

Supporting Information

Self-healable covalently adaptable networks based on disulfide exchange

Xinru Guo^a, Feng Liu^{a*}, Meng Lv^a, Fengbiao Chen^a, Fei Gao^{a*}, Zhenhua Xiong^a,
Xuejiao Chen^a, Xuelang Gao^{b*}

^aJiangxi Engineering Laboratory of Waterborne Coating, School of Chemistry and Chemical Engineering, Jiangxi Science & Technology Normal University, Nanchang, Jiangxi, 330013, P. R. China.

^bDepartment of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, Korea 790-784

E-mail: feng67807@163.com (F. Liu), feigao2016@jxstnu.com.cn (F. Gao); xlanggao@postech.ac.kr (XL. Gao)

Content

| | |
|--|---|
| 1. Solvent swelling..... | 2 |
| 2. Calculating the yield of TMPTAA and PETMPA by ¹ H NMR..... | 2 |
| 2.1 Calculating the yield of trimethylolpropane tris(3-mercaptopropionate) acetoacetate (TMPTAA) by ¹ H NMR | 2 |
| 2.2 Calculating the yield of pentaerythritol tetra(3-mercaptopropionate) acetoacetate (PETMPA) by ¹ H NMR..... | 3 |
| 3. ¹ H NMR and ¹³ C NMR Spectra | 3 |

1. Solvent swelling

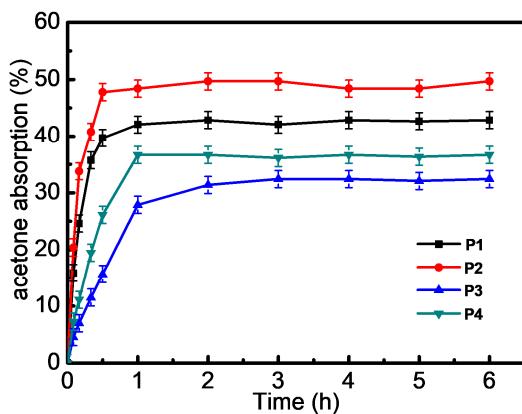


Figure S1. Solvent swelling (acetone absorption-time diagram) of P1, P2, P3 and P4.

2. Calculating the yield of TMPTAA and PETMPA by ^1H NMR

2.1 Calculating the yield of trimethylolpropane tris(3-mercaptacetoacetate) (TMPTAA) by ^1H NMR

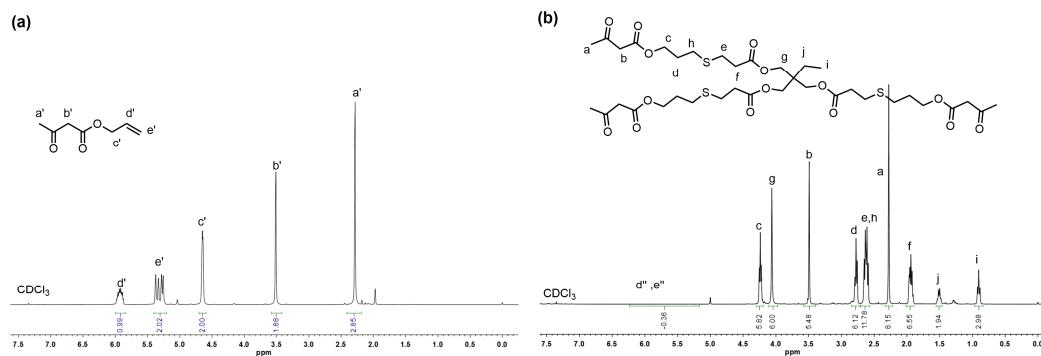


Figure S2. ^1H NMR Spectrum of (a) allyl acetoacetate and (b) trimethylolpropane tris(3-mercaptacetoacetate) (TMPTAA) (400 MHz, CDCl_3 , 7.26 ppm)

Figure S2a shows that the peak areas of c' is 4, and the peak area of d' is 0.99, the peak area of e' is 2.02; thus, the ^1H NMR peak areas correspond to the compound structure. Therefore, we can calculate the conversion yield on the basis of the peak area ratios. the yield of trimethylolpropane tris(3-mercaptacetoacetate) (TMPTAA) can be calculated as: $W(\%) = [3 \times A(d' + e') - A(d'' + e'')] / [3 \times A(d' + e')] = [3 \times (0.99 + 2.02) - 0.36] / [3 \times (0.99 + 2.02)] = 96\%$.

2.2 Calculating the yield of pentaerythritol tetra(3-mercaptopropionate) (PETMPA) by ^1H NMR

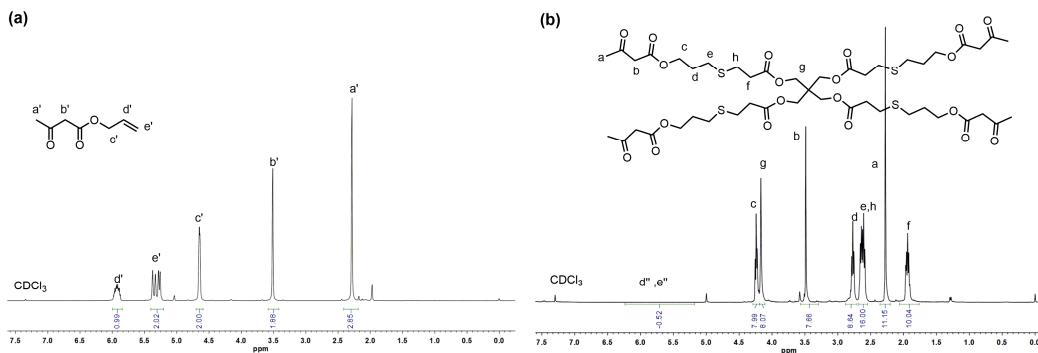


Figure S3. ^1H NMR Spectrum of (a) allyl acetoacetate and (b) pentaerythritol tetra(3-mercaptopropionate) (PETMPA) (400 MHz, CDCl₃, 7.26 ppm)

The yield of modified cardanol is calculated using the same method as described in section 2.1: the yield of pentaerythritol tetra(3-mercaptopropionate) acetoacetate (PETMPA) can be calculated as: W(%) = [4×A(d' + e')-A(d'' + e'')]/[4×A(d' + e')] = [4×(0.99+2.02) - 0.52] / [4×(0.99+2.02)] = 93%.

3. ^1H NMR and ^{13}C NMR Spectra

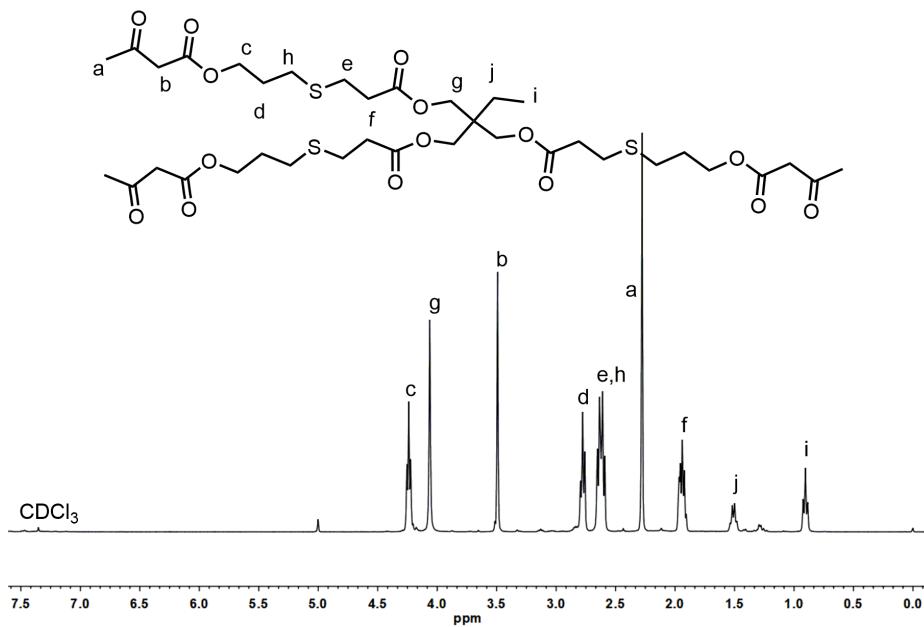


Figure S4. ^1H NMR Spectrum of trimethylolpropane tris(3-mercaptacetoacetate) (TMPTAA)
(400 MHz, CDCl_3 , 7.26 ppm)

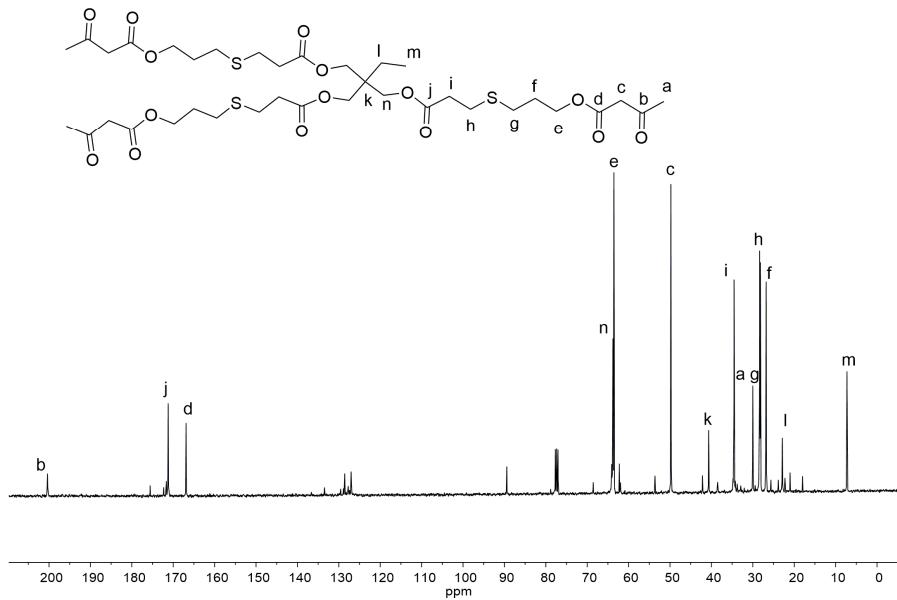


Figure S5. ^{13}C NMR Spectrum of trimethylolpropane tris(3-mercaptacetoacetate) (TMPTAA)
(100 MHz, CDCl_3 , 77 ppm)

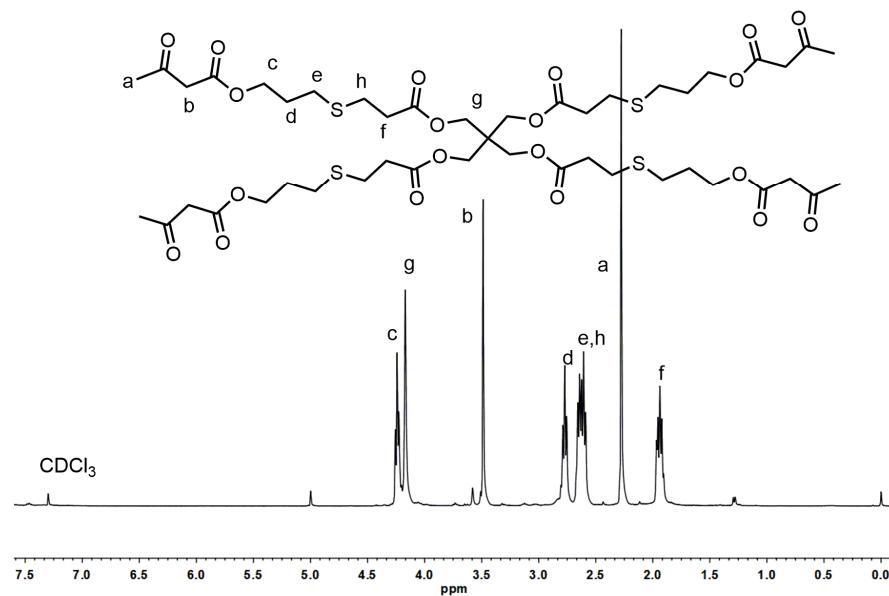


Figure S6. ^1H NMR Spectrum of pentaerythritol tetra(3-mercaptacetoacetate) (PETMPA)
(400 MHz, CDCl_3 , 7.26 ppm)

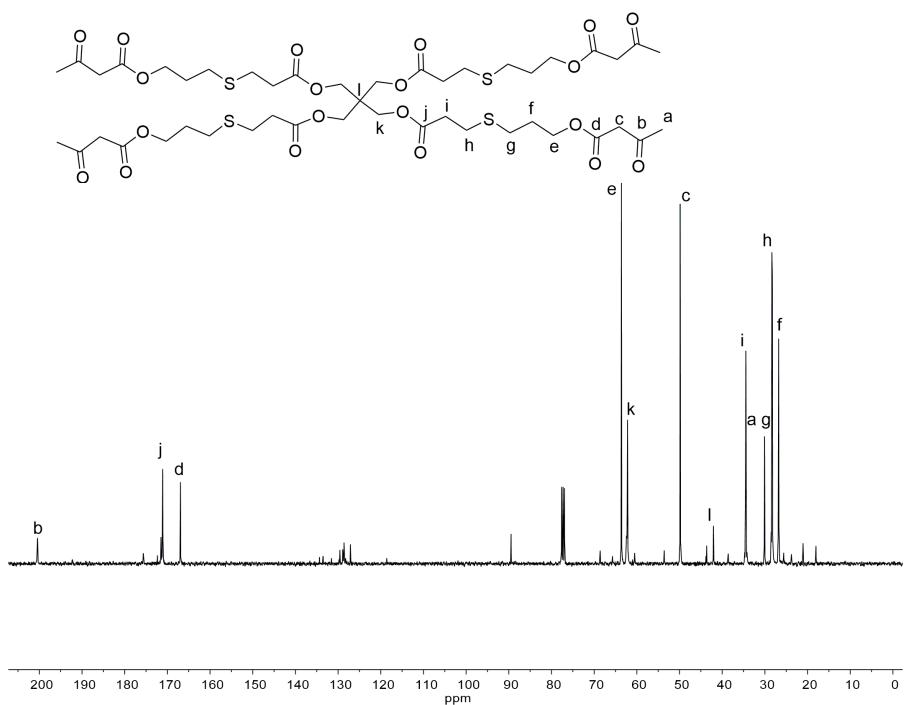


Figure S7. ^{13}C NMR Spectrum of pentaerythritol tetra(3-mercaptacetoacetate) (PETMPA)
(100 MHz, CDCl_3 , 77 ppm)