

SUPPLEMENTARY MATERIALS

RAFT polymerization of *tert*-butyldimethylsilyl methacrylate: Kinetic study and determination of rate coefficients

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PREDICI Workshop

Model: RAFT_ktr_PMASI
 File: RAFT of MASI with preequilibrium.rsy
 Recipe:
 Library:

Simulation mode:
 Distributions
 Moments

Settings | Reactors | Elem. Species | Pol. Species | Coefficients | Reaction steps

Only in Reactor: All

Name	a...	Memo	Type	Files	Reactor
$\text{initiator} \rightarrow \text{I}^* + \text{I}^*$, $k_d f$	X		Elementalreaction		R
$\text{I}^* + \text{M} \rightarrow \text{P}^*(1)$, k_i	X		Initiation(anion)		R
$\text{P}^*(s) + \text{RAFT} \rightarrow \text{Int}^*(s)$, $k_{\beta 2}$	X		Change		R
$\text{Int}^*(s) \rightarrow \text{macroRAFT}(s) + \text{R}^*$, $k_{\beta 2}$	X		Change		R
$\text{Int}^*(s) \rightarrow \text{P}^*(s) + \text{RAFT}$, $k_{\beta 2}$	X		Change		R
$\text{macroRAFT}(s) + \text{R}^* \rightarrow \text{Int}^*(s)$, $k_{\beta 2}$	X		Change		R
$\text{R}^* + \text{RAFT} \rightarrow \text{IntRR}^*$, $k_{\beta 1}$	X		Elementalreaction		R
$\text{IntRR}^* \rightarrow \text{R}^* + \text{RAFT}$, $k_{\beta 1}$	X		Elementalreaction		R
$\text{R}^* + \text{M} \rightarrow \text{P}^*(1)$, k_{prein}	X		Initiation(anion)		R
$\text{P}^*(s) + \text{M} \rightarrow \text{P}^*(s+1)$, k_p	X		Propagation		R
$\text{P}^*(s) + \text{macroRAFT}(r) \rightarrow \text{Q1}(s) + \text{Q2}(r)$, ...	X		d-Termination		R
$\text{Q1}(s) \rightarrow \text{P}^*(s)$, $k_{\beta 2}/2$	X		Change		R
$\text{Q1}(s) \rightarrow \text{macroRAFT}(s)$, $k_{\beta 2}/2$	X		Change		R
$\text{Q2}(s) \rightarrow \text{P}^*(s)$, $k_{\beta 2}/2$	X		Change		R
$\text{Q2}(s) \rightarrow \text{macroRAFT}(s)$, $k_{\beta 2}/2$	X		Change		R
$\text{P}^*(s) + \text{I}^* \rightarrow \text{dead}(s)$, k_t	X		Change		R
$\text{P}^*(s) + \text{R}^* \rightarrow \text{dead}(s)$, k_t	X		Change		R
$\text{P}^*(s) + \text{P}^*(r) \rightarrow \text{dead}(s+r)$, k_{tc} , $\text{P}^*(s)+...$	X		Combination		R
$\text{R}^* + \text{R}^* \rightarrow \text{RR}$, k_t	X		Elementalreaction		R

Buttons: New, Edit, Copy, Delete, Fill with..., Comment, Move up, Move down, Comment, Start, Save, Ok, Cancel, Help

Scheme S1. Reaction scheme of the RAFT process implemented into the PREDICI simulation program.

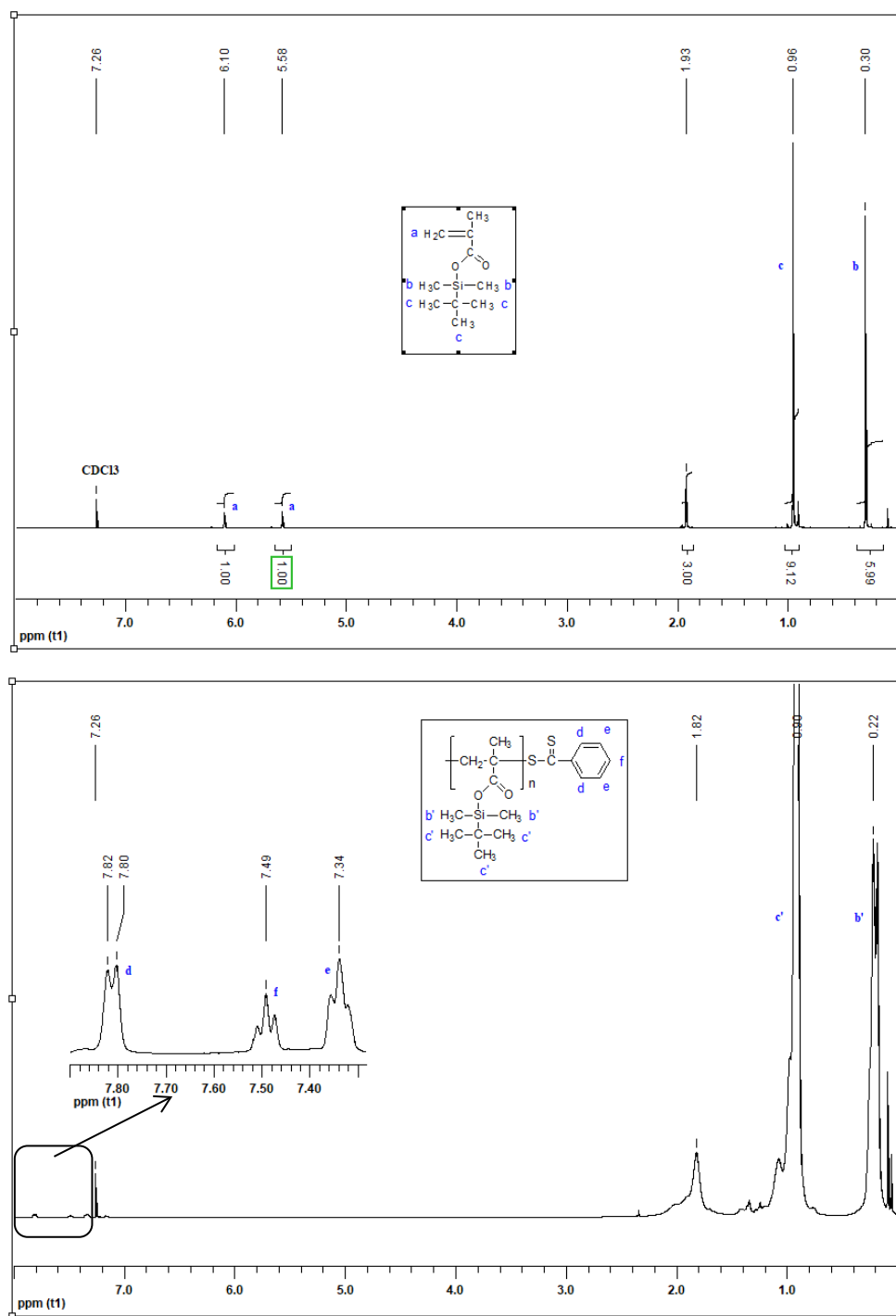


Figure S1. ^1H NMR spectra of TBDMSMA and PTBDMSMA.

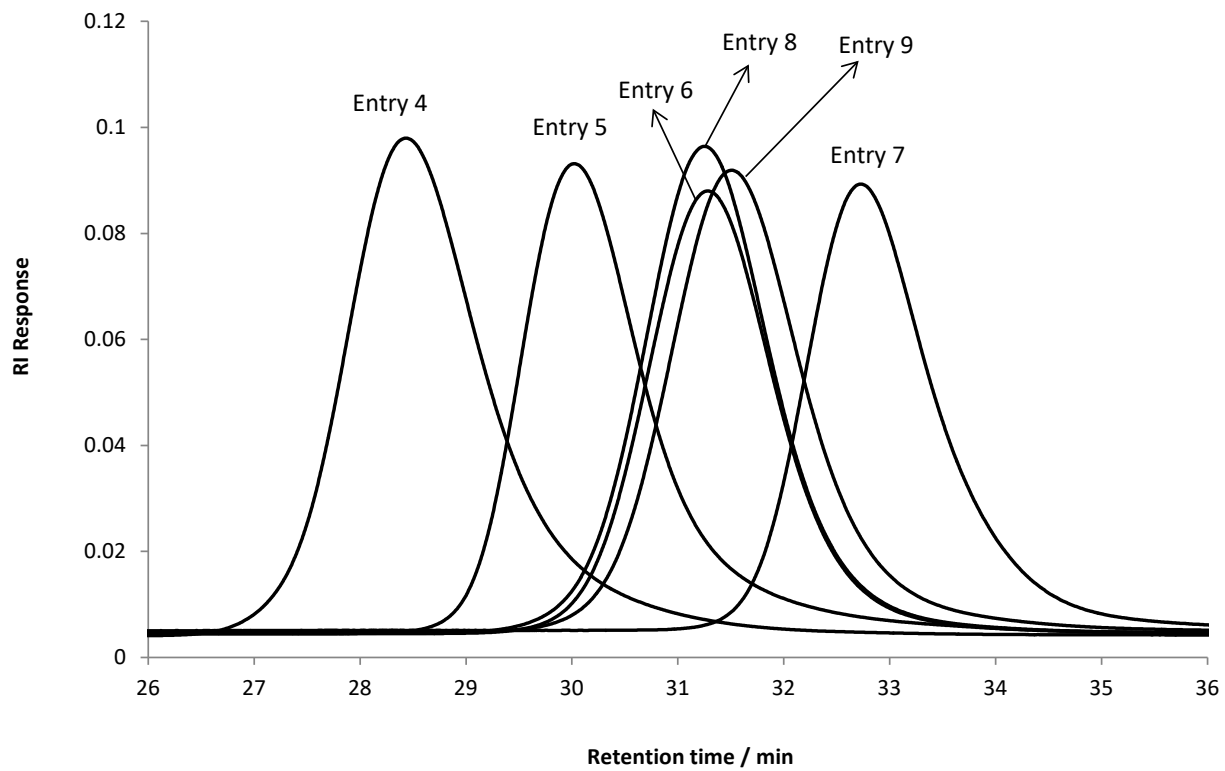


Figure S2. SEC chromatograms of PTBDMSMA.

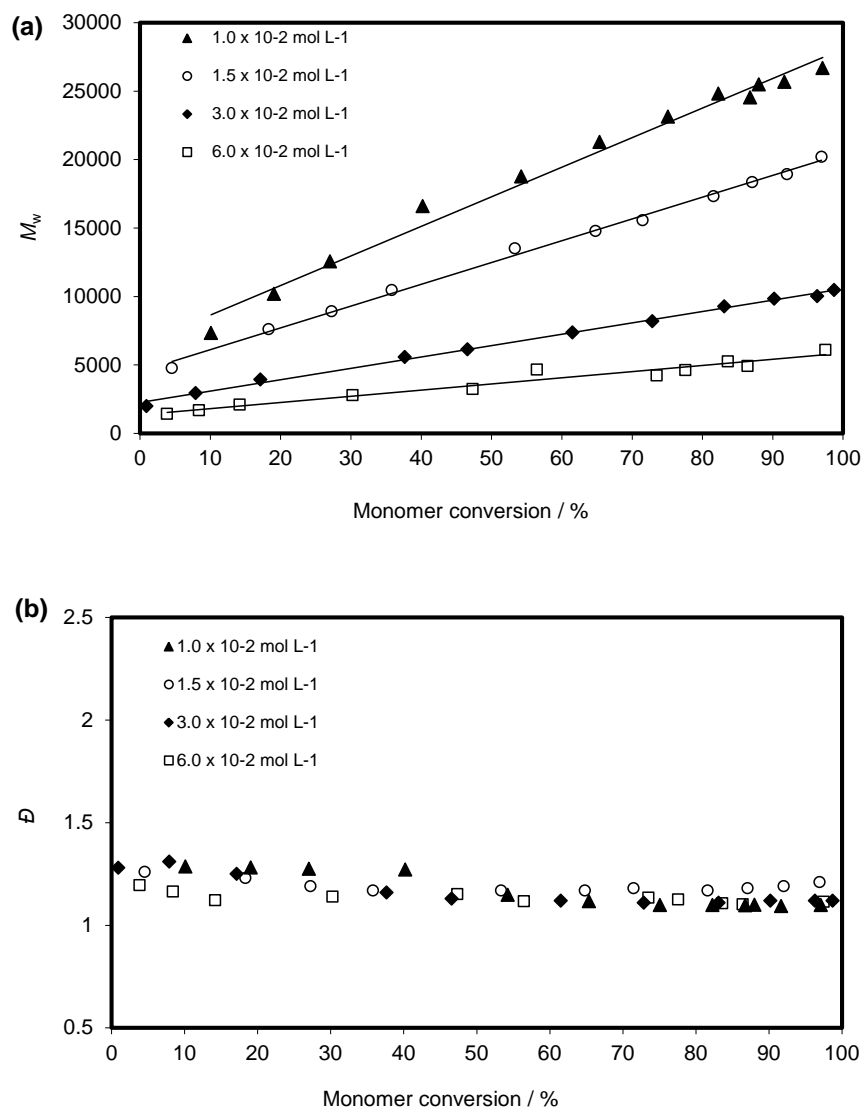


Figure S3. Evolution of M_w (a) and D (b) versus monomer conversion for CPDB-mediated polymerization of TBDMSMA in toluene at 70 °C with initial concentration of CPDB ranging from 1.5×10^{-2} to 6.0×10^{-2} mol L $^{-1}$.