Acrylated Soybean oil: A key intermediate for more sustainable elastomeric materials.

Miguel Melendez-Zamudio, Erin Donahue-Boyle, Yang Chen & Michael A. Brook*

Department of Chemistry and Chemical Biology, McMaster University, 1280 Main St. W., Hamilton, ON, Canada, L8S 4M1, mabrook@mcmaster.ca

Supporting Information

Table S1 Formulations for model aza-Michael reactions between **2** and benzylamine.

Acrylated Soybean oil (ASBO)	Benzylamine	% of modification
g (mmol)	μL (mmol)	
0.5 (0.404)	44.19 (0.40)	25%
0.5 (0.404)	88.39 (0.81)	50%
0.5 (0.404)	132.58 (1.21)	75%
0.5 (0.404)	176.78 (1.62)	100%

	T2	T12	T36	T59
Concentration	Mass %	Mass % of	Mass % of	Mass % of
	of	Silicone	Silicone	Silicone
	Silicone			
10%	2.0	6.7	17.7	26.1
15%	2.9	9.7	24.4	34.6
25%	4.8	15.2	35.0	46.9
50%	9.1	26.4	51.9	63.9
	13.1	-	-	-
	16.7	-	-	-

Table S2 Mass% silicone in the various formulations.



Figure S1. ¹H NMR in CDCl₃ of a) **2** modified with different concentrations of benzylamine: b) 25%, c) 50%, d) 75% and e) 100%.



Figure S2. IR/ATR of **T2-15** → **T2-100** elastomers & **T12-15** → **T2-50**



Figure S3. ¹H NMR for a) **2**, b) ground **T2-25** (swelled) and c) ground **T12-50** (swelled). Note: prior to taking the NMR in CDCl₃, the elastomeric samples were cooled using liquid N_2 and ground to a fine powder.



Figure S4. ${}^{1}H$, ${}^{13}C$ and ${}^{29}Si$ NMR for the degraded aqueous phase (D₂O) **T59-50**.

Aqueous phase: In the ¹H NMR, peaks from 0 to 0.08 ppm correspond to fragments of degraded silicone that are coupled with the degraded soybean oil structure. Signals at 0.90 to 1.68 ppm correspond to the hydrocarbon chain from the degraded soybean oil. In the ¹³C NMR important signals at -167, -179 and - 180 ppm indicate a mixture of carbonyl species, likely to be amides, fatty acids and esters. In the case of the ²⁹ Si NMR, a small peak at -22 ppm indicates that small amounts or degraded silicone structures are present in the sample.





Figure S5. IR spectrum after A: the first base degradation; B: the second base degradation.

A: The peak at 1730 cm⁻¹ that corresponds to the acrylate carbonyl group un the **2** (blue spectrum) disappeared after the 1st degradation. The black spectrum corresponds to the CDCl₃ phase and has 2 peaks in the carbonyl region, one at 1624 cm⁻¹ likely corresponding to the formation of an amide, and also displays peaks characteristic for silicones at 1085 – 1006 cm⁻¹. In the case of the red spectrum, 1649 cm⁻¹ can be assigned to the formation of amides.

B: In this case, the CDCl₃ phase that mostly contained silicone was degraded again using the same basic conditions. Both spectra (red and black) contain a peak at 1646 cm⁻¹, likely an amide. However, the peaks that would correspond to the silicones are gone (near 1000 cm⁻¹), consistent with silicone degradation to volatile products (cyclic monomers or ethoxysilanes).



Figure S6. ¹H, and ¹³C NMR for the degraded organic phase (CDCl₃) **T59-50**.

CDCl₃ phase: In the ¹H NMR a strong peak at 0.06 ppm was observed that corresponds to the methyl units from the silicone backbone. Small peaks were observed in the region from 0.8-1.6 ppm that correspond to the hydrocarbon chains from soybean oil constituents that are still interacting with the silicone chain. In the ¹³C NMR a single peak at 1.06 ppm was seen and is assigned to the methyl group from the silicone; the CDCl₃ phase is clearly rich in silicone.



Figure S7. TGA measurements for T2-100, T12-50 and T36-15.



Figure S8. ¹H NMR of epoxidized soybean oil **1** in CDCl₃.



Figure S9. ¹³C NMR of epoxidized soybean oil **1** in CDCl₃.



Figure S10. ¹H NMR of acrylated soybean oil **2** in CDCl₃.



Figure S11. ¹³C NMR of acrylated soybean oil **2** in CDCl₃.