

Biological and Mechanical Evaluation of Novel Prototype Dental Composites

H.L. Van der Laan, S.L. Zajdowicz, K. Kuroda, B.J. Bielajew, T.A. Davidson, J. Gardinier, D.H. Kohn, S. Chahal, S. Chang, J. Liu, J. Gerszberg, T.F. Scott, and B.H. Clarkson

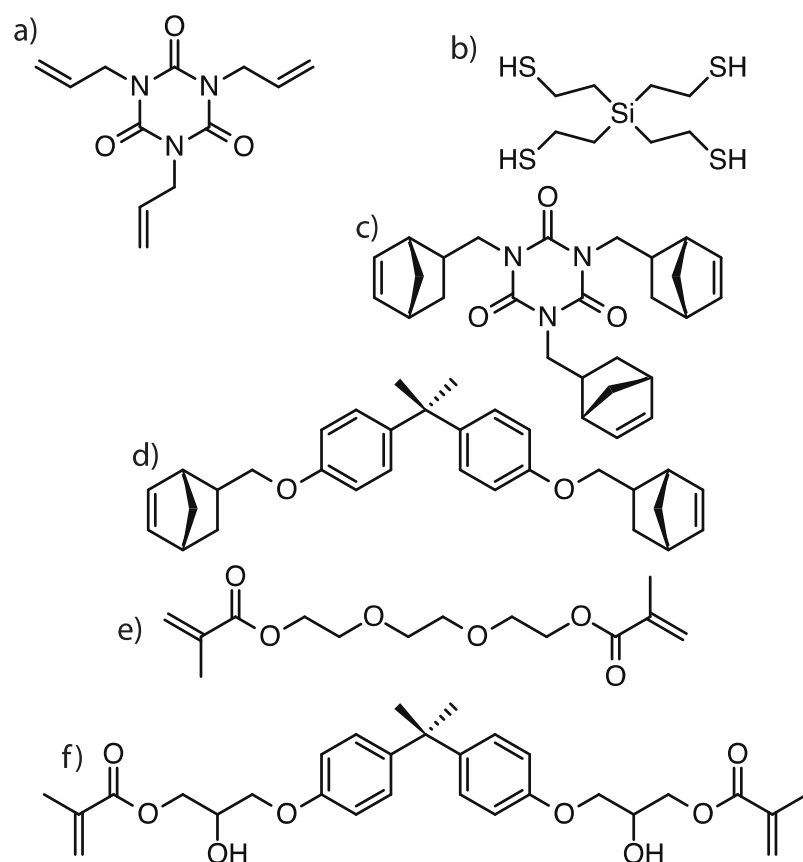
Appendix

Calculating Oligomer formulation

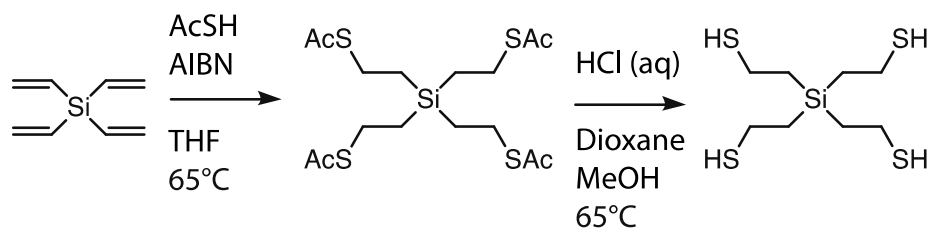
The thiol-ene polymerization follows a step-growth mechanism, and as a result the gelation point of this system can be predicted. Following the Flory-Stockmayer theory, the gelation point of multifunctional monomer systems can be predicted according to the following equation.

$$\alpha = \frac{1}{\sqrt{r(f_a - 1)(f_b - 1)}}$$

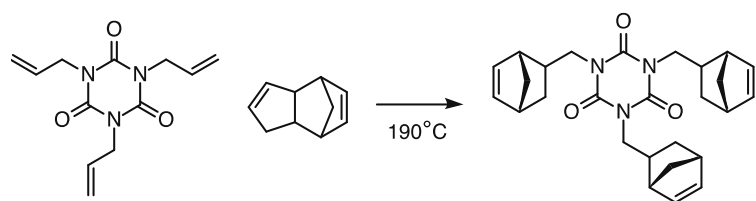
In which f_a and f_b are the functionalities of the 2 monomers, r is the molar ratio of the monomers ($r = N_a/N_b \leq 1$), and α is the extend of reaction at which gelation occurs. α was set to be ~ 1.02 , so that the maximum amount of oligomerization would occur, while maintaining a flowable oligomer. For the TMES/TNTATO system, $f_a = 3$, and $f_b = 4$, r was calculated to be 0.16. For TMES/DNBPA, $f_a = 2$, and $f_b = 4$, resulting in $r = 0.3$.



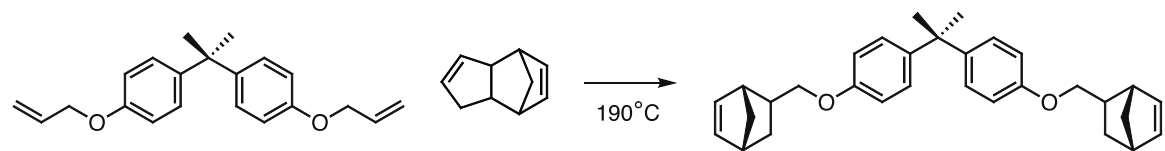
Appendix Figure 1. Structures of monomers used in this study. a) 1,3,5-Triallyl-1,3,5-triazine-2,4,6-trione (TATATO), b) Tetra(2-mercaptoethyl)silane (TMES), c) trinorbornyl triazine trione (TNTATO), d) dinorbornyl bisphenol A (DNBPA), e) Triethyleneglycol dimethacrylate (TEGDMA), f) bisphenol A-glycidyl methacrylate (bisGMA)



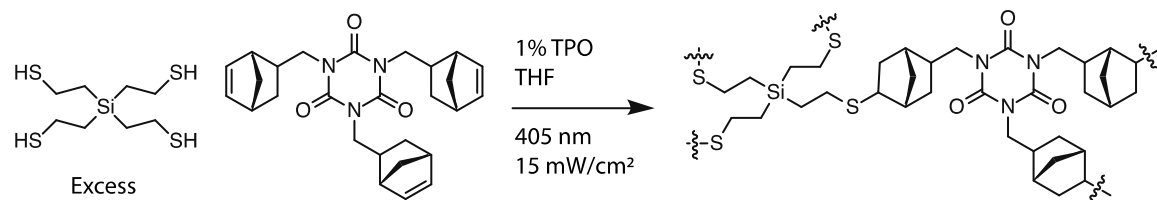
Appendix Figure 2. Synthesis of TMES from tetravinylsilane and thioacetic acid followed by hydrolysis.



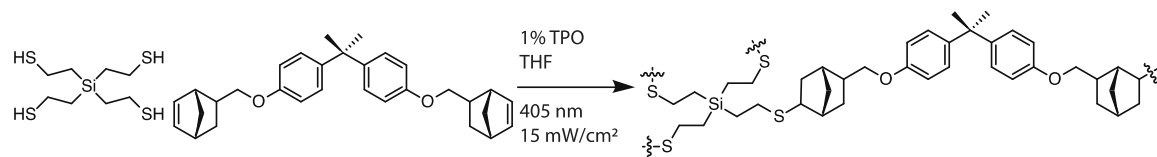
Appendix Figure 3. Synthesis of TNTATO from TATATO and dicyclopentadiene.



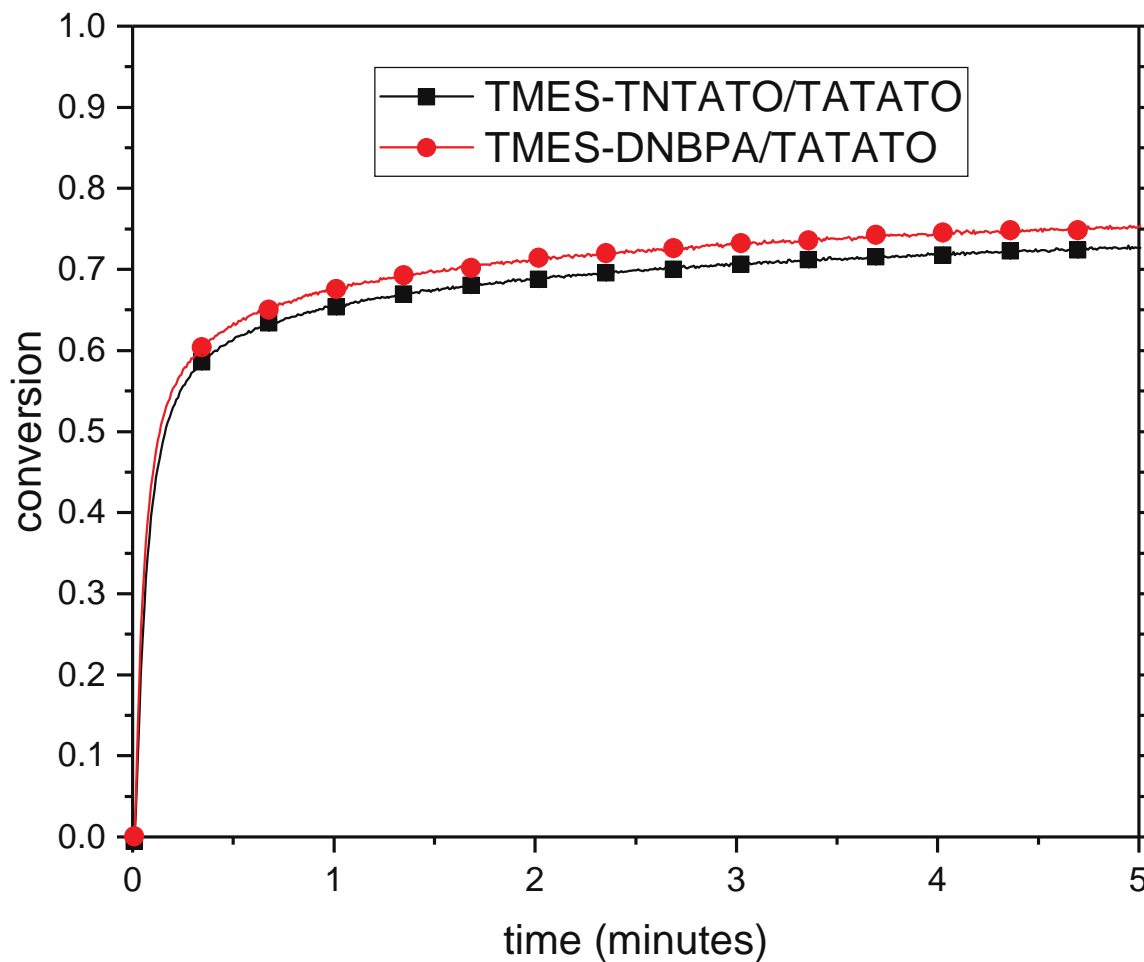
Appendix Figure 4. Synthesis of DNBPA from Diallyl bisphenol A and dicyclopentadiene.



Appendix Figure 5. Oligomerization reaction of TMES with TNTATO in Tetrahydrofuran.



Appendix Figure 6. Oligomerization reaction of TMES with DNBPA in Tetrahydrofuran.



Appendix Figure 7. Time/conversion plots of unfilled TMES-TNTATO/TATATO (black, squares), and TMES-DNBPA/TATATO (red, circles) formulated with 1% TPO and irradiated at 405 nm with 10 mW/cm². Conversions are obtained from monitoring the TATATO C=C in the FTIR spectrum at 3083 cm⁻¹.