFT agents and hemi-telechelic cationomers

Longhe Zhang,^a Lydia R. Cool,^b Chrys Wesdemiotis,^b R. A. Weiss^a and Kevin A. Cavicchi,*^a

^a Department of Polymer Engineering, The University of Akron, Akron, OH, 44325-0301,

USA. Fax: +1 330 972 3406; Tel: +1 330 972 8368; E-mail: kac58@uakron.edu

^b Department of Chemistry, The University of Akron, Akron, OH, 44325-3601, USA.

This supporting information contains a) the ¹H NMR and ESI spectra of synthesized compounds (Br-NMe₃, Br-NBu₃, RAFT-NMe₃, RAFT-NBu₃); b) the pseudo-first order kinetic curve of bulk styrene polymerization with RAFT-NMe₃ and RAFT-NBu₃; c) the kinetic data of bulk styrene polymerization with RAFT-NEt₃ at 65 °C; d) the ¹H NMR data of PBA and PDMAEA.



Figure S1. ¹H NMR spectrum in CDCl₃ of Br- Ph-NMe₃.



Figure S2. ESI mass spectrum of Br- Ph-NMe₃.



Figure S3. ¹H NMR spectrum in CDCl₃ of Br- Ph-NBu₃.



Figure S4. ESI mass spectrum of Br- Ph-NBu₃. The peak at m/z 237.1 is due to the di-substituted compounds.



Figure S5. Chemical Structure of RAFT-NEt₃ and the potential sulfide by-product.



Figure S6. ¹H NMR spectrum in CDCl₃ of RAFT-NMe₃.



Figure S7. ESI mass spectrum of RAFT-NMe₃.



Figure S8. ¹H NMR spectrum in CDCl₃ of RAFT-NBu₃.



Figure S9. ESI mass spectrum of RAFT-NBu₃.



Figure S10. Pseudo first-order kinetic plot for the RAFT bulk polymerization of styrene at 120 °C with a) RAFT-NMe₃ and b) RAFT-NBu₃. Target molecular weight is 25 kDa. The solid line is a linear fit to the data.



Figure S11. (a) Pseudo first-order kinetic plot for the RAFT bulk polymerization of styrene at 65 °C with RAFT-NEt₃. Target molecular weight is 25 kDa. The solid line is a linear fit to the data. (b) Plot of M_n (SEC) and \tilde{D} versus monomer conversion and (c) SEC traces as a function of polymerization time for the same polymerization.



Figure S12. ¹H NMR spectrum of purified PBA (acetone fraction).



Figure S13. ¹H NMR spectrum of PDMAEA.