

Supplementary Information

Mechanical properties and structure under deformation of thiophene copolymers with cyclic siloxane units

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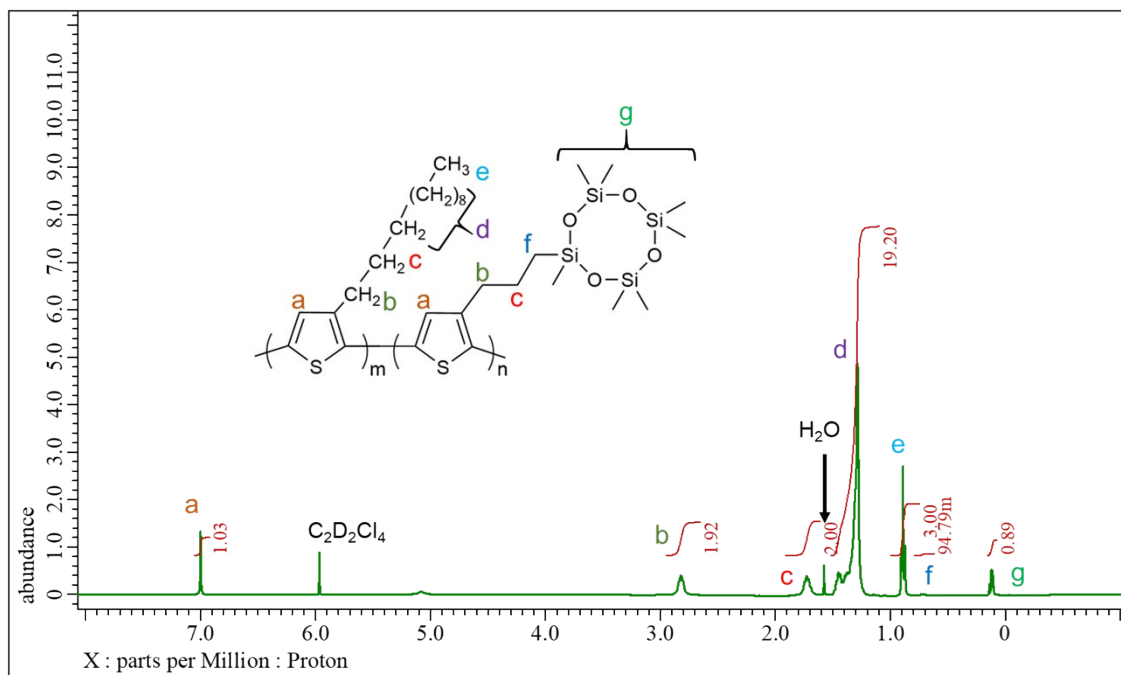


Figure S1. ^1H NMR spectrum of P(3DDT-3CSiT).

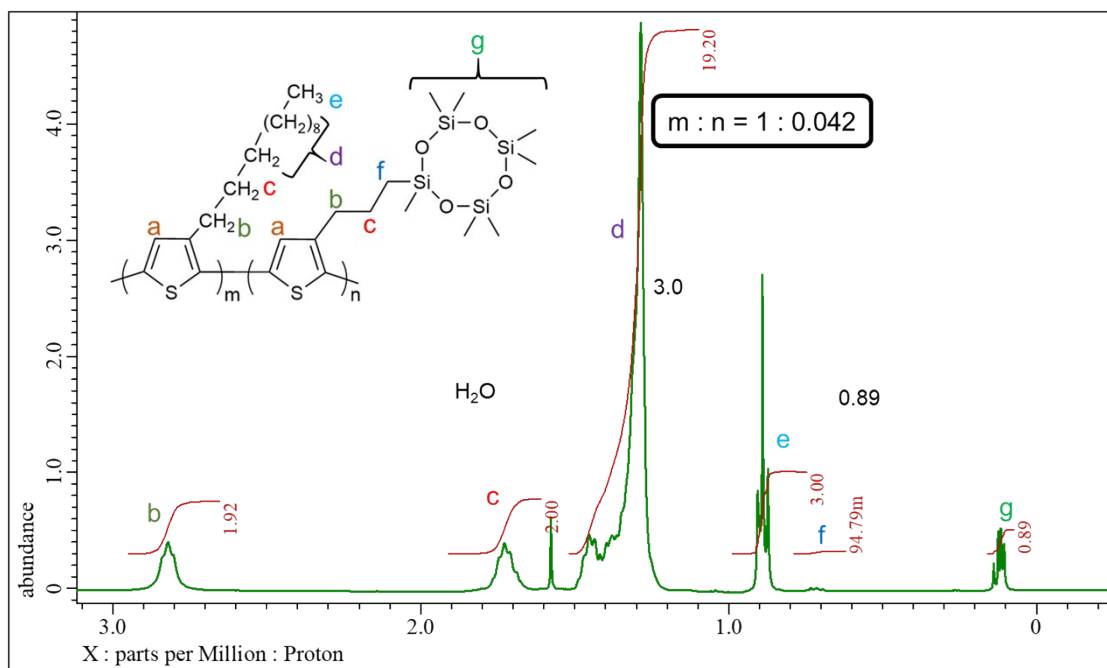


Figure S2. Expanded ^1H NMR spectrum of P(3DDT-3CSiT).

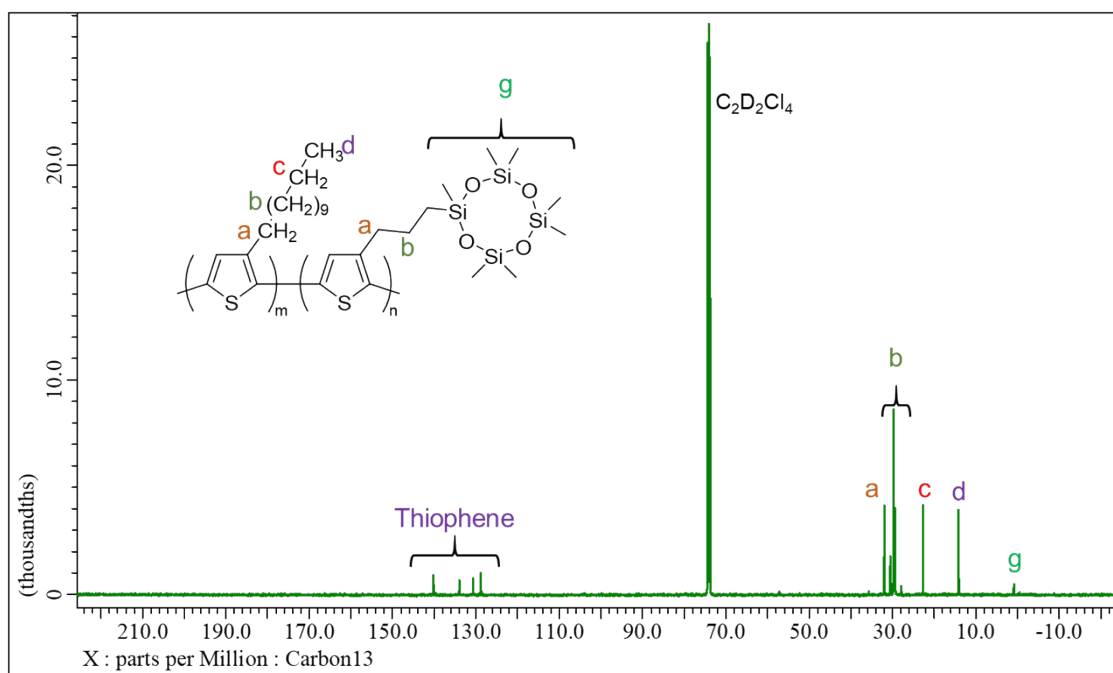


Figure S3. ^{13}C NMR spectrum of P(3DDT-3CSiT).

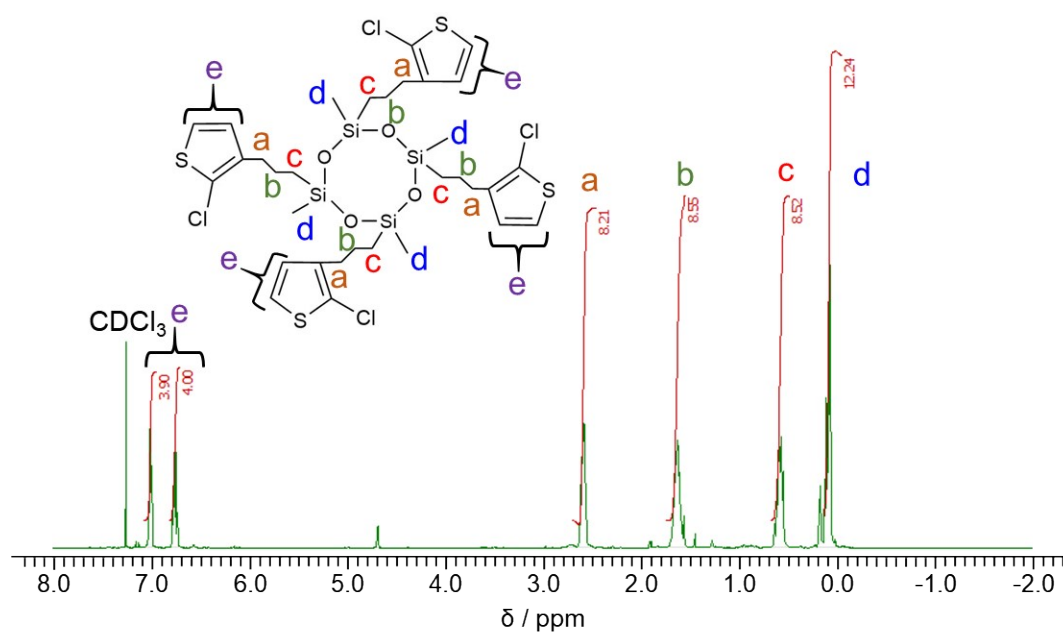


Figure S4. ^1H NMR spectrum of 3tetraCSiT.

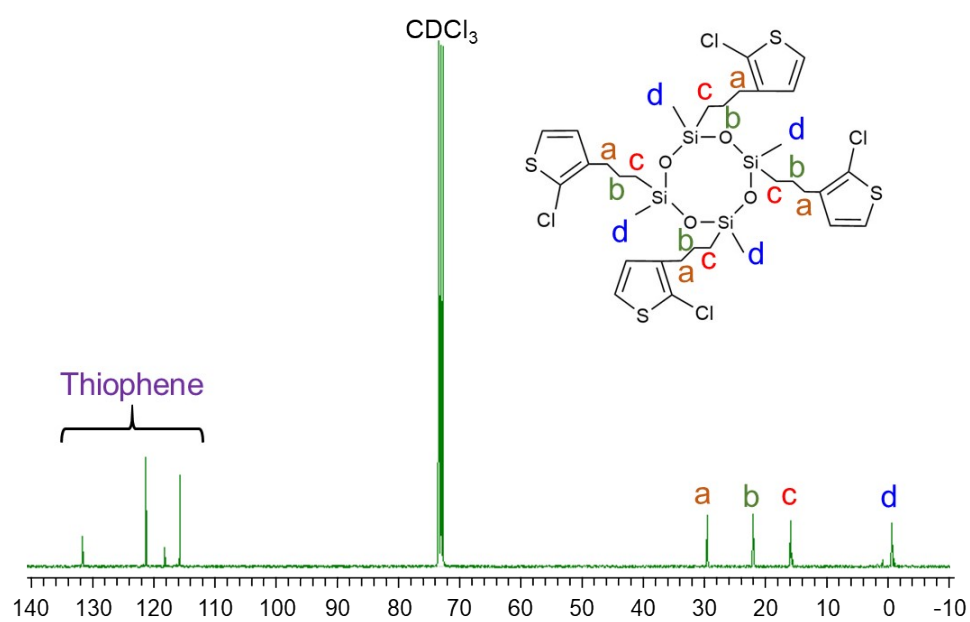


Figure S5. ^{13}C NMR spectrum of 3tetraCSiT.

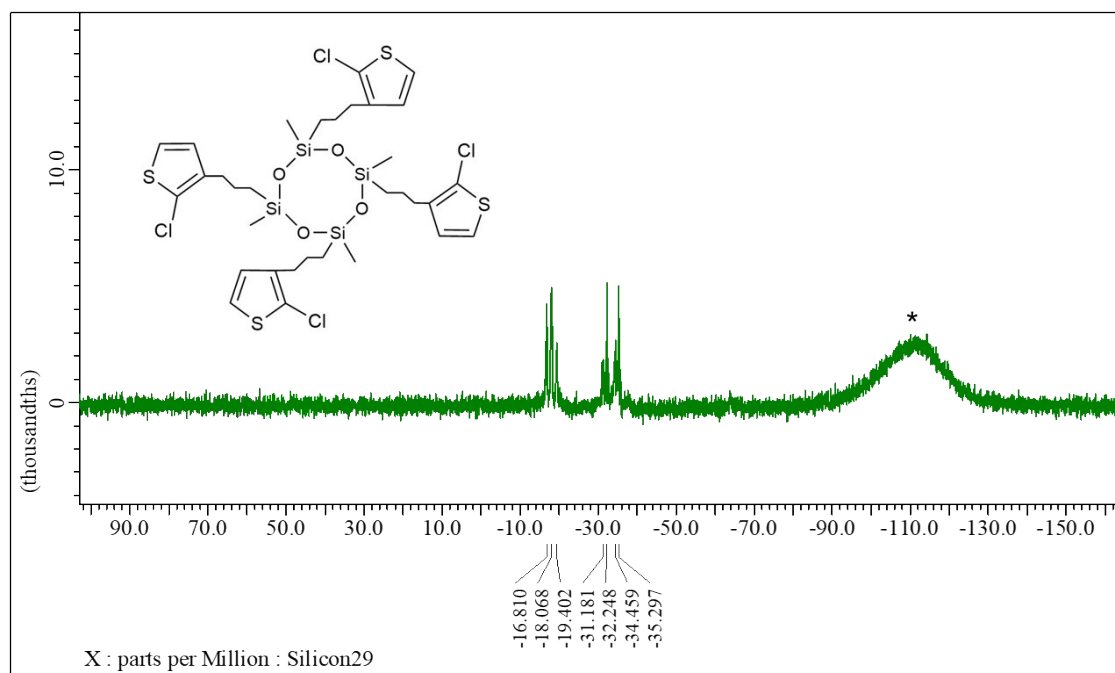


Figure S6. ^{29}Si NMR spectrum of 3tetraCSiT (* peak from SiO_2 of a NMR tube).

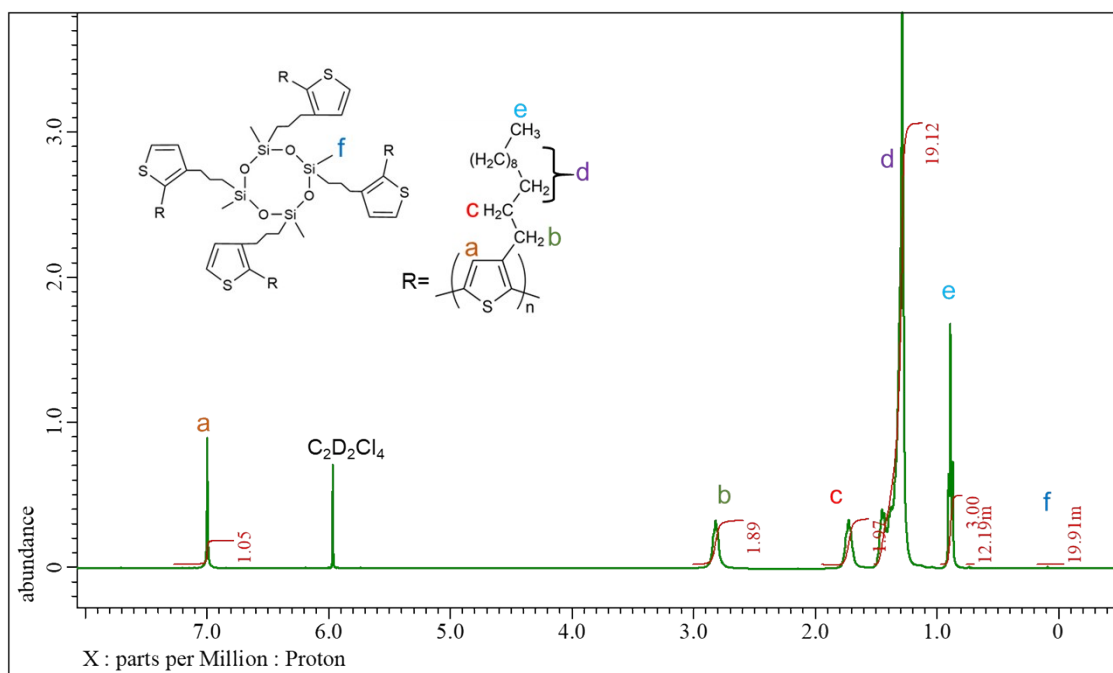


Figure S7. ^1H NMR spectrum of P(3DDT-3tetraCSiT).

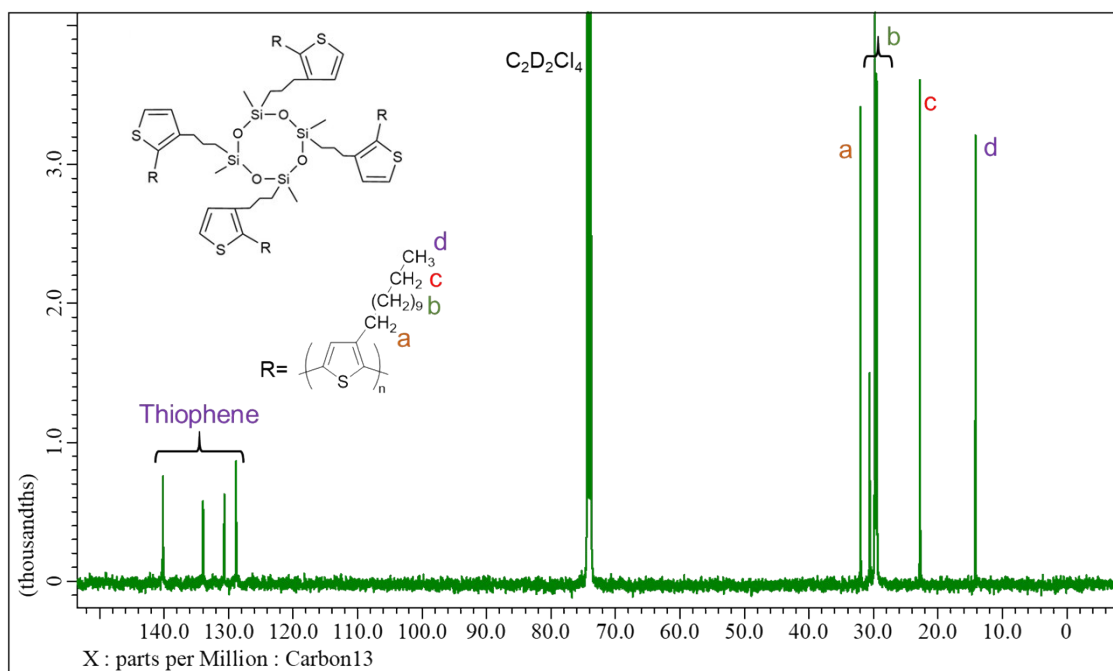


Figure S8. ^{13}C NMR spectrum of P(3DDT-3tetraCSiT).

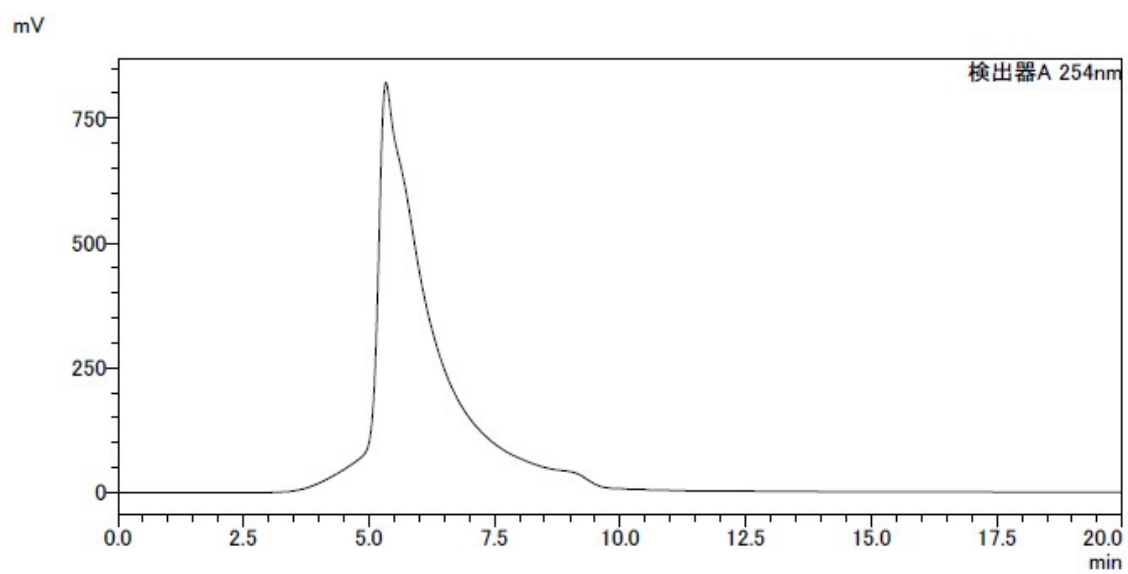


Figure S9. GPC chart of P(3DDT-3CSiT).

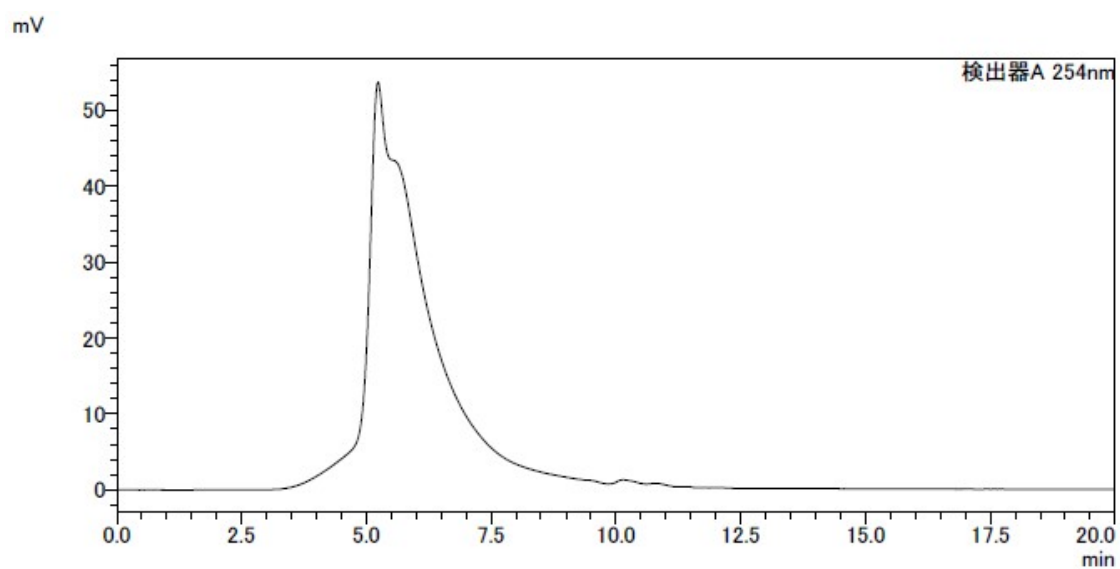


Figure S10. GPC chart of P(3DDT-3tetraCSiT).

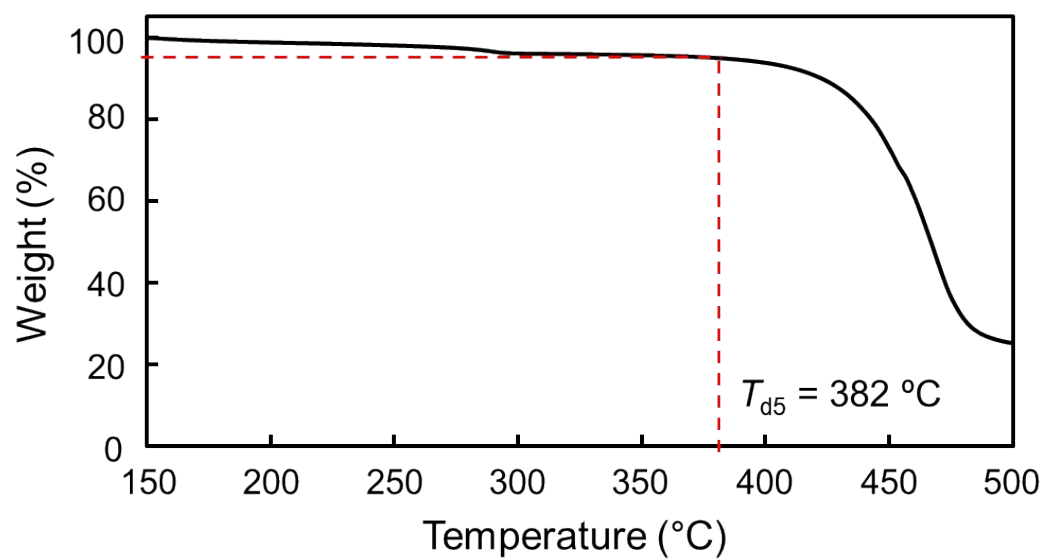


Figure S11. Thermogravimetric curve of P(3DDT-3CSiT).

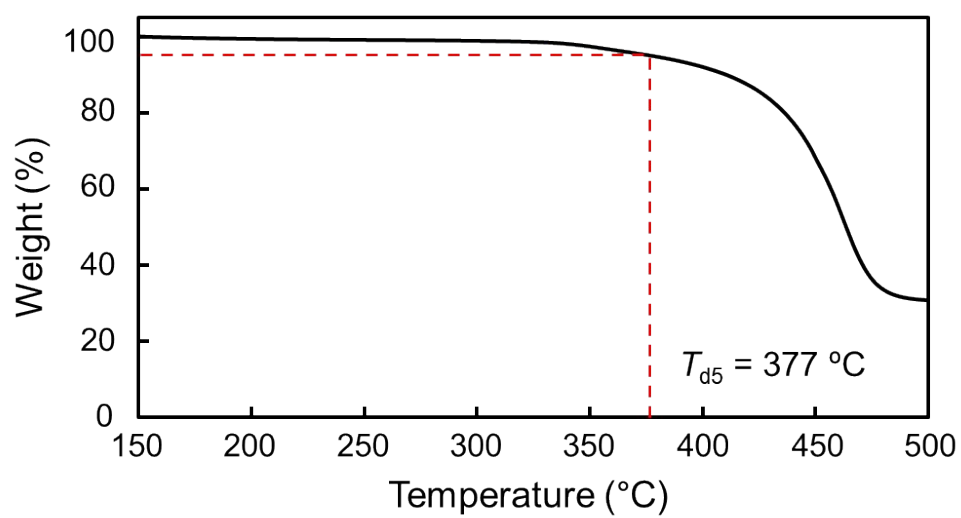


Figure S12. Thermogravimetric curve of P(3DDT-3tetraCSiT).

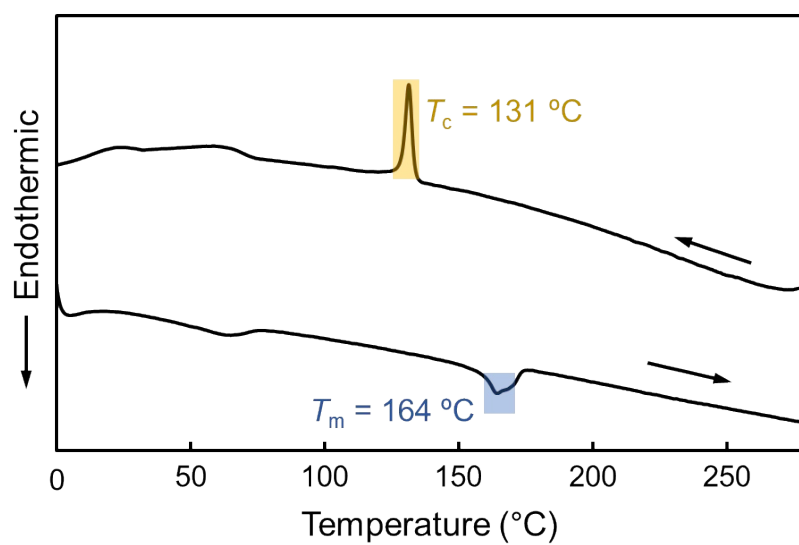


Figure S13. DSC thermogram of P3DDT.

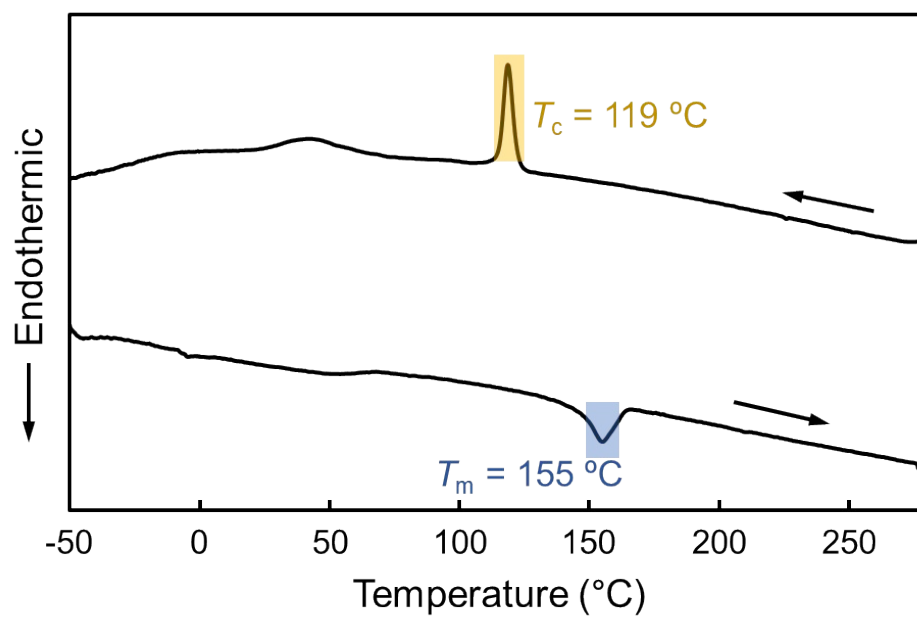


Figure S14. DSC thermogram of P(3DDT-3CSiT).

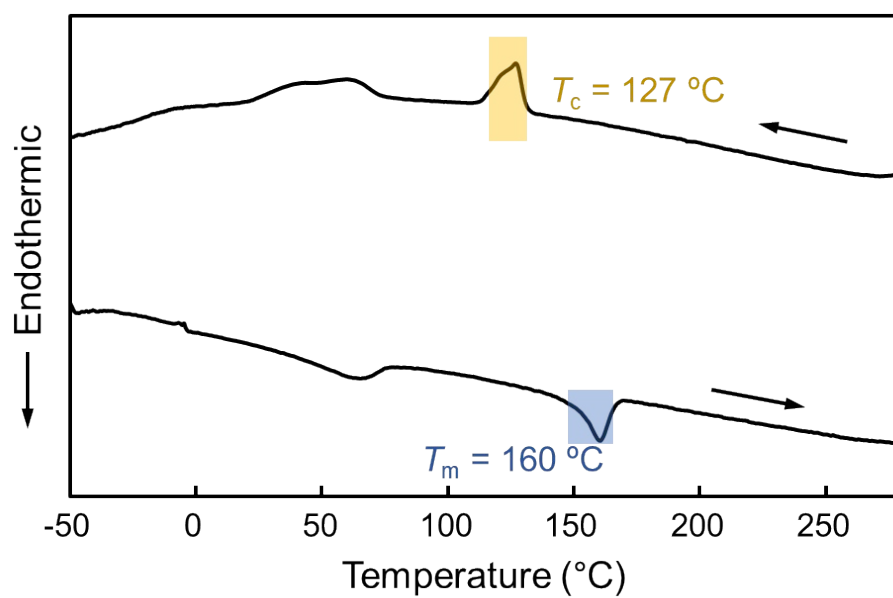


Figure S15. DSC thermogram of P(3DDT-3tetraCSiT).

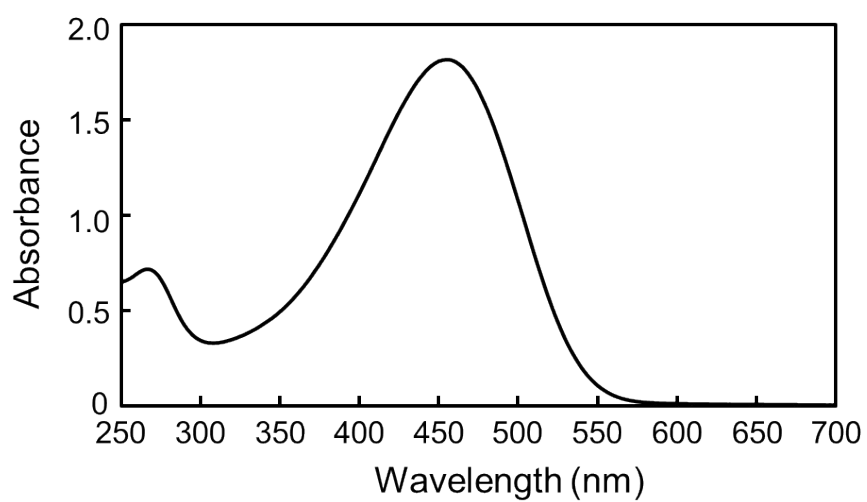


Figure S16. UV—vis absorption spectrum of 2.1×10^{-4} mol/L P(3DDT-3CSiT) in chloroform.

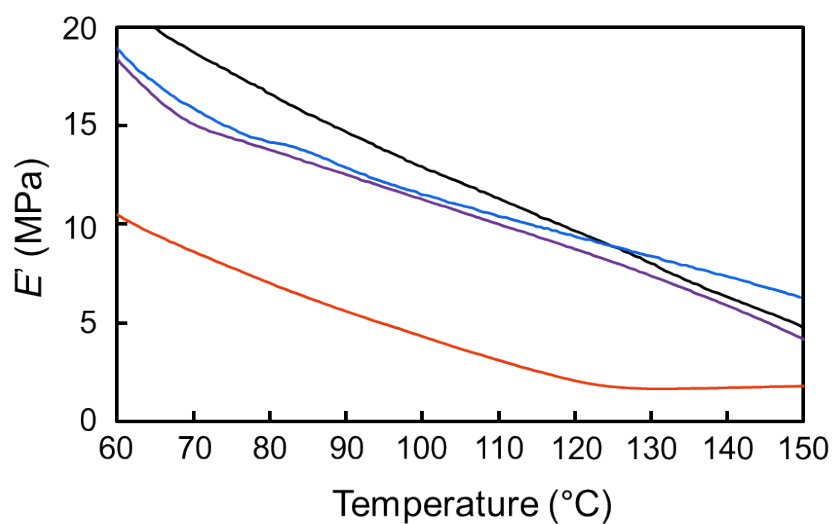


Figure S17. Expanded storage modulus of (black line) Noacid_P(3DDT-3CSiT), (blue line) Acid_anneal_P(3DDT-3CSiT), (red line) Acid_melt_P(3DDT-3CSiT) and (blue line) Melt_P(3DDT-3tetraCSiT) from 60 °C to 150 °C.

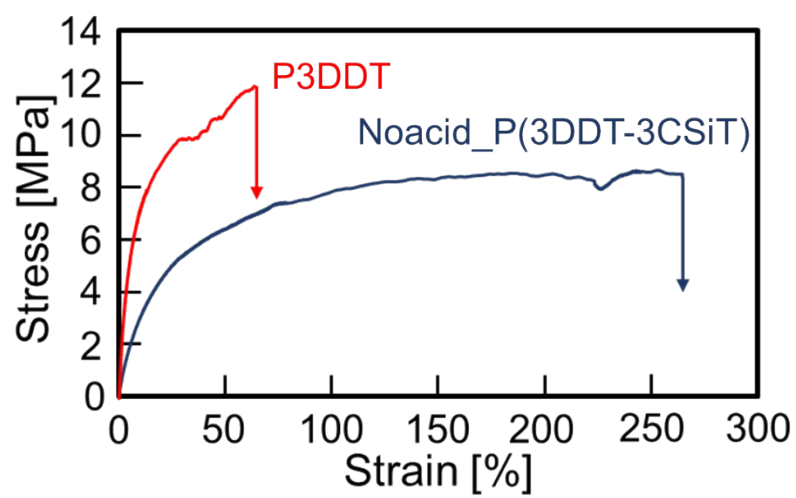


Figure S18. Strain-stress curves of P3DDT and Noacid_P(3DDT-3CSiT).

Table S1. Mechanical properties of Noacid_P(3DDT-3CSiT), Acid_anneal_P(3DDT-3CSiT), Acid_melt_P(3DDT-3CSiT) and Melt_P(3DDT-3tetraCSiT).

| Sample | Young's modulus | Tensile strength | Strain at beaking | Toughnes s |
|---------------------------|--------------------|---------------------|----------------------|-------------------|
| | MPa | MPa | % | MJ/m ³ |
| Noacid_P(3DDT-3CSiT) | 39±2.3 | 9.4±1.2 | 313±47 | 23 ±5.2 |
| Acid_anneal_P(3DDT-3CSiT) | 46±2.5 | 12.0±1.5 | 74±23 | 5.9±2.7 |
| Acid_melt_P(3DDT-3CSiT) | 41±3.8 | 8.1±1.5 | 64± 7.3 | 3.7±079 |
| Melt_P(3DDT-3tetraCSiT) | 43±4.3 | 8.9±1.1 | 104±12 | 7.4±1.4 |

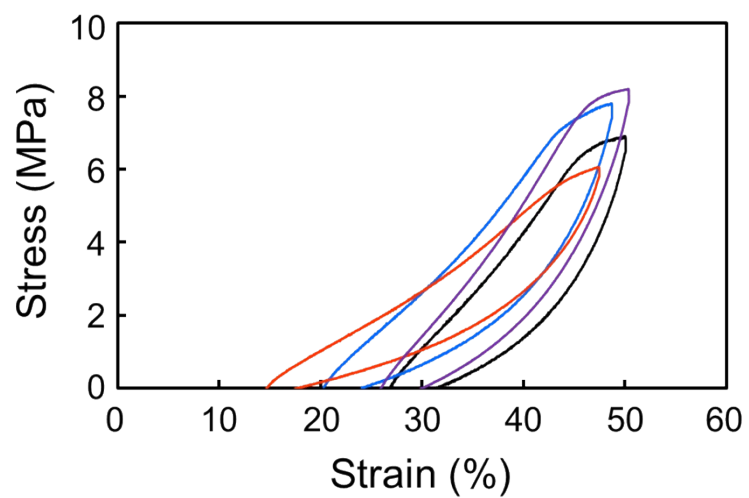


Figure S19. Strain-stress curves of cyclic tensile tests of (black line) Noacid_P(3DDT-3CSiT), (blue line) Acid_anneal_P(3DDT-3CSiT), (red line) Acid_melt_P(3DDT-3CSiT) and (blue line) Melt_P(3DDT-3tetraCSiT) in the 50% strain region.

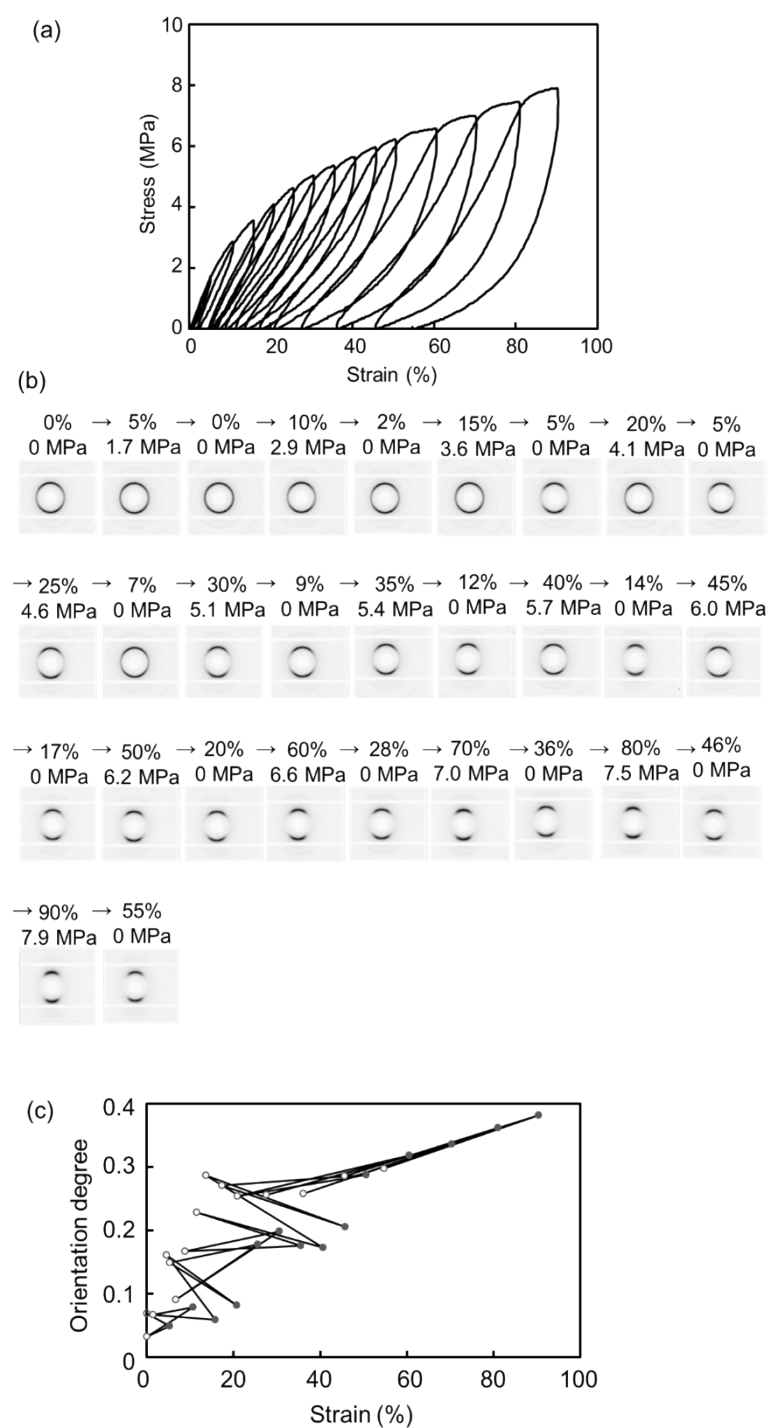


Figure S20. (a) Stress-strain curves, (b) 2D X-ray diffraction images, (c) orientation degrees of Noacid_P(3DDT-3CSiT) in *in situ* X-ray diffraction pattern measurements under cyclic tensile tests (black circles : loading states, and white circles : unloading states).

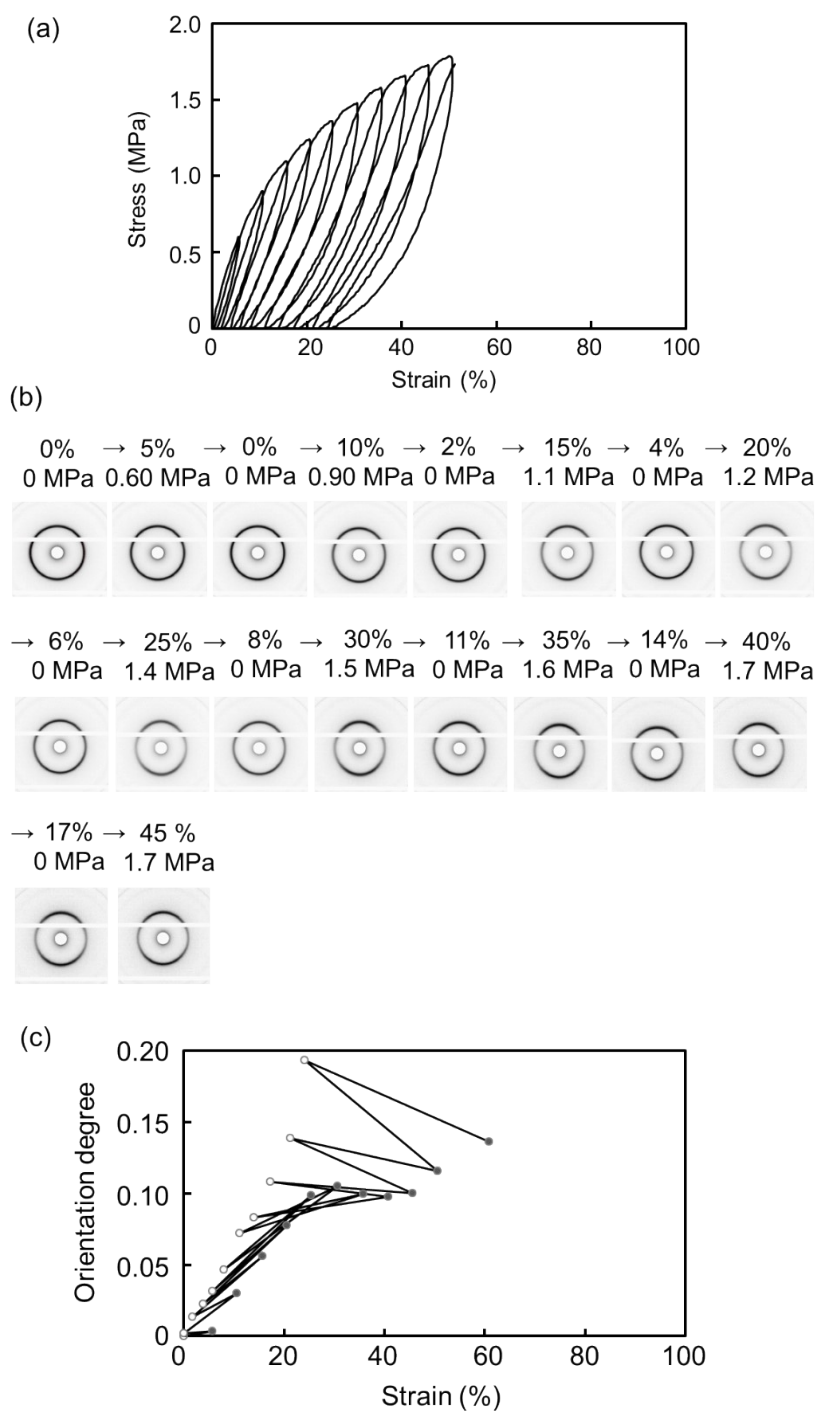


Figure S21. (a) Stress-strain curves, (b) 2D X-ray diffraction images, (c) orientation degrees of Melt_P(3DDT-3tetraCSiT) in *in situ* X-ray diffraction pattern measurements under cyclic tensile tests (black circles : loading states, and white circles : unloading states).

Electronic conductive measurements

The electrical resistances of cross-linked polythiophene films were measured in ambient atmosphere by two-point measurement using Keysight Technologies B1500A with voltage ranges of $-10 \sim 10$ V. VE-2030 (Vacuum Device Equipments) was utilized to deposit Au electrodes onto polymer cast film surfaces under vacuum. The length and thickness of the Au electrodes was 3 mm and 100 nm. The electrical resistivity (R) of these samples as function of voltage were calculated by Ohm's law. The average value in the range of the electrical resistivity levelling off were employed as the experimental results of these samples.

Table S2. Electrical resistivity and conductivity of Noacid_P(3DDT-3CSiT) and Acid_anneal_P(3DDT-3CSiT).

| | Electrical resistance | Electrical conductivity |
|---------------------------|-----------------------|-------------------------|
| | $G\Omega$ | 10^{-8} S/cm |
| Noacid_P(3DDT-3CSiT) | 3.0 | 0.065 |
| Acid_anneal_P(3DDT-3CSiT) | 0.19 | 1.0 |