Supplementary information

Bioderived copolymer alternatives to poly(styrene-*co*-maleic anhydride) *via* RAFT-mediated copolymerization

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Contents

Materials

Styrene (99.9%, 10-15 ppm 4-tert-butylcatechol inhibitor, Merck) and indene (>99%, 10-15 ppm 4-tert-butylcatechol inhibitor, Merck) were eluted through an aluminium oxide column thrice, 30 minutes before polymerizations commenced. Maleic anhydride (99%, Merck) was purified *via* recrystallization in freshly distilled chloroform. AIBN was recrystallized in methanol. 1,3,5-Trioxane (>99%, Merck) was utilized as an internal standard and was purified *by* vacuum sublimation at 50 °C overnight in a sealed Schlenk flask. Carbon disulfide (>99.9%, Merck), (1-bromoethyl)benzene (97%, Merck), triethylamine (>99.5%, Merck), 1-butanethiol (99%, Merck), dimethylsulfoxide (anhydrous, >99.9%, Merck), 3,5-dimethylpyrazole (99%, Merck), 1,4-dioxane (>99.5%, anhydrous, Merck), $(CD_3)_2CO$ (deuteration degree min. 99.9% for NMR spectroscopy, MagniSolv™, Merck) and $CDCl_3$ (deuteration degree min. 99.8% for NMR spectroscopy, MagniSolv™, Merck) were used as received.

Characterization

Size Exclusion Chromatography (SEC)

SEC analyses employed THF (5 v/v% AcOH with 0.125% BHT, Merck, for HPLC, ≥99.9%) as the mobile phase with samples dissolved at 2 mg/mL and filtered using 0.45 µm RC filters (Sartorius) prior to analysis. The analysis was performed on an Agilent 1260 HPLC instrument fitted with a quaternary pump, a column compartment thermostated at 30 °C, a differential refractometer set at 30 °C and a diode array UV detector set at 254 and 320 nm. The columns utilized were two Agilent Technologies PLgel 5 Mixed-C columns (300 × 7.5 mm i.d.) and a PLgel 5 Guard column (50 × 7.5 mm i.d.). The flow rate during analysis was 1.0 mL/min and the injection volume per sample was 100 µL. The system was calibrated using narrow PS calibration standards with a molar mass range of 580–2.0 ×106 g/mol.

Nuclear Magnetic Resonance (NMR) Spectroscopy

Samples were diluted/dissolved using $(CD_3)_2CO$ or $CDCl_3$ (specified per sample) and analyzed using a 400 MHz and 600 MHz Ascend Bruker spectrometer. Data analysis was performed using Maestronova v11.3.

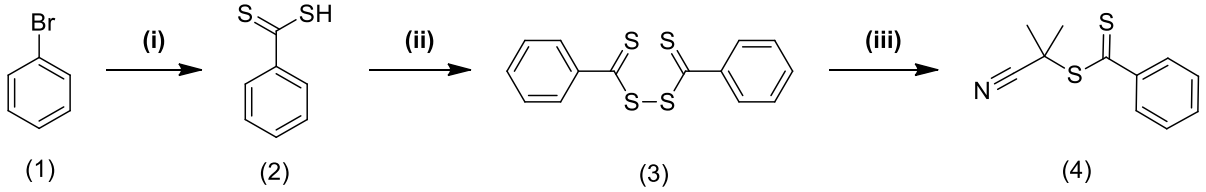
Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) spectroscopy

Analyses was conducted on a Thermo Scientific Nicolet iS10 Smart iTR spectrometer using 128 scans over the wavelength range of 600–4000 cm^{-1}, with a background spectrum (64 scans) obtained prior to each sample analyzed.

Experimental procedures

RAFT agent synthesis

Synthesis of the dithiobenzoate RAFT agent (2-cyanopropan-2-yl benzodithioate)



Scheme s1: *i) a) Mg(0), I_2, THF, 25 °C; b) CS_2, 0 °C - 25 °C; c) H_3O^+, 25 °C; ii) I_2, DMSO, 25 °C; iii) AIBN, ethyl acetate, 85 °C.*

Step i

An oven dried 250 mL flask was attached to an argon line *via* an adaptor. To this was added a Teflon stir bar, a crystal of iodine and oven dried magnesium turnings (1.3 g, 51 mmol, 1.0 eq.). A reflux condenser was attached to the central neck of the flask. To the top of the condenser, was added an anhydrous, oven dried, drying tube containing anhydrous calcium chloride. To the other side neck of the flask was added a 100 mL pressure equalizing dropping funnel with a stopper slightly ajar with some tissue paper. The entire apparatus was flashed with argon for 10 minutes. After this anhydrous THF (20 mL) was added in a single portion to the reaction setup *via* the dropping funnel and the mixture stirred for 2 minutes. During this time a mixture of bromobenzene (7.9 g, 50 mmol, 1 eq.) and anhydrous THF (40 mL) was prepared. This mixture was added to the closed dropping funnel and 2-3 mL of the solution added to the flask *via* the dropping funnel. The flask was heated with a water bath at 38 °C, the mixture was left to stir for 10 minutes. During this time the reaction changed from a brown colour (consumption of iodine) to a metallic, cloudy colour. The reaction was not heated at this point and was left to stir at 25°C (it was ensured that the reaction did not increase temperature past 40 °C). The rest of the solution in the dropping funnel was added dropwise (2 drops per second) and the reaction mixture left to stir for a further 2 h till the flask was cool to the touch, the solution was a metallic grey colour and all the magnesium turnings were consumed. The flask was thereafter placed in an ice bath for 5 minutes. Carbon disulfide (3.8 g, 50 mmol, 1eq.) was added to the dropping funnel and added to the cooled reaction dropwise (2 drops per second). During this process the reaction changed to a deep red colour. Once all the carbon disulfide was added, the reaction was left to stir for 1 h at ambient temperature. To quench the reaction, water (50 mL) was added to the dropping funnel and added to the reaction mixture dropwise (2 drops per second) until the reaction stopped generating heat (~40 mL water). The solution was filtered to collect any residual magnesium

turnings and the THF evaporated under reduced pressure at 30 °C. The solution was acidified with a 30 w/v% HCl solution. This was done *via* dropwise addition of ~5 mL of the acid or until a deep purple colour was observed and remained. The acidified mixture was then placed into a 500 mL separatory funnel and extracted with diethyl ether (3×50 mL) (the extracted solution should become progressively less purple and eventually become completely clear). The combined organic layers were then washed with water (50 mL). The organic layer was collected and dried with anhydrous magnesium sulfate for 3 minutes. The mixture was then filtered and concentrated at 30 ℃ yielding **compound 2** as a purple oil.

Step ii

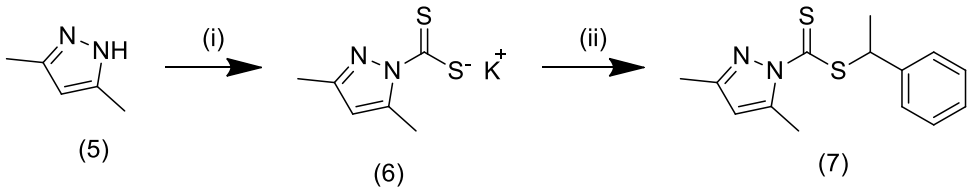
An oven dried one necked 250 mL flask was charged with the purple oil from step 1. To this flask was added a stirrer bar and absolute ethanol (40 mL). A crystal of iodine and DMSO (7.8 g, 100 mmol, 2 eq.) were added and the reaction stirred at 25 ℃ for 1 hour. The reaction was then left in the freezer overnight to crystallize. The product was collected *via* filtration and dried further in a vacuum oven at 25℃ for 24 h. This reaction afforded **compound 3** as a deep purple solid, 70%.

Step iii

To an oven-dried 250 mL two necked flask, fitted with a Teflon stirrer bar, was added **compound 3** (8.7 g, 28 mmol, 1 eq.) and the flask purged with dry argon gas. AIBN (7.0 g, 43 mmol, 1.5 eq.) and ethyl acetate (45 mL) were added to the solution and the flask fitted with a reflux condenser (stoppered with an oven-dried anhydrous calcium chloride drying tube). The setup was purged with argon for 2 minutes after which the argon adaptor was removed and replaced with a glass stopper. The reaction mixture was refluxed at 85℃ for 6 h and subsequently concentrated *via* evaporation (30℃) and purified *via* column chromatography on silica gel with 100% hexane to 10% ethyl acetate/90% hexane to yield 67% of **compound 4** as a deep purple oil. Purity was determined *via* ^{1}H NMR spectroscopy in C*D*Cl$_3$ to be 88%.

^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.91 (d, J = 4.0 Hz, 2H), 7.56 (t, J = 4.0 Hz, 1H), 7.40 (t, J = 4.0 Hz, 2H), 1.94 (s, 6H). This matches the literature signals.[1]

Synthesis of dithiocarbamate RAFT agent (1-phenylethyl 3,5-dimethyl-1*H*-pyrazole-1-carbodithioate)



Scheme S2: *i) a) KOH, THF, 4 ℃; b) CS_2, 0 ℃ - 25 ℃; ii) 1-Bromoethyl benzene, acetone, H_2O, 4 ℃.*

Step i

CTA synthesis was adapted from literature.[2] To a 250 mL oven-dried flask was added KOH (3.98 g, 70.9 mmol) in THF (60 mL). This mixture was thereafter stirred at 4 °C and 3,5-dimethylpyrazole (6.19 g, 64.4 mmol) in THF (27 mL) added to the solution which was stirred for an additional 5 minutes at 4 °C. CS_2 (6.38 g, 83.8 mmol) was thereafter added dropwise while stirring at 4 °C,

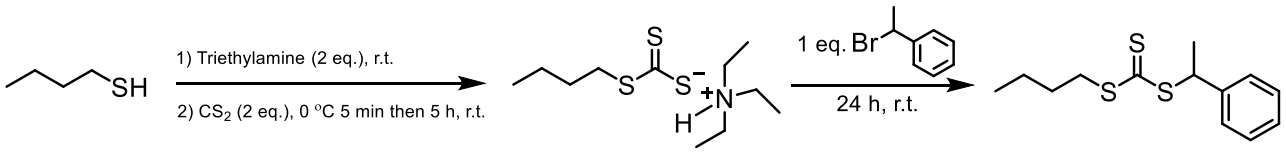
resulting in a colour change from a colorless to bright yellow and subsequently the solution was allowed to stir at ambient temperature for 1 h to afford a dark orange suspension. The mixture was filtered and the solid potassium 3,5-dimethyl-1*H*-pyrazole-1-carbodithioate (KPC) was washed with diethyl ether and dried under vacuum.

Step ii

A solution of KPC (7.43 g, 35.3 mmol) in acetone (65 mL) and DI water (65 mL) was prepared in a 250 mL round bottom flask and stirred at 4 °C, followed by the slow addition of 1-bromoethyl benzene (6.53 g, 35.3 mmol). After 5 minutes, the solution was stirred at ambient temperature for 3 h resulting in a colour change from dark orange to pale yellow. The acetone was evaporated under reduced pressure and the aqueous dispersion was further diluted with 100 mL DDI water. The product was extracted using diethyl ether (3 × 100 mL), stirred over $MgSO_4$ overnight and then concentrated. **Compound 7** was recrystallized from methanol to afford a yellow solid which was collected *via* filtration and thereafter dried under vacuum at 40 °C overnight resulting in bright yellow crystals with a 70% yield. Purity was determined with ^{1}H NMR in $(CD_3)_2CO$ to be 94%.

^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ: 7.50–7.46 (m, 2H, *m*-aromatic), 7.39–7.33 (m, 2H, *o*-aromatic), 7.30–7.25 (m, 1H, *p*-aromatic), 6.26 (s, 1H, -N-C(CH_3)-C**H**-C(CH_3)-N-N-), 5.05–4.99 (q, 1H, -S-C**H**(CH_3)-Ph), 2.66 (s, 3H, -N-C(C**H$_3$**)-CH-C(CH_3)-N-N-), 2.18 (s, 3H, -N-C(CH_3)-CH-C(C**H$_3$**)-N-N-), 1.77–1.74 (d, 3H, -S-CH(C**H$_3$**)-Ph).

Synthesis of trithiocarbonate RAFT agent (butyl (1-phenylethyl) carbonotrithioate)



Scheme S3. *Synthesis of butyl (1-phenylethyl) carbonotrithioate*

Butanethiol (5.00 g, 55.4 mmol) and triethylamine (11.2 g, 111 mmol) were dispersed in dry chloroform (40 mL) and stirred at ambient temperature for 0.5 h. The solution was cooled to 0 °C and carbon disulphide (8.44 g, 111 mmol) added dropwise. The solution was stirred at 0 °C for an additional 10 minutes, followed by 5 h at ambient temperature. 1-Bromoethylbenzene (10.3 g, 55.4 mmol) was added dropwise while cooling at 0 °C, followed by stirring at ambient temperature for 24 h. The reaction mixture was transferred to a 500 mL separatory funnel and washed with DI water (2×150 mL), H2SO4 (2 M) (1×100 mL), brine (2×100 mL) and finally DI water (2×150 mL). The organic phase was dried over MgSO4 for 1 h at ambient temperature, filtered and subsequently concentrated under vacuum, yielding a viscous dark orange oil. The product was further purified via column chromatography (95 v/v% pentane, 5 v/v% ethyl acetate), the fractions concentrated and the product dried under high vacuum for 24 h. The product was obtained in good yield (90%) and purity was determined to be 95% via ^{1}H NMR spectroscopy.

^{1}H NMR (600 MHz, $(CD_3)_2CO$): δ 7.454–7.423 (m, 2H, *m*-aromatic), 7.378–7.338 (m, 1H, *p*-aromatic), 7.305–7.271 (m, 2H, *o*-aromatic), 5.373–5.328 (q, 1H, $CH_3CH_2CH_2CH_2SC(=S)SC\mathbf{H}CH_3Ph$), 3.409–3.373 (t, 2H, $CH_3CH_2CH_2C\mathbf{H_2}SC(=S)SCHCH_3Ph$), 1.759–1.732 (d, 3H, $CH_3CH_2CH_2CH_2SC(=S)SCHC\mathbf{H_3}Ph$), 1.694–1.637 (q, 2H,

$CH_3CH_2C\mathbf{H_2}CH_2SC(=S)SCHCH_3Ph$), 1.456–1.388 (sext, 2H, $CH_3C\mathbf{H_2}CH_2CH_2SC(=S)SCHCH_3Ph$), 0.937–0.902 (t, 3H, $C\mathbf{H_3}CH_2CH_2CH_2SC(=S)SCHCH_3Ph$).

Polymerization procedures

A 100 mL oven-dried flask was charged with styrene (or indene) (50 eq.) and maleic anhydride (or itaconic anhydride) (50 eq.). Thereafter AIBN (0.2 eq.), the RAFT agent (1.0 eq.) and 1,3,5-trioxane as the internal standard (0.05 eq.) were added. Lastly, 1,4-dioxane was included to afford a polymerization concentration of 30 w/v%. The mixture was thereafter sparged with argon for 30 minutes. Near the end of this time interval (2 minutes left of sparging), a T_0 sample was collected. Once the sparging was complete the polymerization was placed into a preheated silicon oil bath (70 °C) and the polymerization commenced for 24 h. At each kinetic time interval, a sparged needle was utilized to collect 0.5 mL of the polymerization medium (0.1 mL for ^{1}H NMR spectroscopic analysis and 0.4 mL to be dried for SEC analysis). The remaining copolymerization mixture could be isolated *via* precipitation into isopropanol (for IAnh comprising copolymers) or pentane (for MAnh comprising copolymers).

The SEC samples were dried in a vacuum oven overnight at 40 °C, where the samples were thereafter analyzed within the week of the experiment to ensure minimum ring opening of the anhydride groups along the polymer backbone. The 0.1 mL kinetic samples collected for ^{1}H NMR spectroscopic analysis were diluted with either $CDCl_3$ (0.5 mL) or $(CD_3)_2CO$ (0.5 mL) and thereafter analyzed on the 400 MHz Bruker Ascend spectrometer.

Calculations and equations utilized for kinetic analysis

Equation S1. Comonomer conversion was calculation using vinylic proton integrals determined *via* ^{1}H NMR spectroscopic analysis of polymerization kinetic samples, with 1,3,5-trioxane as internal standard. Using SMAnh as a representative copolymerization; integral ranges for the vinylic protons were determined and used to calculate α.

$$\alpha = \left(1 - \frac{I_{tx}^{STY/MAnh}}{I_{t0}^{STY/MAnh}}\right) \times 100$$

$$\int STY1 = 5.824 - 5.784\ ppm, \int STY2 = 5.247 - 5.215\ ppm, \int MAnh = 7.323 - 7.319\ ppm$$

Equation S2. M_n^{theo} calculation using monomer conversions calculated using the above equation.

$$M_n^{theo} = \frac{[STY] \times MW_{STY} \times \alpha_{STY}}{[CTA]} + \frac{[MAnh] \times MW_{MAnh} \times \alpha_{MAnh}}{[CTA]} + MW_{CTA}$$

Where MW_{STY}, MW_{MAnh}, MW_{CTA} are the molecular weights of STY, MAnh and the CTA respectively, for a representative SMAnh copolymerization. $\alpha_{STY/MAnh}$ is the monomer conversion calculated using **Equation S1**.

Experimental data

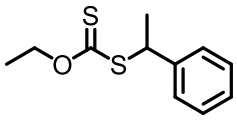
***Table S1**: Kinetic data of copolymer systems*

Copolymer [a]	α 24 h (%) [b]	M_n^{theo} (g/mol) [c]	M_n^{SEC} (g/mol) [d]	$Đ$ [d]	k_p^{app} (h^{-1}) [e]
SMAnh**1**	93	9 700	9 200	1.18	(0.02) 0.16
SMAnh**2**	98	10 000	10 200	1.13	0.54
SMAnh**3**	93	10 100	9 500	1.17	0.37
IMAnh**1**	51	5 300	3 600	1.26	(0.02) 0.09
IMAnh**2**	97	9 900	6 100	1.37	0.28
IMAnh**3**	98	9 100	6 200	1.25	0.28
IMAnh**X**	95	10 400	13 700	2.07	-
SIAnh**1**	STY – 93 IAnh – 97	10 400	8 000	1.15	STY – 0.14 IAnh – 0.16
SIAnh**2**	STY –93 IAnh – 97	10 600	7 700	1.25	STY – 0.15 IAnh – 0.18
SIAnh**3**	STY – 39 IAnh – 79	6 700	4 500	1.37	STY – 0.04 IAnh – 0.10
SIAnh**X**	98	10 800	22 100	1.36	-
IIAnh**1**	Ind – 20 IAnh – 45	3 800	3 400	1.29	Ind – 0.007 IAnh – (0.003) 0.002
IIAnh**2**	Ind – 47 IAnh – 74	6 900	3 100	1.64	Ind – 0.05 IAnh – 0.10
IIAnh**3**	Ind – 57 IAnh – 83	7 900	3 600	1.55	Ind – 0.04 IAnh – 0.12
IIAnh**X**	64	7 200	15 700	1.45	-

a – Copolymer legend provided in **Figure 1**, where the number in bold indicates the CTA utilized. The codes including **X**, indicate the use of a xanthate (structure provided below).
b – Monomer conversion determined *via* ^{1}H NMR spectroscopy using 1,3,5-trioxane as internal reference and **Equation S1**
c – Calculated using **Equation S2**
d – Determined *via* SEC analysis using THF (5% AcOH) as mobile phase and PS calibration standards
e – Calculated using the semilogarithmic curves presented in **Figures S1–4**.

Xanthate-mediated copolymerizations of bio-derived monomers

Xanthates generally provide poor control over the RAFT-mediated polymerization of "more activated" monomers (such as those investigated in this study). While it is known that xanthates cannot be successfully employed for the RAFT-mediated synthesis of SMAnh, little is known about the RAFT-mediated synthesis of SIAnh, IMAnh and IIAnh. Therefore, three preliminary copolymerizations were performed (IMAnh**X**, SIAnh**X** and IIAnh**X**, **Table S1**) using the xanthate indicated below. The well-controlled RAFT-mediated synthesis of IMAnh**X** was unsuccessful and IMAnh with high $Đ$ was obtained. The SIAnh**X** and IIAnh**X** copolymerizations exhibited slightly better control, as $Đ$<1.5 could be obtained, but as M_n^{SEC} was considerably larger then M_n^{theo}, it was concluded that the xanthate had not provided adequate control over the copolymerizations. This RAFT agent was therefore not utilized for the subsequent kinetic investigation.



Kinetic analyses

SMAnh

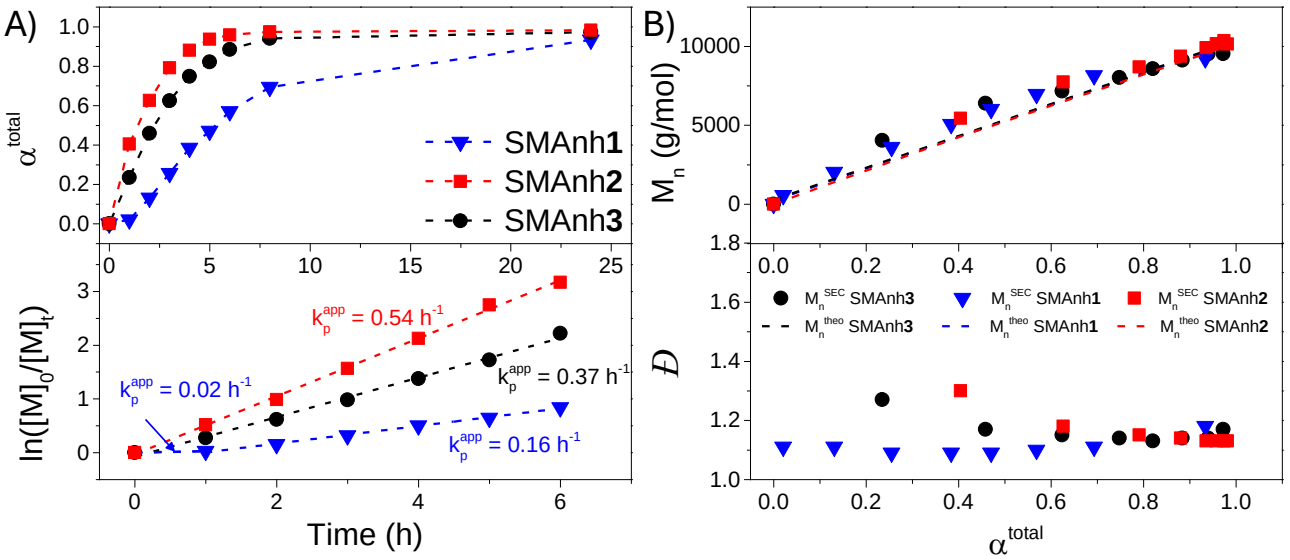


Figure S1: *A) Monomer conversion and ln(M_0/M_n) as a function of time for the copolymerization of styrene and maleic anhydride using a dithiobenzoate (SMAnh**1**), a dithiocarbamate (SMAnh**2**) and trithiocarbonate (SMAnh**3**) CTA. B) M_n and dispersity (Đ) as a function of the total monomer conversion (α^{total}) for the copolymerization of styrene and maleic anhydride, using a dithiobenzoate (SMAnh**1**), a dithiocarbamate (SMAnh**2**) and trithiocarbonate (SMAnh**3**) CTA. Total monomer conversions are employed as these copolymerizations exhibited strong alternating characteristics (equimolar comonomer consumption).*

IMAnh

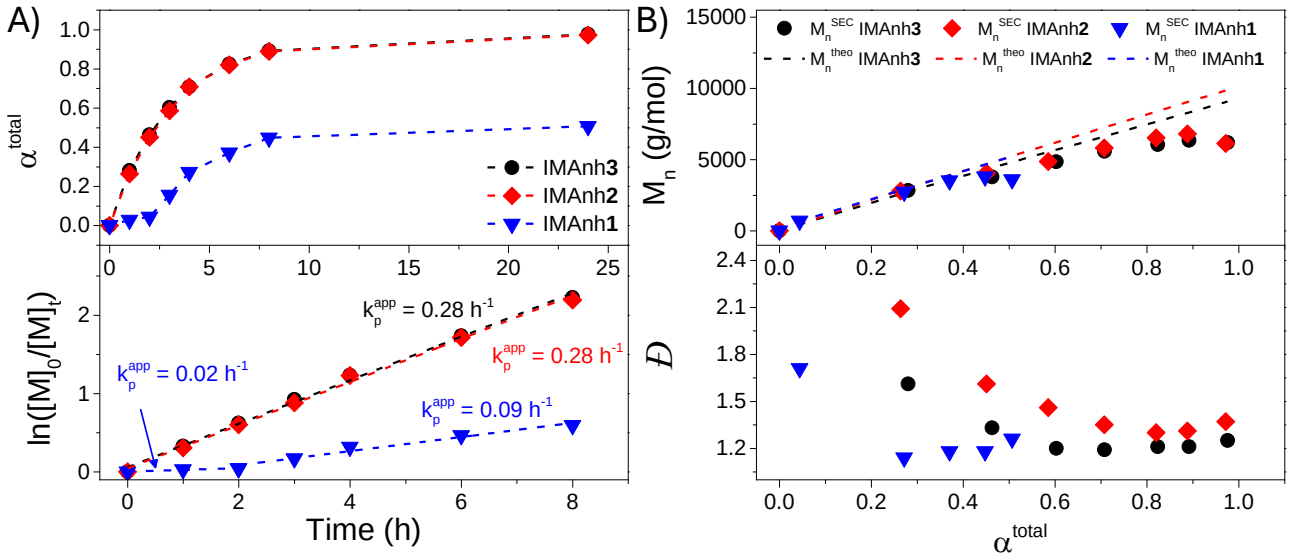


Figure S2: *A) Monomer conversion and ln(M_0/M_n) as a function of time for the copolymerization of indene and maleic anhydride using a dithiobenzoate (IMAnh**1**, trithiocarbonate (IMAnh**3**) and dithiocarbamate (IMAnh**2**) CTA. B) M_n and dispersity (Đ) as a function of the total monomer conversion (α^{total}) for the copolymerization of indene and maleic anhydride, using a dithiobenzoate (IMAnh**1**), trithiocarbonate (IMAnh**3**) and dithiocarbamate (IMAnh**2**) CTA. Total monomer conversions are employed as these copolymerizations exhibited strong alternating characteristics (equimolar comonomer consumption).*

SIAnh

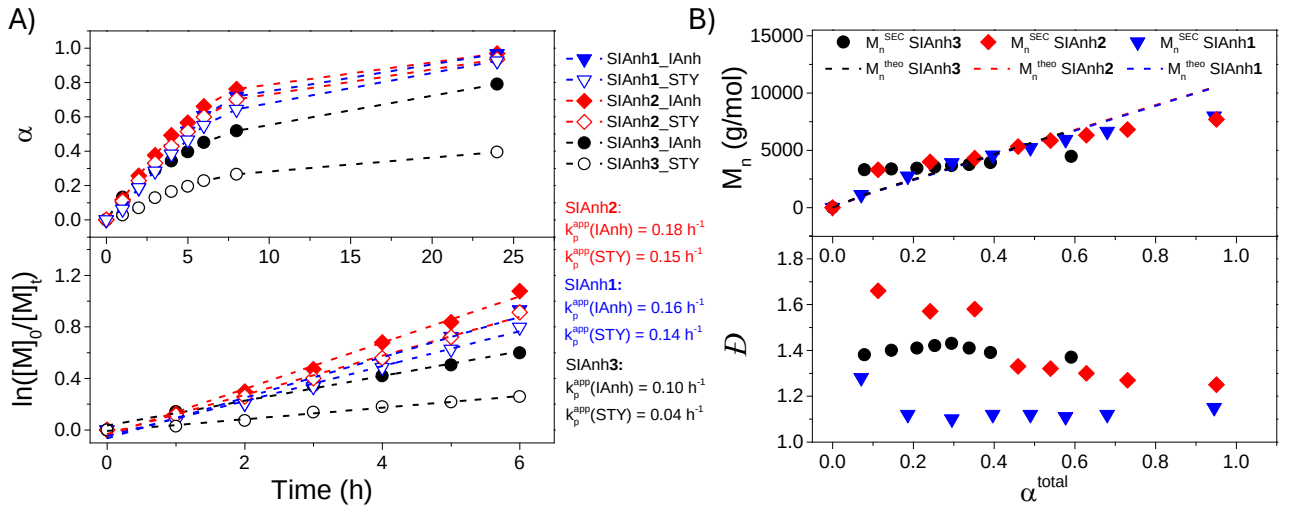


Figure S3: *A) Monomer conversion and ln(M_0/M_n) as a function of time for the copolymerization of styrene and itaconic anhydride using a dithiobenzoate (SIAnh**1**, trithiocarbonate (SIAnh**3**) and dithiocarbamate (SIAnh**2**) CTA. B) M_n and dispersity (Đ) as a function of the total monomer conversion (α^{total}) for the copolymerization of styrene and itaconic anhydride, using a dithiobenzoate (SIAnh**1**), trithiocarbonate (SIAnh**3**) and dithiocarbamate (SIAnh**2**) CTA.*

IIAnh

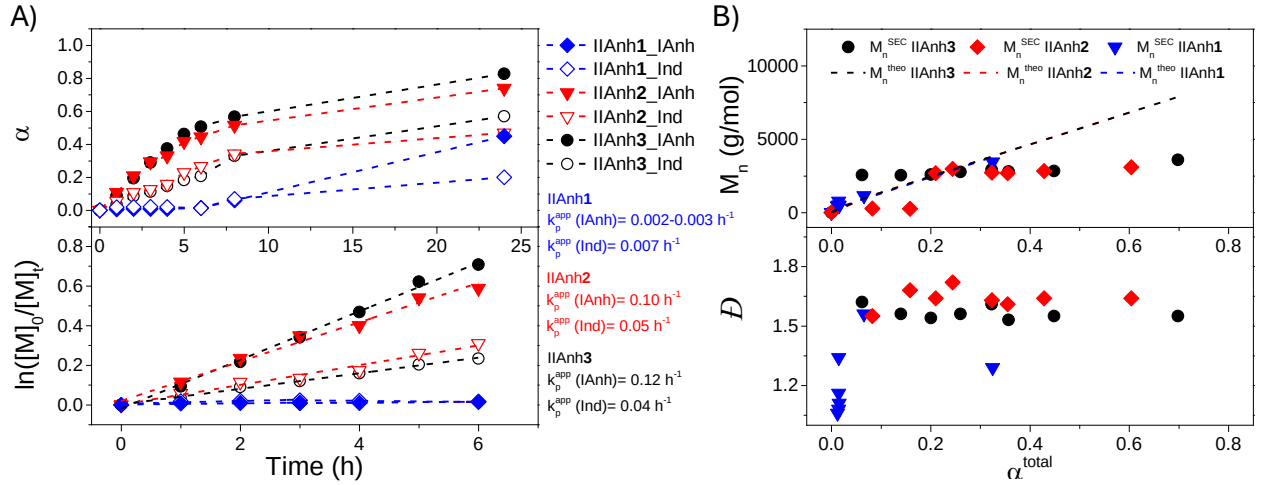


Figure S4: *A) Monomer conversion and ln(M_0/M_n) as a function of time for the copolymerization of indene and itaconic anhydride using a dithiobenzoate (IIAnh**1**, trithiocarbonate (IIAnh**3**) and dithiocarbamate (IIAnh**2**) CTA. B) M_n and dispersity (Đ) as a function of the total monomer conversion (α^{total}) for the copolymerization of indene and itaconic anhydride, using a dithiobenzoate (IIAnh**1**), trithiocarbonate (IIAnh**3**) and dithiocarbamate (IIAnh**2**) CTA.*

CTA consumption analysis

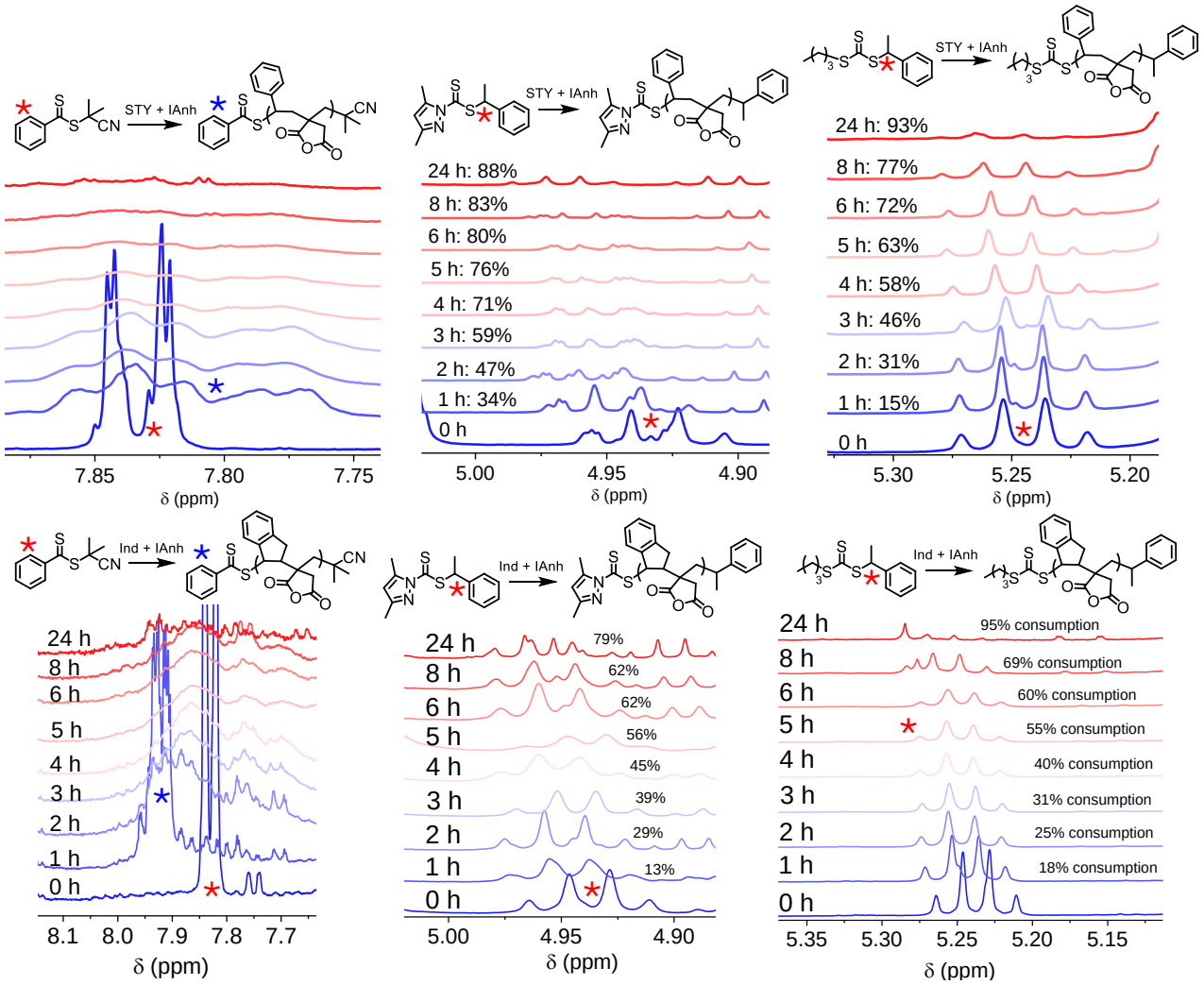


Figure S5: *^{1}H NMR spectroscopic analysis of kinetic samples withdrawn from SIAnh**1** (top left), SIAnh**2** (top middle), SIAnh**3** (top right), IIAnh**1** (bottom left) and IIAnh**2** (bottom middle) and IIAnh**3** (bottom right) copolymerizations, in $(CD_3)_2CO$.*

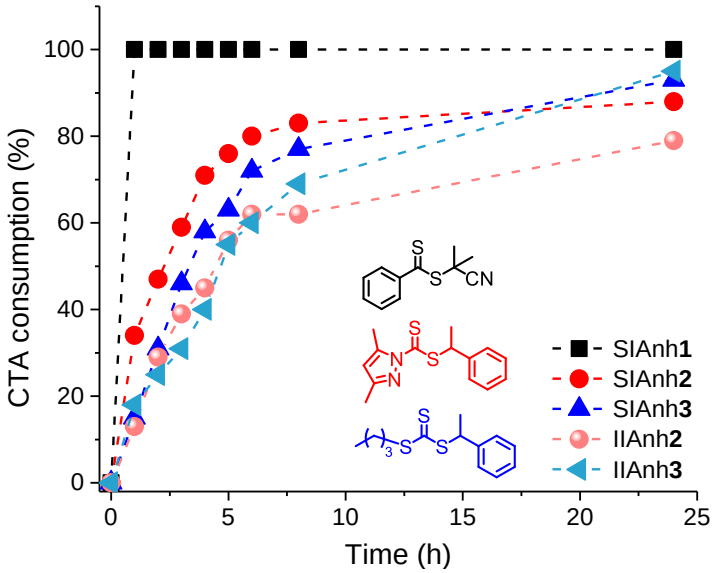


Figure S6: *Consumption of CTA**1**, CTA**2** and CTA**3** during SIAnh and IIAnh copolymerizations.*

The consumption of CTA**2** and CTA**3** was calculated throughout SIAnh and IIAnh copolymerizations using the internal standard 1,3,5-trioxane. The methine proton of the 1-phenyl ethyl R-group

decreases in intensity as it re-initiates the copolymerization and thus provides insight into the relative efficiency of the CTA for each copolymerization. Protons associated with the CTA**1** Z- and R-group do not shift upon addition of monomer to CTA**1** and subsequent fragmentation and re-initiation of the polymerization. The signals associated with these protons simply broaden as they exhibit a change in multiplicity, characteristic of their incorporation at the ω-chain end of macro-CTAs. Despite this, it is visually obvious in **Figure S5** that CTA**1** is consumed rapidly (within 1 h for SIAnh and 2 h for IIAnh). This rapid consumption occurs during an initialization period, where very low monomer conversion is observed as CTA**1** is converted to a single monomer adduct. After initialization for ~5 h k_p^{app} increases, and a linear evolution of M_n^{SEC} with increasing monomer conversion is obtained, with the final isolated IIAnh copolymer having a relatively low *Đ* (1.29). Conversely, CTA**2** and CTA**3** are consumed slowly throughout the IIAnh copolymerizations, which could suggest that the 1-phenyl ethyl R-group is a poor leaving group and re-initiating radical for these copolymerizations. As a result, IIAnh**2** and IIAnh**3** did not exhibit characteristics of a well-controlled RAFT-mediated copolymerization.

For SIAnh copolymerizations, CTA**1** was rapidly consumed, and the kinetic analysis of the copolymerization exhibited characteristics of a well-controlled RAFT-mediated copolymerization (**Figure S3**). Conversely, CTA**2** and CTA**3** were consumed slowly throughout the SIAnh copolymerizations (albeit faster than that observed for IIAnh copolymerizations), and therefore less control over these copolymerizations was obtained. CTA**3** was the least efficient for SIAnh copolymerizations as it was consumed slower than CTA**2**. The effects of this could be observed in **Figure S3** as M_n^{SEC} was higher than M_n^{theo} at low monomer conversion, but lower then M_n^{theo} at higher monomer conversions (with a high *Đ* of ~1.4 obtained throughout the copolymerization). Both SIAnh**2** and SIAnh**3** exhibited somewhat similar evolution of M_n^{SEC} with increasing monomer conversion.

Polymer Characterization

ATR-FTIR spectra

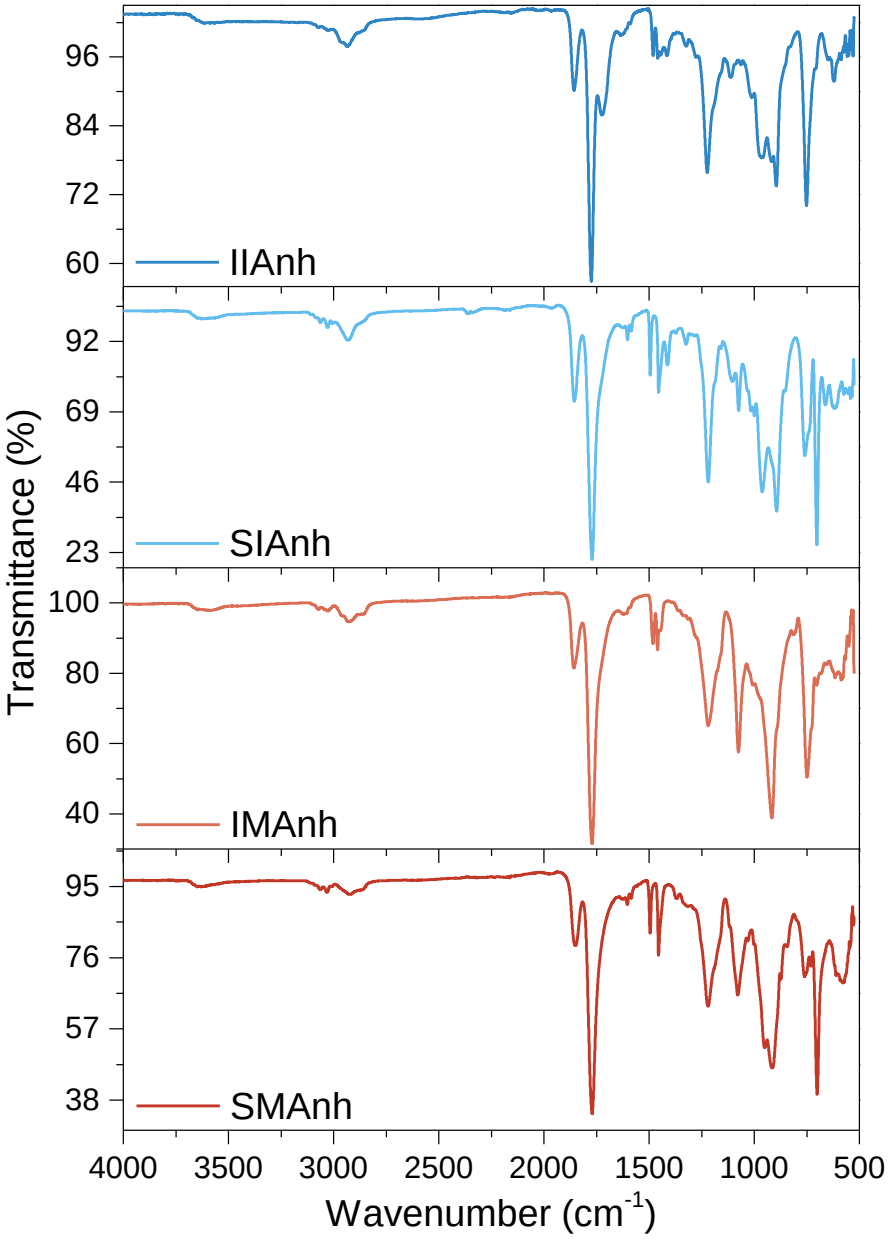


***Figure S7**: ATR-FTIR spectra of the purified copolymer powders (poly(styrene-alt-maleic anhydride) (SMAnh), poly(styrene-alt-itaconic anhydride) (SIAnh), poly(indene-co-itaconic anhydride) (IIAnh), poly(indene-alt-maleic anhydride) (IMAnh)). In each instance, it can be noted that each of the polymers contains the characteristic anhydride signal at 1780 cm^{-1} which confirms the incorporation of these monomers within the polymer backbone. It can be also noted in the 1500 cm^{-1} – 500 cm^{-1} regions that there are slight differences in signals between the indene and the styrene-containing copolymer systems.*

^{1}H NMR spectra

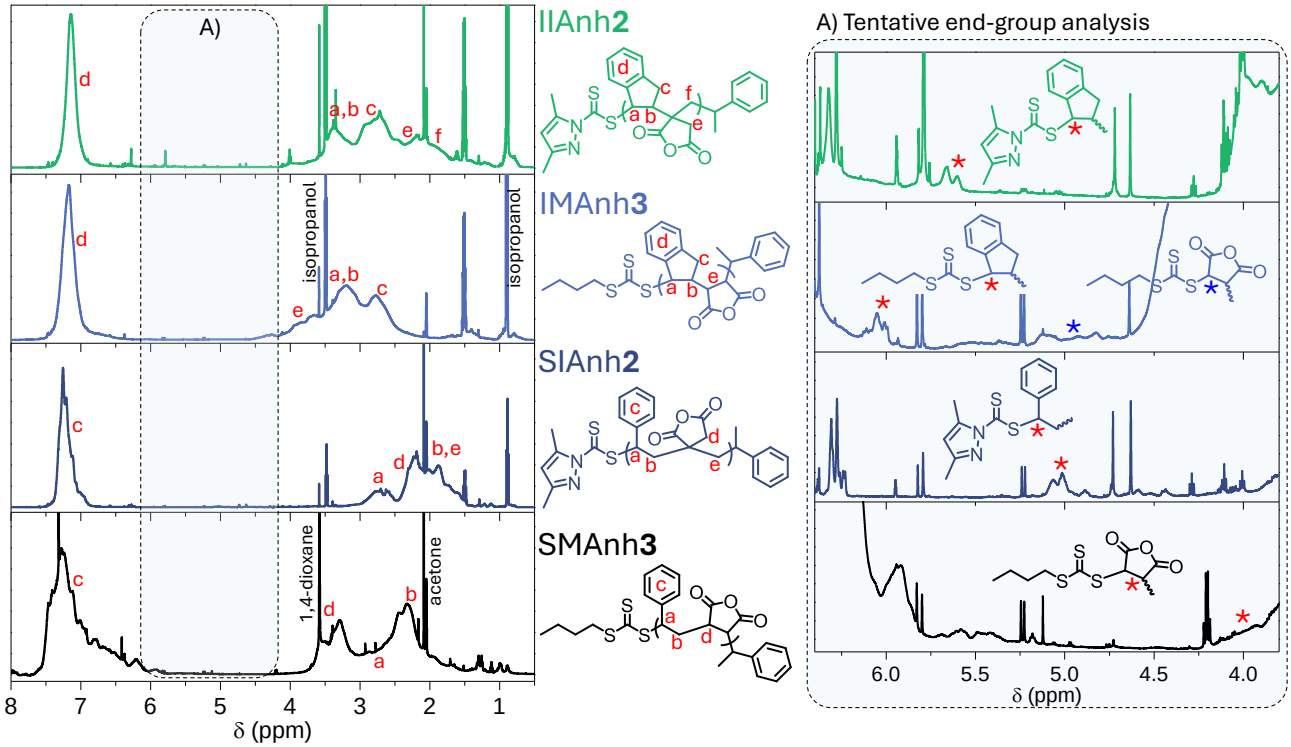


Figure S8: *^{1}H NMR spectra of the poly(styrene-alt-maleic anhydride) (SMAnh), poly(styrene-alt-itaconic anhydride) (SIAnh), poly(indene-co-itaconic anhydride) (IIAnh), poly(indene-alt-maleic anhydride) (IMAnh), in $(CD_3)_2CO$.*

Tentative proton assignments were made for the terminal monomer unit adjacent to each Z-group (inset A). Based on these assignments, SMAnh**3** appears to have predominantly MAnh units at ω-chain ends; SIAnh**2** appears to have predominantly STY units at ω-chain ends (although it is possible to have IAnh units, but the terminal IAnh protons cannot be observed); IMAnh**3** appears to have a mixture of Ind and MAnh units at the ω-chain end; and lastly IIAnh**2** appears to have predominantly Ind at ω-chain ends (but once again IAnh terminal monomer units are possible and cannot be directly observed). This corresponds well with the computational analysis of the bond dissociation energy (BDE) of the C-S bond connecting the thiocarbonylthio moiety to the terminal monomer unit (**Figure S13**). For SMAnh, BDE(MAnh) > BDE(STY) and therefore a large proportion of the macro-CTAs will have MAnh at the ω-chain end. For SIAnh, BDE(STY) > BDE(IAnh) and therefore it is likely that a large proportion of SIAnh macro-CTAs have STY at the ω-chain end, despite the protons of potential IAnh terminal monomer units being undetectable. For IMAnh, BDE(Ind) ≈ BDE(MAnh) and as such it is possible to observe protons associated with both Ind and MAnh at ω-chain ends. For IIAnh, BDE(Ind) > BDE(IAnh) and therefore only protons associated with Ind at ω-chain ends are observed.

SEC analysis - **SMAnh**

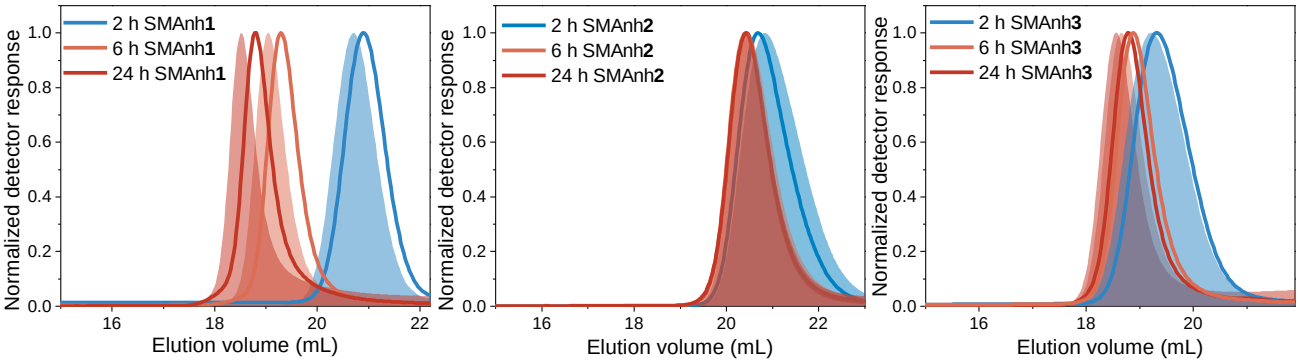


Figure S9: *SEC analysis of SMAnh**1**, SMAnh**2**, and SMAnh**3** copolymerization kinetic samples (2, 6 and, 24 h). The solid lines correspond to normalized RI detector signals while the filled curves correspond to normalized UV detector signals (320 nm).*

SIAnh

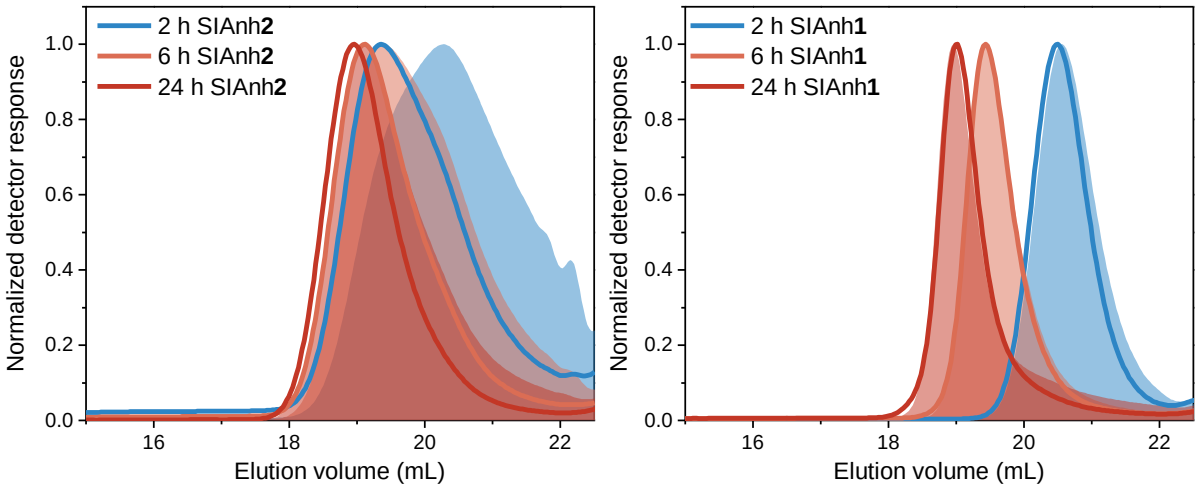


Figure S10: *SEC analysis of SIAnh**1** and SIAnh**2** copolymerization kinetic samples (2, 6 and, 24 h). The solid lines correspond to normalized RI detector signals while the filled curves correspond to normalized UV detector signals (320 nm).*

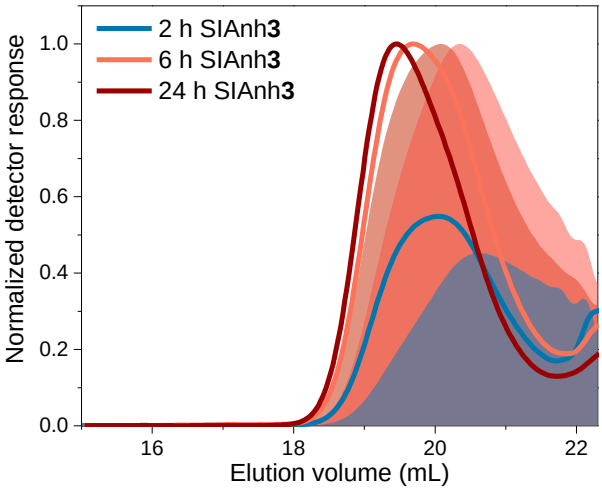


Figure S11: *SEC analysis of SIAnh**3** copolymerization kinetic samples (2, 6 and, 24 h). The solid lines correspond to normalized RI detector signals while the filled curves correspond to normalized UV detector signals (320 nm).*

IMAnh

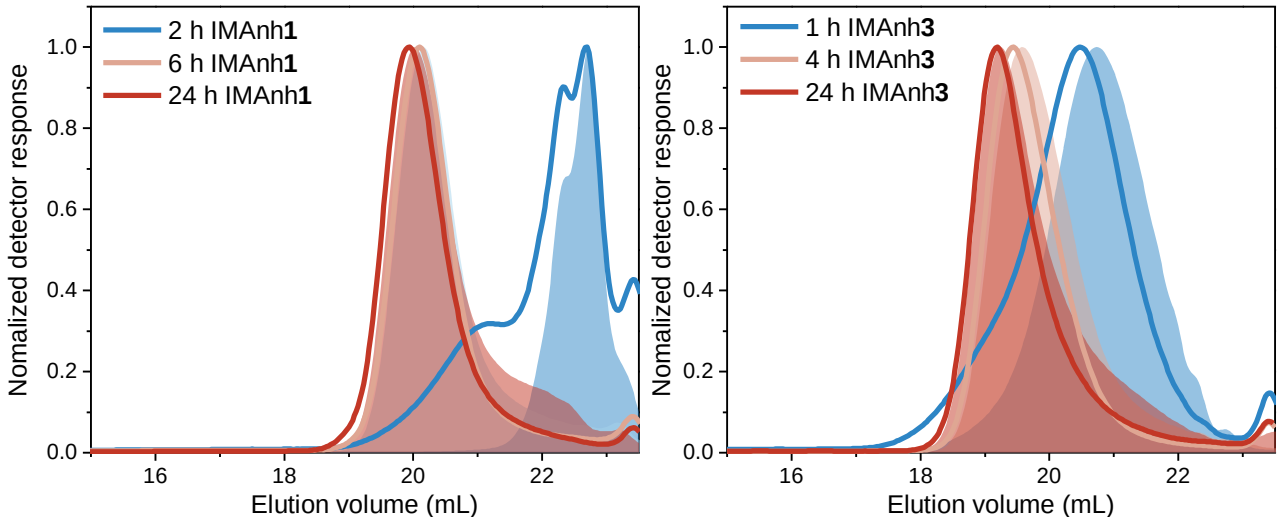


Figure S12: *SEC analysis of IMAnh**1** and IMAnh**3** copolymerization kinetic samples (2, 6 and, 24 h for IMAnh**1** and 1, 4 and 24 h for IMAnh**3**). The solid lines correspond to normalized RI detector signals while the filled curves correspond to normalized UV detector signals (320 nm).*

IIAnh

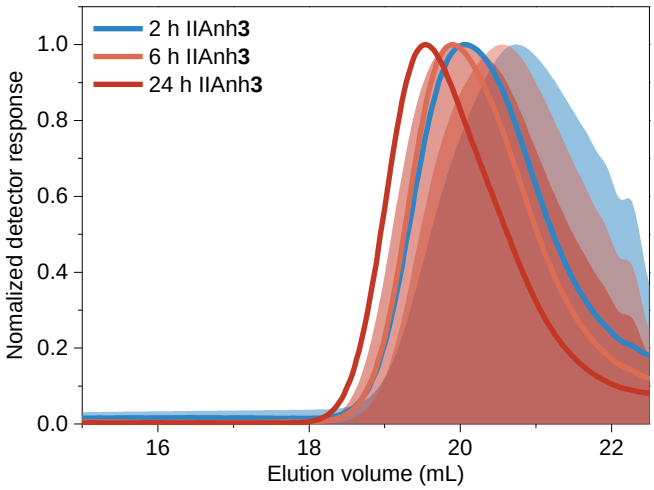


Figure S13: *SEC analysis of the IIAnh**3** copolymerization kinetic samples (2, 6 and, 24 h). The solid lines correspond to normalized RI detector signals while the filled curves correspond to normalized UV detector signals (320 nm).*

Reactivity ratio data

Table S2: *Reactivity ratio data of each copolymer system with various RAFT agents as indicated.*

monomer 1	monomer 2	RAFT agent	r_1	r_2
STY	MAnh	CTA 3	0.01	0.01
STY	IAnh	CTA 3	0.12	0.01
STY	IAnh	CTA 2	0.02	0.01
Ind	MAnh	CTA 3	0.01	0.01
Ind	IAnh	CTA 3	0.01	0.13

Reactivity ratios of the various comonomer pairs were determined *via* parameter estimation for the terminal monomer model in accordance with the published IUPAC recommended method.[3] These results (**Table S2**) indicate that there is a significant tendency towards alternation for each of the comonomer systems. The observed variations in reactivity ratios are within the error margin with which we can estimate the values. This also means that based on the current measurements, the RAFT agent does not appear to have a significant effect on the reactivity ratios.

Computational data

Bond dissociation energy/free energy (kcal/mol) of the C-S bond between the representative trithiocarbonate Z group and monomer (representative terminal monomer unit)

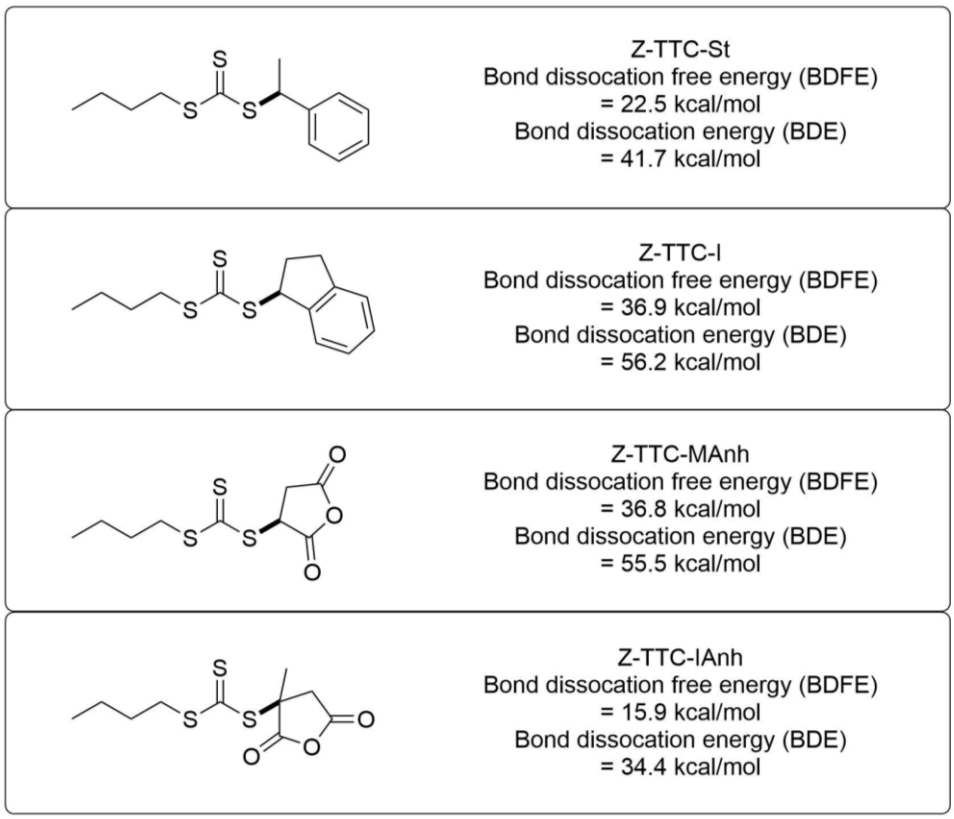


Figure S14*: Bond dissociation free energy (kcal/mol) of the C-S bond (bolded in structures) between the trithiocarbonate Z group and the respective monomer. Conducted with B3LYP/6-31+G*. Where St = styrene, I = indene, MAnh = maleic anhydride and IAnh = itaconic anhydride.*

It is noted that that the bond dissociation free energy (BDFE) of maleic anhydride is higher compared to styrene (36.8 kcal·mol^{-1} and 22.5 kcal·mol^{-1} respectively). This indicates that during a copolymerization of styrene and maleic anhydride, the ω-chain ends will predominantly be MAnh-functional as result of the higher BDFE compared to the C-S bond of styrene and the Z group. This agrees with what has been previously reported.[4]

Gibbs free energy (kcal/mol) investigation for the binding or cleaving of monomers from the RAFT agent (trithiocarbonate)

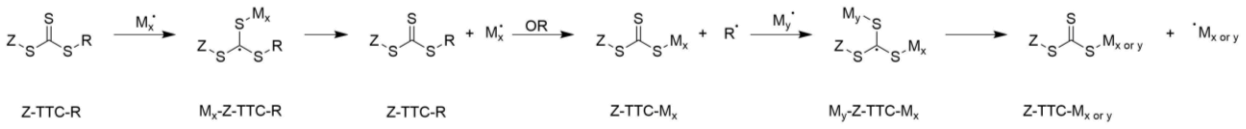


Figure S15: *Codes, nomenclature and structures for the figures to follow in this subsection. Where M_x and M_y are comonomers in the copolymerization i.e. maleic anhydride and styrene for the synthesis of SMAnh.*

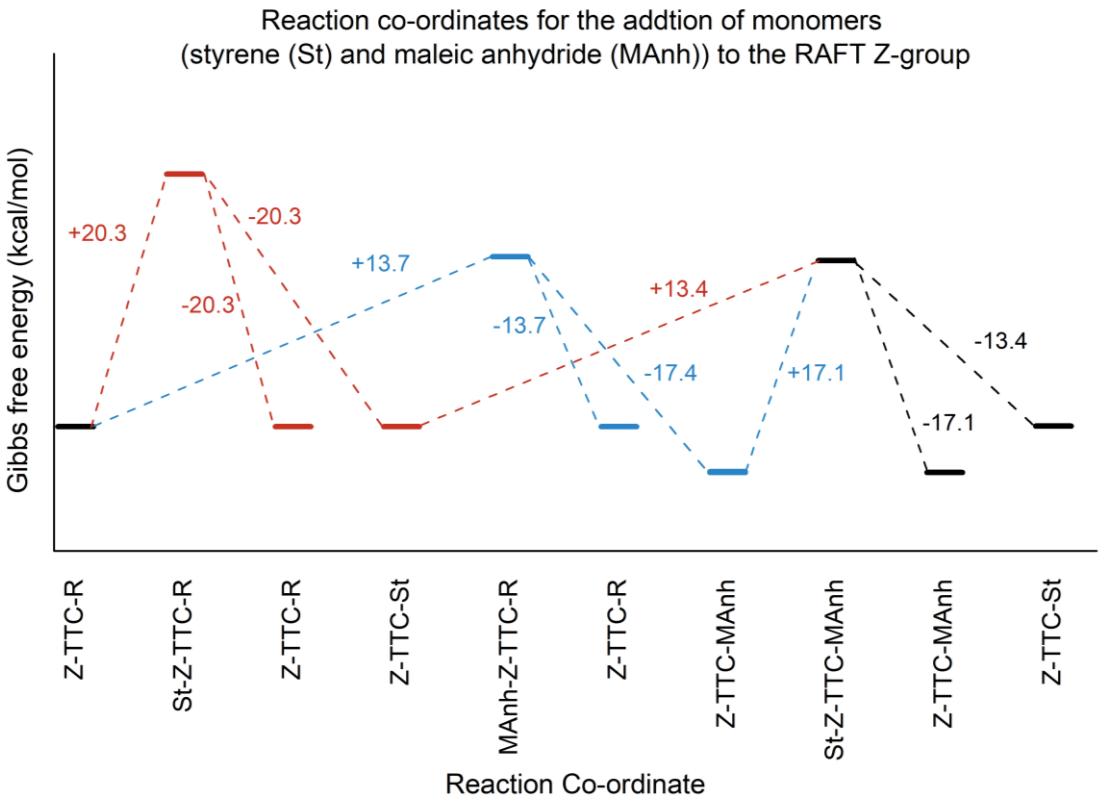


Figure S16: *Gibbs free energy (kcal/mol) investigation for the binding or cleaving of styrene and maleic anhydride from the RAFT agent (trithiocarbonate). Conducted with B3LYP/6-31+G*. Where St = styrene and MAnh = maleic anhydride.*

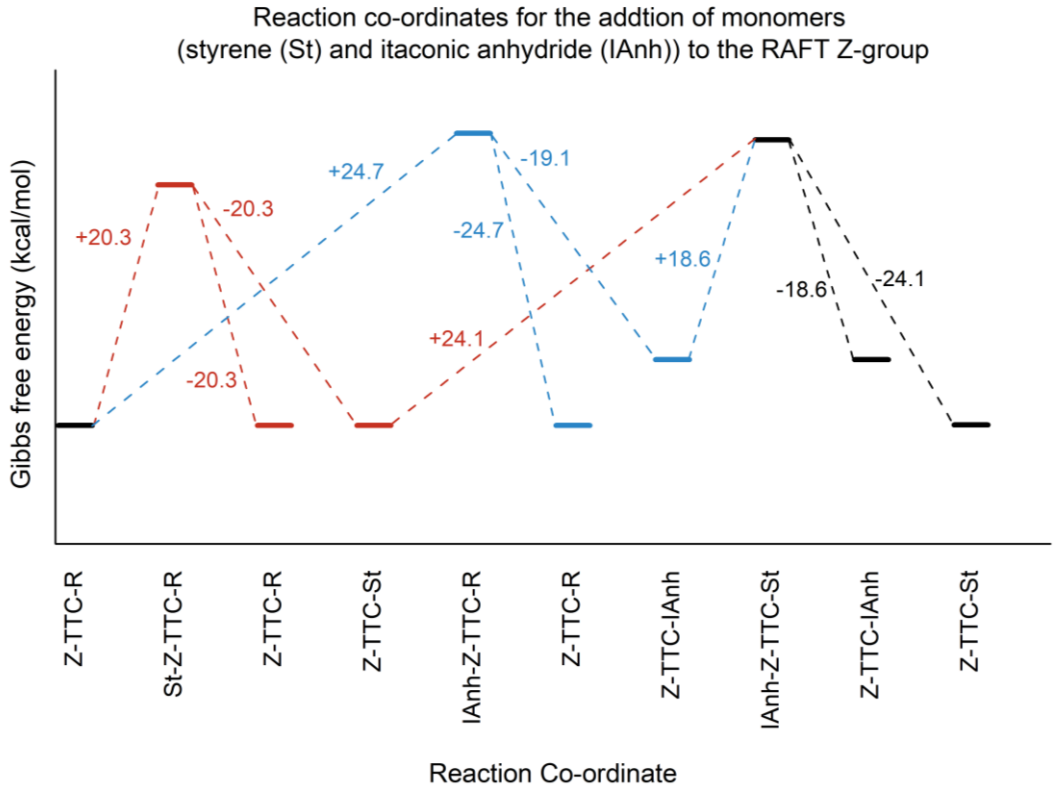


Figure S17: *Gibbs free energy (kcal/mol) investigation for the binding or cleaving of styrene and itaconic anhydride from the RAFT agent (trithiocarbonate). Conducted with B3LYP/6-31+G*. Where St = styrene and IAnh = itaconic anhydride.*

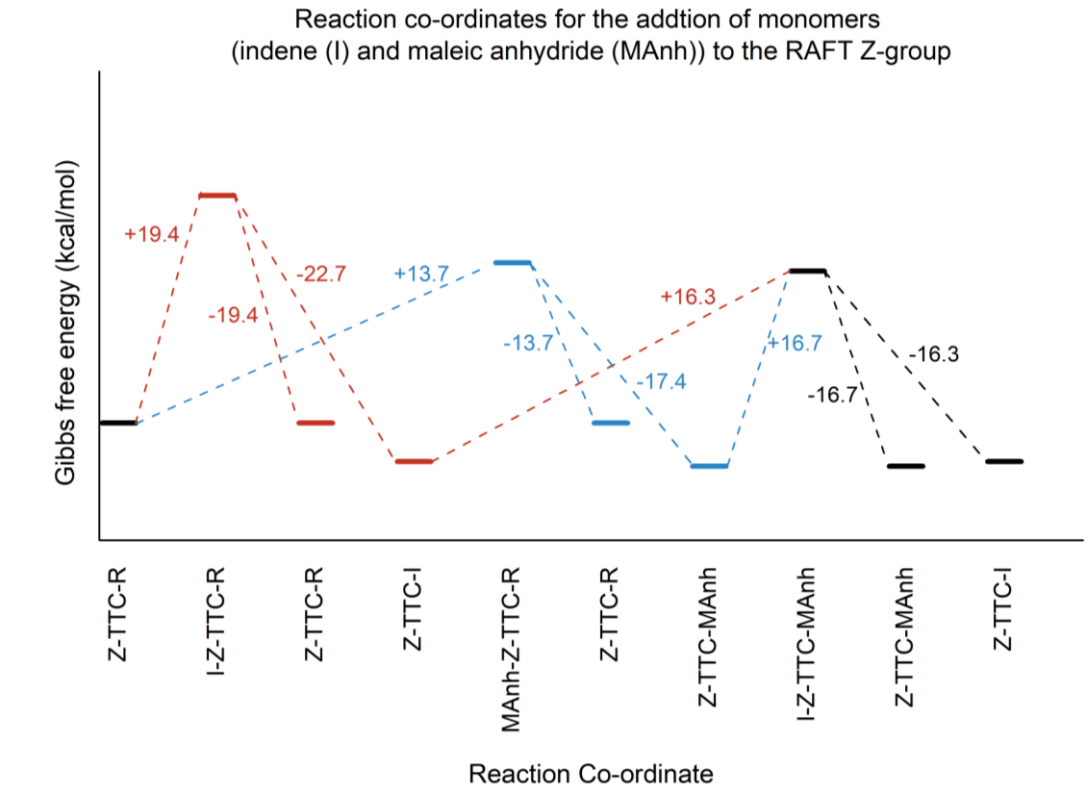


Figure S18: *Gibbs free energy (kcal/mol) investigation for the binding or cleaving of indene and maleic anhydride from the RAFT agent (trithiocarbonate). Conducted with B3LYP/6-31+G*. Where I = indene and MAnh = maleic anhydride.*

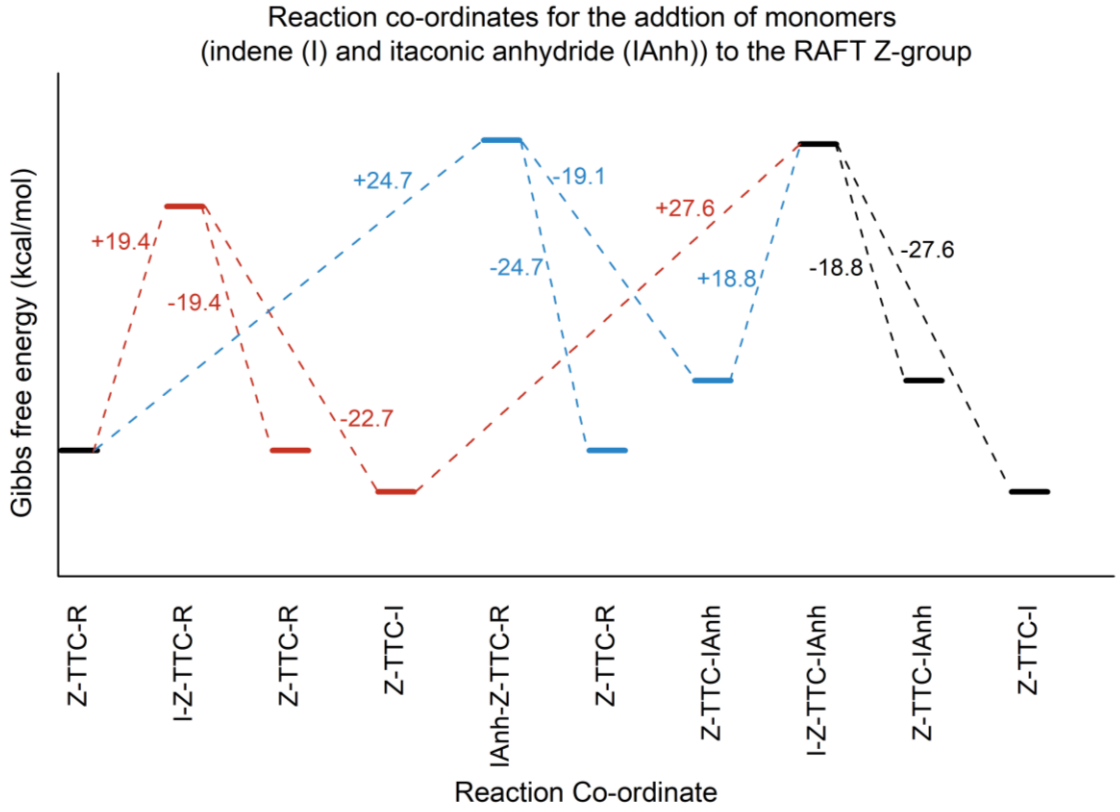
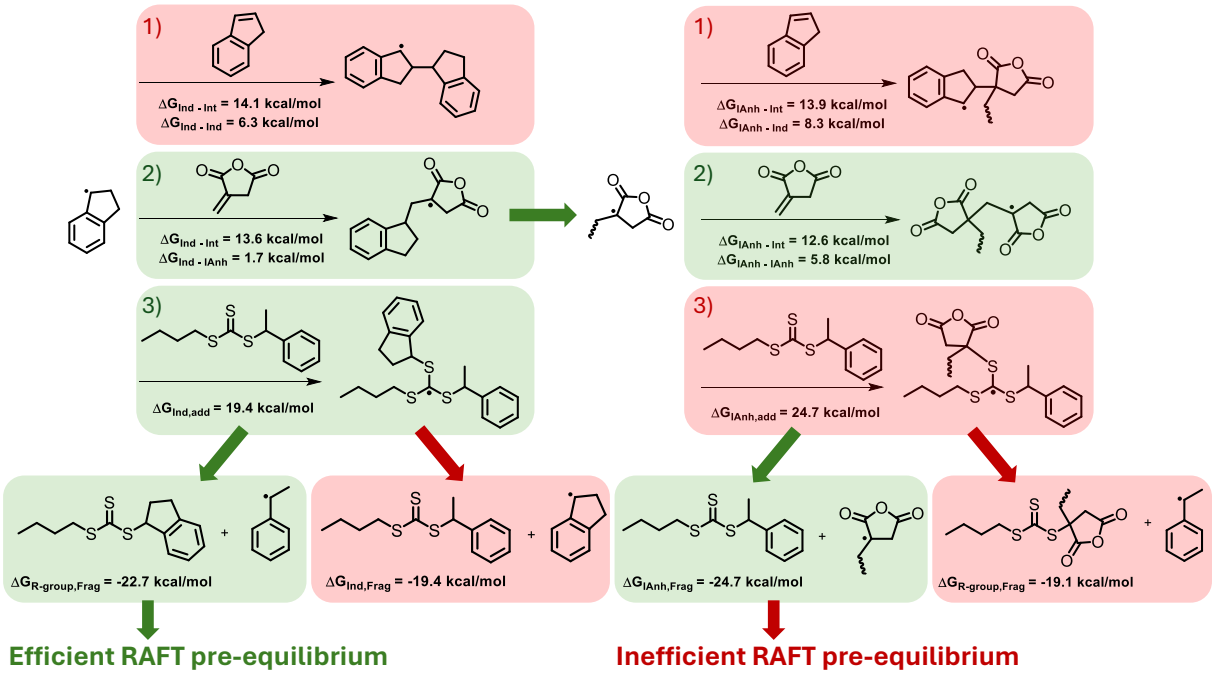


Figure S19: *Gibbs free energy (kcal/mol) investigation for the binding or cleaving of indene and itaconic anhydride from the RAFT agent (trithiocarbonate). Conducted with B3LYP/6-31+G*. Where I = indene and IAnh = itaconic anhydride.*

None of the CTAs investigated in this study provided adequate control over the RAFT-mediated copolymerization of Ind and IAnh. The RAFT pre-equilibrium was assessed computationally to probe where the inefficiencies of the RAFT-mediated synthesis of IIAnh originate (**Figure S19**). Excluding termination events, three scenarios exist which describe the reaction of propagating monomer radicals. For Ind-based radicals, addition to Ind can occur; addition to IAnh can occur and addition to the CTA can occur. The former scenario is unlikely as it is more energetically favourable for the addition of an Ind-based radical to an IAnh monomer as opposed to an Ind monomer ($\Delta G_{Ind\text{-}IAnh}$ = 1.7 kcal·mol^{-1} *vs*. $\Delta G_{Ind\text{-}Ind}$ = 6.3 kcal·mol^{-1}) (**Figure S24**, scenario IIAI *vs*. II). Furthermore, the addition of IAnh-based radicals to IAnh monomer as opposed to Ind monomer is energetically more favourable ($\Delta G_{IAnh\text{-}IAnh}$ = 5.8 kcal·mol^{-1} *vs*. $\Delta G_{IAnh\text{-}Ind}$ = 8.3 kcal·mol^{-1}) (**Figure S24**, scenario IIAI *vs*. IAIA). The addition of Ind-based radicals to CTA**3** is energetically more favourable than the addition of IAnh-based radicals ($\Delta G_{IAnh,add}$ = 24.7 kcal·mol^{-1} *vs*. $\Delta G_{Ind,add}$ = 19.4 kcal·mol^{-1}), but due to the favourable cross propagation of Ind-based radicals with IAnh monomer, it is plausible that a higher proportion of IAnh-based radicals are available for addition to CTA. While the fragmentation of the Ind-based intermediate radical (I-Z-TTC-R, **Figure S19**) favours the R-group leaving (which improves the efficiency of the RAFT pre-equilibrium), the IAnh-based intermediate radical (IAnh-Z-TTC-R, **Figure S19**) favours the fragmentation of the IAnh-based group instead of the R-group. This corresponds to the observed bond dissociation energies, whereby the IAnh-based leaving group had by far the lowest bond dissociation energy (**Figure S14**). If the IAnh-based group has higher efficiency as the leaving group compared to the R-group, the slow consumption of CTA**3** would result, which is observed experimentally in **Figure S5–6** and summarized in **Scheme S4** below.



Scheme S4: *Computational analysis of the RAFT-mediated copolymerization of Ind and IAnh using CTA3.*

HOMO and LUMO orbital instigation of monomers

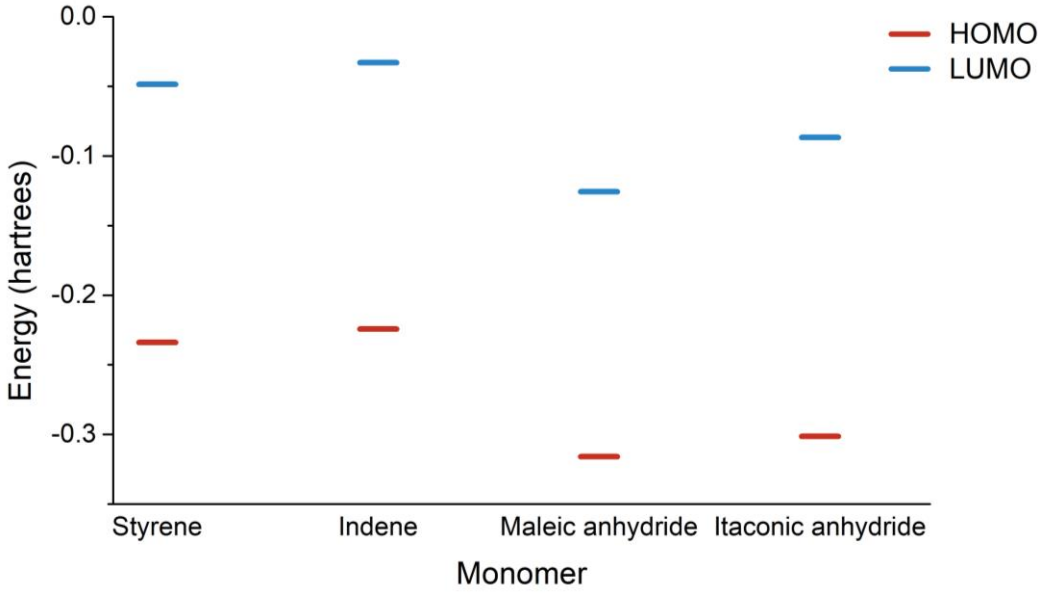


Figure S20: *HOMO and LUMO energies (hartrees) of the monomers utilized in this study. Conducted with B3LYP/6-31+G*.*

It can be noted that both indene and itaconic anhydride have a higher HOMO and LUMO energy compared to their respective petroleum-derived counterparts.

Gibbs free energy (kcal/mol) investigation during polymerization propagation

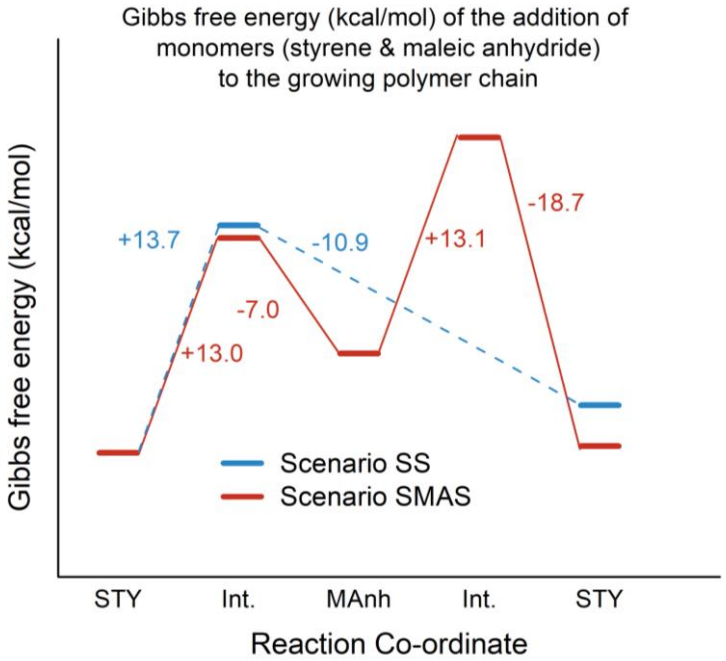


Figure S21: *Gibbs free energy diagram for the addition of monomers (styrene and maleic anhydride) to the chain end of a growing polymer chain. Different addition patterns are indicated with different colours for either copolymerization or homopolymerization of monomers where possible (proven experimentally). Conducted with B3LYP/6-31+G*. Where St = styrene, MAnh = maleic anhydride and Int. = intermdiate structure.*

It can be noted that the addition of maleic anhydride to a styrenic radical is more favourable than the addition of a styrene monomer (on comparison of the intermediates energies). Thereafter, the addition of a styrene monomer to a chain end containing maleic anhydride is more favoured with an overall negative Gibbs free energy *via* an unstable intermediate.

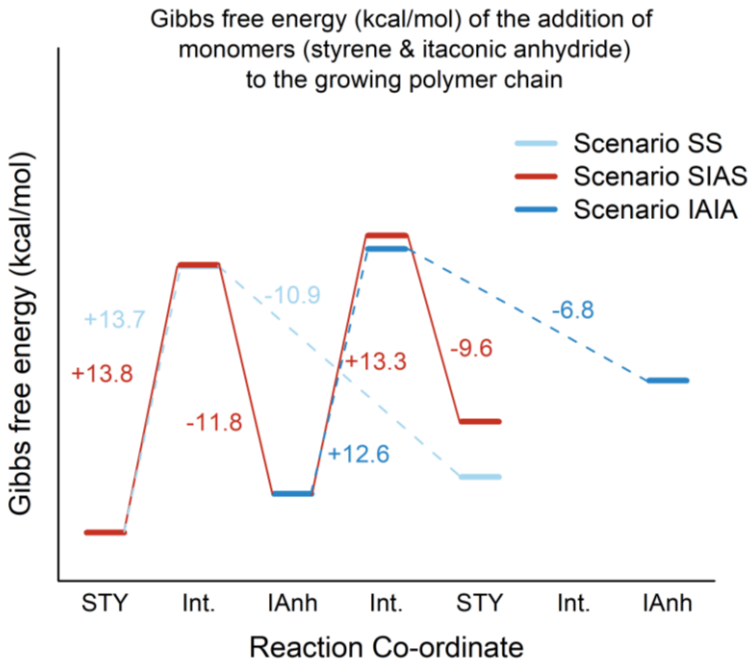


Figure S22: *Gibbs free energy diagram for the addition of monomers (styrene and itaconic anhydride) to the chain end of a growing polymer chain. Different addition patterns are indicated with different colours for either copolymerization or homopolymerization of monomers where possible (proven experimentally). Conducted with B3LYP/6-31+G*. Where St = styrene, IAnh = itaconic anhydride and Int. = intermediate structure.*

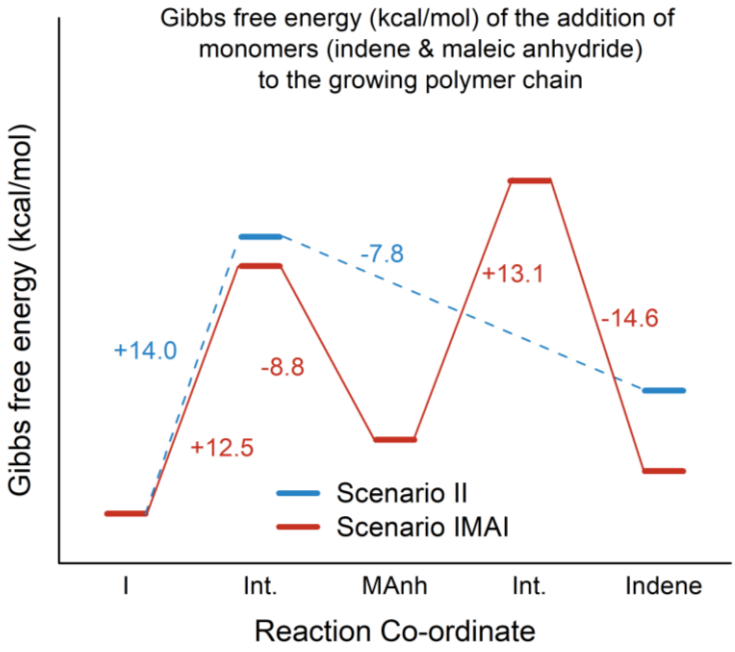


Figure S23: *Gibbs free energy diagram for the addition of monomers (indene and maleic anhydride) to the chain end of a growing polymer chain. Different addition patterns are indicated with different colours for either copolymerization or homopolymerization of monomers where possible (proven experimentally). Conducted with B3LYP/6-31+G*. Where I = indene, MAnh = maleic anhydride and Int. = intermediate structures.*

The addition of maleic anhydride to an indene chain end is more favourable in terms of the intermediate formed as well as the final molecule. This suggests that this copolymerization is rather alternating in character.

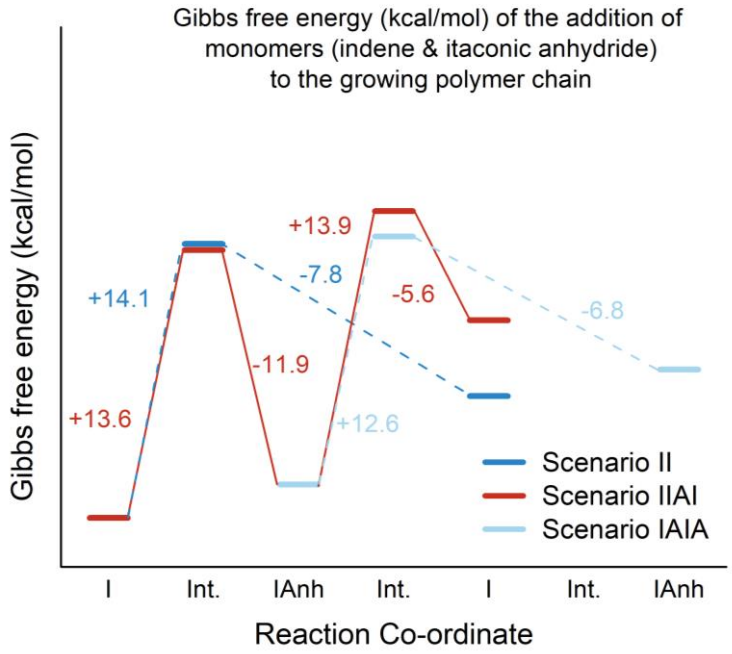


Figure S24: *Gibbs free energy diagram for the addition of monomers (styrene and maleic anhydride) to the chain end of a growing polymer chain. Different addition patterns are indicated with different colours for either copolymerization or homopolymerization of monomers where possible (proven experimentally). Conducted with B3LYP/6-31+G*. Where I = indene, IAnh = itaconic anhydride and Int. = intermediate structures.*

In this system, it can be noted that the addition of itaconic anhydride compared to indene (to an indene terminated polymer chain end) is slightly more favoured (0.5 kcal·mol^{-1} based on the energy differences of the intermediates). This highlights that this system may not be strictly alternating during the copolymerization. It can be noted that the energy of the final product of the addition of an itaconic anhydride is lower than that the addition of a second indene monomer (4.6 kcal/mol lower acquired by comparing 13.6-11.9 = 1.7 kcal·mol^{-1} compared to 14.1-7.8 = 6.3 kcal·mol^{-1}). This suggests that once an indene monomer has been added to the chain end, an itaconic anhydride is preferentially added. Interestingly, it can be noted that the addition of an indene or itaconic anhydride unit to an itaconic anhydride polymer chain end does not afford the same pattern. It can be noted that both the intermediate (1.3 kcal·mol^{-1} higher acquired by comparing 13.9 kcal·mol^{-1} to 12.6 kcal·mol^{-1}) and the final product (2.5 kcal·mol^{-1} higher acquired by 12.6-6.8 = 5.8 kcal·mol^{-1} compared to 13.9-5.6 = 8.3 kcal·mol^{-1}) of the addition of indene are higher than that of the addition of another itaconic anhydride. This suggests that once an itaconic anhydride has been added to the growing polymer chain, it is energetically more favourable for another itaconic anhydride unit to be added.

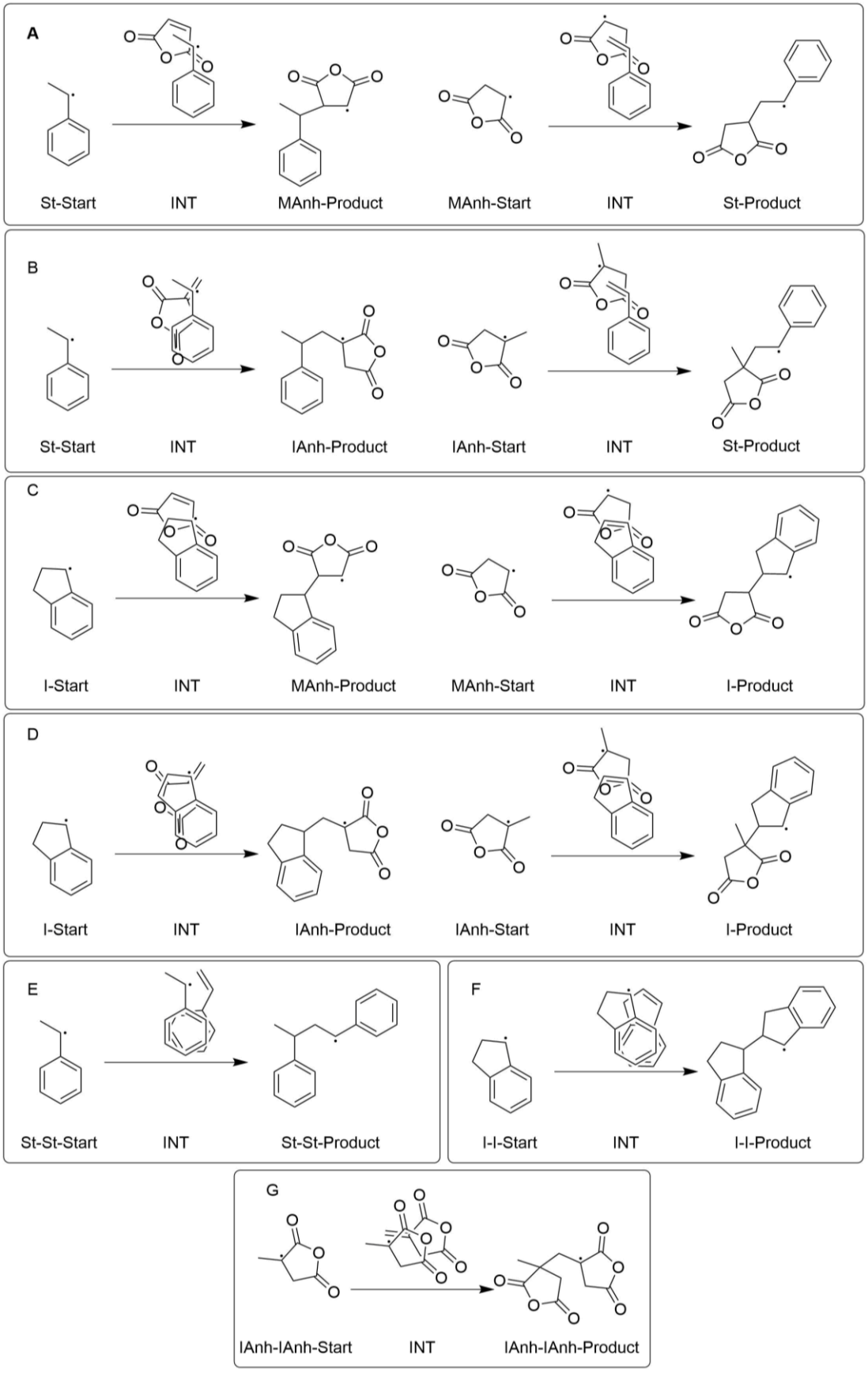


Figure S25: *Reaction modelled via DFT calculations to determine the energy of the propagation steps of the monomer pairs from Figures S21– S24.*

Computational methodology

The Jaguar module of the Schrödinger Suite (2021-4),[5] was utilized for all calculations in this study through the utilization of the Maestro graphical interface.[6] The geometries of all compounds/monomers investigated in this study were optimized using density functional theory at the B3LYP level,[7-10] using the 6-31+G* basis set.[11-14] The check_min=1 function of Jaguar in the Maestro interface was used to confirm that all geometries corresponded to minimum energy structures for all relevant molecules. All calculations were undertaken with unrestricted spin. The THF solvent environment was modeled using the conductor-like polarizable continuum model (CPCM) and thereafter compared to the gas-phase optimized structure.[15-17]

All basis sets were obtained from the Basis Set Exchange.[18-20]

Optimized atom coordinates

Z-TTC-St BDFE output

C	-10.60980	2.04590	-0.36780
C	-11.04080	3.47000	-0.74930
S	-8.74330	2.04590	-0.36780
C	-8.26130	0.37000	-0.65620
S	-9.22730	-0.84870	-1.20960
S	-6.54770	0.23140	-0.26960
C	-6.04740	-1.41860	-0.90770
C	-4.54660	-1.59870	-0.65550
C	-4.03510	-2.98700	-1.07730
C	-4.08650	-3.25500	-2.58510
C	-10.87410	2.20810	2.16080
C	-11.18440	1.57190	0.95110
C	-11.45670	1.78730	3.35330
C	-12.36080	0.72300	3.35610
C	-12.67620	0.08420	2.15880
C	-12.08970	0.50580	0.96440
H	-10.89280	1.35220	-1.15960
H	-12.13280	3.51060	-0.77400
H	-10.69750	4.21260	-0.02420
H	-10.66090	3.74450	-1.73620
H	-6.63360	-2.17420	-0.38350
H	-6.29850	-1.45050	-1.96790
H	-3.98500	-0.82560	-1.19180
H	-4.33970	-1.45880	0.41050
H	-3.00000	-3.07810	-0.73210
H	-4.60230	-3.75780	-0.54270
H	-3.64820	-4.22840	-2.82190
H	-5.11090	-3.25780	-2.96720
H	-3.52630	-2.49500	-3.13940
H	-10.16540	3.03050	2.17630
H	-11.20450	2.28860	4.28220
H	-12.81260	0.39450	4.28640
H	-13.37560	-0.74560	2.15130
H	-12.33710	0.00280	0.03520
C	4.57700	4.80490	0.56010
C	3.89210	3.95210	-0.46110
C	5.05180	6.71380	-0.97100
C	5.11300	6.09040	0.30960
C	5.58840	7.97590	-1.17870

C	6.20580	8.67160	-0.13200
C	6.27930	8.08100	1.13760
C	5.74740	6.82150	1.35730
H	4.67230	4.41500	1.56940
H	3.00000	4.44060	-0.87640
H	4.54260	3.72870	-1.31730
H	3.57490	3.00000	-0.03180
H	4.57870	6.19520	-1.79750
H	5.52790	8.42720	-2.16440
H	6.62340	9.65800	-0.30150
H	6.75640	8.61410	1.95400
H	5.80850	6.37130	2.34390
S	3.06750	-3.00000	0.96520
C	3.96660	-4.38530	0.58380
S	3.00000	-5.51160	-0.22050
S	5.62990	-4.53460	0.99990
C	6.10630	-6.19190	0.34740
C	7.60490	-6.39450	0.59150
C	8.08200	-7.79350	0.16740
C	7.96050	-8.07980	-1.33310
H	5.51210	-6.94370	0.87150
H	5.86110	-6.20580	-0.71500
H	8.17230	-5.63190	0.04590
H	7.82250	-6.25470	1.65570
H	9.12890	-7.89390	0.47100
H	7.52680	-8.54900	0.73520
H	8.38350	-9.05840	-1.57540
H	6.91950	-8.08380	-1.66800
H	8.49750	-7.32960	-1.92250

Z-TTC-I BDFE calculation output

C	-4.71280	0.99680	0.09800
C	-4.09950	0.58770	1.45690
S	-6.58060	0.99680	0.09800
C	-7.04760	-0.68850	-0.15040
S	-6.02040	-1.95770	-0.40800
S	-8.80770	-0.78740	-0.09800
C	-9.19950	-2.54150	-0.48720
C	-10.72060	-2.70520	-0.53420
C	-11.12050	-4.15070	-0.86180
C	-12.63860	-4.33850	-0.92970
C	-3.91460	1.90850	2.24150
C	-3.82030	2.95030	1.14870
C	-4.27930	2.43530	-0.06930
C	-3.36260	4.26480	1.22130
C	-3.37030	5.05160	0.06730
C	-3.83240	4.53360	-1.14720
C	-4.29510	3.21910	-1.22240
H	-4.42470	0.34210	-0.72330
H	-4.69320	-0.15580	1.98810
H	-3.12150	0.14030	1.25300
H	-8.73960	-2.78230	-1.44650
H	-8.75020	-3.16830	0.28410
H	-11.15710	-2.41770	0.42860
H	-11.14270	-2.03300	-1.28910
H	-10.67120	-4.44110	-1.81810
H	-10.69940	-4.82220	-0.10500
H	-12.89890	-5.37470	-1.16170
H	-13.11140	-4.08070	0.02270
H	-13.08110	-3.70210	-1.70230
H	-4.77640	2.11170	2.88830

H	-3.03270	1.88700	2.88630
H	-3.00000	4.67420	2.15970
H	-3.01100	6.07500	0.11100
H	-3.82700	5.15680	-2.03550
H	-4.65620	2.81570	-2.16380
S	9.60270	9.32230	0.79960
C	9.01210	7.72140	0.46670
S	10.05850	6.43790	0.21190
S	7.27260	7.63460	0.43550
C	6.88480	5.87940	0.07360
C	5.36570	5.70280	0.03450
C	4.97800	4.24890	-0.26590
C	3.46190	4.04190	-0.30790
H	7.34850	5.62610	-0.88250
H	7.34500	5.26930	0.85410
H	4.93240	6.00380	0.99520
H	4.93490	6.35970	-0.72980
H	5.41830	3.94950	-1.22370
H	5.41910	3.59420	0.49410
H	3.21150	3.00000	-0.52400
H	3.00110	4.30480	0.64930
H	3.00000	4.66390	-1.08070
C	4.91770	-3.91990	-0.27770
C	4.55070	-4.10140	-1.72510
C	4.03240	-5.56880	-1.82290
C	4.14310	-6.10540	-0.41110
C	4.66940	-5.09620	0.45270
C	3.81760	-7.35580	0.08270
C	4.00990	-7.63020	1.44790
C	4.52710	-6.64590	2.30530
C	4.85910	-5.38450	1.82810
H	5.31710	-3.00000	0.13280
H	3.78790	-3.37890	-2.04320
H	5.40980	-3.92840	-2.38640
H	3.00000	-5.61000	-2.18490
H	4.63030	-6.16270	-2.52170
H	3.41620	-8.12400	-0.57300
H	3.75740	-8.60840	1.84340
H	4.66800	-6.87780	3.35660
H	5.25820	-4.62770	2.49670

Z-TTC-MAnh BDFE calculation output

O	-12.97280	-3.83670	0.91790
C	-11.87010	-3.45760	0.17690
C	-11.29460	-2.18490	0.78350
C	-11.98300	-2.06710	2.14650
C	-13.13460	-3.03970	2.05100
O	-14.06510	-3.20220	2.77630
O	-11.52560	-4.06860	-0.78610
S	-9.47260	-2.18490	0.78350
C	-9.05810	-0.61880	0.01930
S	-10.12180	0.44700	-0.64920
S	-7.31880	-0.43250	0.10960
C	-6.96810	1.14880	-0.76590
C	-5.47110	1.44940	-0.65710
C	-5.11260	2.76690	-1.36020
C	-3.62520	3.11190	-1.23850
H	-11.58370	-1.35980	0.11760
H	-11.34440	-2.39070	2.97510
H	-12.35170	-1.06600	2.37460
H	-7.28410	1.03430	-1.80380

H	-7.56960	1.92800	-0.29670
H	-5.18190	1.51170	0.39760
H	-4.89140	0.63230	-1.10020
H	-5.38990	2.69860	-2.41830
H	-5.71350	3.57840	-0.93390
H	-3.39490	4.05090	-1.74940
H	-3.32960	3.22150	-0.19050
H	-3.00000	2.32970	-1.68010
O	3.88280	3.00000	-0.38010
C	4.86840	3.54520	-1.23560
C	5.42540	4.70350	-0.58910
C	4.76780	4.89360	0.72240
C	3.77780	3.74190	0.77820
O	3.00000	3.44850	1.63740
O	5.10100	3.02630	-2.29850
H	6.20550	5.30660	-1.03230
H	5.45550	4.83560	1.57730
H	4.23440	5.84920	0.82040
S	3.52020	-9.17310	1.56050
C	4.06520	-7.71150	0.79310
S	3.00000	-6.68780	0.00290
S	5.78230	-7.46510	0.94880
C	6.12270	-5.88700	0.08030
C	7.61970	-5.58420	0.16530
C	7.96640	-4.26910	-0.54500
C	9.45960	-3.94020	-0.47620
H	5.78800	-5.99750	-0.95370
H	5.52250	-5.10870	0.55730
H	7.92720	-5.52240	1.21550
H	8.19030	-6.40350	-0.28680
H	7.64990	-4.33120	-1.59230
H	7.38770	-3.45400	-0.09610
H	9.68090	-3.00000	-0.98820
H	9.79480	-3.84270	0.56100
H	10.05890	-4.72590	-0.94630

Z-TTC-MAnh BDFE calculation output

C	-11.69500	2.18360	-0.02280
C	-12.07090	3.68190	-0.12450
S	-9.84810	2.18360	-0.02280
C	-9.31800	0.49110	-0.10800
S	-10.29210	-0.81870	-0.33720
S	-7.56980	0.47360	0.07770
C	-7.08020	-1.28190	-0.18310
C	-5.56720	-1.39760	0.02540
C	-5.07570	-2.83840	-0.17740
C	-3.56800	-2.98060	0.05580
C	-12.29960	1.48130	-1.24610
O	-13.40440	0.75410	-0.84030
C	-13.52000	0.72390	0.54560
C	-12.37820	1.49310	1.16810
O	-12.00940	1.58430	-2.39680
O	-14.42020	0.14150	1.06620
H	-13.15950	3.78470	-0.14550
H	-11.69240	4.22690	0.74310
H	-11.66540	4.12540	-1.03540
H	-7.63370	-1.89410	0.52990
H	-7.37310	-1.56560	-1.19550
H	-5.04230	-0.73550	-0.67170
H	-5.30770	-1.06660	1.03690
H	-5.61700	-3.50410	0.50420

H	-5.32370	-3.16570	-1.19350
H	-3.24030	-4.01340	-0.09340
H	-3.00000	-2.34800	-0.63280
H	-3.29670	-2.68880	1.07520
H	-11.74010	0.77560	1.68820
H	-12.76560	2.19440	1.91040
C	4.37530	6.03200	-0.17680
C	4.94600	7.39500	-0.21810
C	4.18220	5.20110	-1.33680
O	3.62850	3.96710	-0.91760
C	3.45440	3.95420	0.44870
C	3.91860	5.27990	1.02240
O	4.40750	5.39580	-2.50700
O	3.00000	3.00000	1.00990
H	4.26110	8.12090	0.23920
H	5.88030	7.44200	0.35800
H	5.15240	7.70050	-1.24500
H	4.70930	5.10720	1.76560
H	3.08940	5.76330	1.55750
S	3.11560	-3.00000	0.07930
C	4.01130	-4.43320	-0.05260
S	3.00000	-5.72610	-0.44550
S	5.71430	-4.46800	0.19600
C	6.17300	-6.23550	-0.06340
C	7.68500	-6.37430	0.12380
C	8.13980	-7.82600	-0.07440
C	9.65070	-7.99550	0.10230
H	5.62400	-6.83630	0.66430
H	5.86910	-6.51800	-1.07320
H	8.20720	-5.72750	-0.59020
H	7.96700	-6.03730	1.12760
H	7.61020	-8.46960	0.63690
H	7.84490	-8.16270	-1.07450
H	9.94900	-9.03690	-0.04420
H	10.20340	-7.38460	-0.61810
H	9.96690	-7.69470	1.10590

Z-TTC-R

Final Energy = -1700.824099 hartree

S	0.06980	0.57690	0.15910
C	1.81350	0.51530	-0.10600
S	2.34560	-1.15110	0.18220
S	2.76990	1.78680	-0.56770
C	4.20140	-1.06360	0.31770
C	-0.41980	2.25400	-0.41370
C	4.67230	-0.49250	1.64160
C	4.71410	-2.49090	0.06380
C	4.26340	-1.03750	2.87020
C	4.75670	-0.53010	4.07420
C	5.67080	0.53030	4.07020
C	6.08590	1.07790	2.85260
C	5.58650	0.57120	1.64770
C	-1.94340	2.39060	-0.31110
C	-2.42960	3.81330	-0.64710
C	-2.17700	4.25220	-2.09590
H	4.52490	-0.40920	-0.49430
H	0.08790	2.98960	0.21940
H	-0.06330	2.37470	-1.43850
H	5.80820	-2.48270	0.10860
H	4.35160	-3.19410	0.82160
H	4.40840	-2.84870	-0.92290

H	3.54910	-1.85650	2.89050
H	4.42560	-0.96010	5.01740
H	6.05220	0.92740	5.00920
H	6.79240	1.90530	2.83800
H	5.90760	1.00900	0.70560
H	-2.42660	1.66910	-0.98300
H	-2.26560	2.14220	0.71070
H	-3.50820	3.85470	-0.44120
H	-1.95800	4.52870	0.04430
H	-2.61340	5.24220	-2.28030
H	-1.10720	4.31960	-2.32530
H	-2.63050	3.54910	-2.80490

St-Z-TTC-R

Final Energy = -2011.069543 hartree

C	1.06640	5.07260	1.63600
C	1.52430	6.47220	2.06350
S	2.49840	4.31860	0.66020
C	1.81680	2.83100	0.00140
S	0.55230	2.84010	-1.21340
S	2.56690	1.36600	0.62700
C	1.60890	-0.04640	-0.06560
C	2.34380	-1.36570	0.22020
C	3.52110	-1.67430	-0.72200
C	3.08550	-2.07380	-2.13840
C	1.27680	3.86180	-2.63370
C	0.12060	4.11330	-3.60830
C	2.49360	3.20850	-3.24490
C	3.76590	3.74560	-2.99600
C	4.91300	3.16710	-3.55090
C	4.80370	2.03770	-4.36610
C	3.53910	1.49250	-4.62060
C	2.39710	2.07090	-4.06370
C	0.61440	4.18480	2.77210
C	1.41130	3.96820	3.90940
C	0.96500	3.15020	4.94860
C	-0.28740	2.52870	4.87010
C	-1.08680	2.73340	3.74300
C	-0.63680	3.55460	2.70360
H	0.25070	5.16880	0.91370
H	0.70950	6.97330	2.59840
H	2.39290	6.43580	2.72960
H	1.78610	7.07970	1.19050
H	0.63140	-0.03800	0.40990
H	1.46930	0.11790	-1.12980
H	2.68760	-1.37300	1.26100
H	1.60520	-2.17350	0.14190
H	4.19230	-0.80560	-0.77220
H	4.10790	-2.49360	-0.28410
H	3.95640	-2.28830	-2.77280
H	2.45940	-2.97330	-2.11010
H	2.50680	-1.27770	-2.63840
H	1.57300	4.80950	-2.17540
H	0.47500	4.73380	-4.44020
H	-0.27880	3.18410	-4.02660
H	-0.69860	4.64360	-3.11010
H	3.86010	4.62590	-2.36360
H	5.88870	3.60060	-3.34450
H	5.69220	1.58540	-4.79860
H	3.44320	0.61420	-5.25340
H	1.42520	1.62770	-4.26480

H	2.39180	4.43200	3.98060
H	1.59520	2.99490	5.82050
H	-0.63290	1.89130	5.67920
H	-2.06050	2.25570	3.66890
H	-1.26580	3.70920	1.82920

MAnh-Z-TTC-R

Final Energy = -2080.726618 hartree

C	0.78950	4.74970	1.55030
C	0.93670	6.09510	2.27070
S	2.39210	4.46180	0.58050
C	1.89980	3.41190	-0.73490
S	0.81510	3.96360	-2.00460
S	2.56060	1.81240	-1.01520
C	3.12650	1.21730	0.63900
C	3.38220	-0.29530	0.60100
C	2.11950	-1.16280	0.49780
C	2.43260	-2.66290	0.54520
C	1.68410	5.45680	-2.74120
C	0.77960	6.12850	-3.77800
C	0.47600	3.58030	2.45560
C	-0.57510	2.70800	2.13210
C	-0.88270	1.61730	2.95430
C	-0.14070	1.38250	4.11480
C	0.91100	2.24590	4.44740
C	1.21610	3.33270	3.62570
C	2.88730	5.01420	-3.54170
O	2.60410	5.11650	-4.90230
C	1.37580	5.72930	-5.11070
O	0.94770	5.88840	-6.22230
O	3.95490	4.60910	-3.16480
H	0.01390	4.83450	0.78420
H	0.03070	6.29460	2.85480
H	1.78920	6.10640	2.95890
H	1.06960	6.90730	1.54860
H	4.04100	1.75830	0.89540
H	2.35420	1.47020	1.37050
H	4.07390	-0.53820	-0.21840
H	3.91330	-0.54430	1.53100
H	1.43990	-0.90250	1.32180
H	1.58310	-0.93150	-0.43210
H	1.51540	-3.26070	0.47890
H	3.08530	-2.95790	-0.28700
H	2.94150	-2.93230	1.48040
H	1.98750	6.10140	-1.91500
H	-0.27320	5.83440	-3.73560
H	0.81770	7.22120	-3.69700
H	-1.16030	2.88440	1.23200
H	-1.70190	0.95450	2.68620
H	-0.37710	0.53630	4.75530
H	1.49480	2.07140	5.34820
H	2.04290	3.98620	3.89420

I-Z-TTC-R

Final Energy = -2049.177952 hartree

C	0.26010	4.33300	1.56980
C	-0.29660	5.76100	1.48050
S	1.64970	4.17550	0.28250
C	1.34710	2.65430	-0.54570
S	0.80900	2.58490	-2.21830
S	1.62770	1.18800	0.39340
C	0.62840	-0.12250	-0.44130

C	0.51870	-1.34670	0.47420
C	-0.26320	-2.48910	-0.19400
C	-0.44660	-3.70020	0.72910
C	1.81350	3.91720	-3.10210
C	1.29350	4.01430	-4.55900
C	3.27020	3.56430	-3.27210
C	3.52060	3.12560	-4.58400
C	4.81200	2.76540	-4.97190
C	5.85390	2.84870	-4.03850
C	5.60420	3.28860	-2.73200
C	4.30920	3.65070	-2.34080
C	0.73140	3.96850	2.96120
C	1.80240	4.64260	3.57300
C	2.21030	4.31220	4.86680
C	1.54940	3.30320	5.57790
C	0.47890	2.63080	4.98280
C	0.07540	2.96130	3.68420
C	2.24720	3.13300	-5.40280
H	-0.50170	3.62150	1.24130
H	-1.09620	5.88920	2.22070
H	0.47600	6.50940	1.69020
H	-0.70720	5.95750	0.48510
H	-0.36360	0.29020	-0.65140
H	1.10790	-0.38180	-1.39010
H	1.52250	-1.70340	0.74500
H	0.01910	-1.05940	1.40940
H	-1.24910	-2.11760	-0.50900
H	0.26040	-2.79960	-1.10940
H	-0.99770	-4.50210	0.22300
H	0.52200	-4.10790	1.04710
H	-1.00740	-3.42680	1.63270
H	1.64600	4.83200	-2.53010
H	0.24060	3.73160	-4.66020
H	1.38220	5.06090	-4.87480
H	5.01330	2.43540	-5.98900
H	6.86540	2.58000	-4.33370
H	6.42220	3.35990	-2.01950
H	4.12500	4.00290	-1.32910
H	2.33330	5.42150	3.03050
H	3.04670	4.83970	5.31910
H	1.86920	3.04350	6.58400
H	-0.04140	1.84470	5.52480
H	-0.75480	2.42710	3.22730
H	1.85270	2.11280	-5.51080
H	2.39310	3.52820	-6.41420

IAnh-Z-TTC-R

Final Energy = -2120.038236 hartree

C	0.87590	5.12180	1.86410
C	1.30570	6.53220	2.28590
S	2.29830	4.42980	0.82900
C	1.67920	2.88420	0.24340
S	0.29360	2.78450	-0.82060
S	2.63650	1.50490	0.77700
C	1.76480	-0.04140	0.25100
C	2.63440	-0.97210	-0.60210
C	2.84340	-0.50670	-2.04810
C	3.65580	-1.50490	-2.88160
C	0.77800	3.73880	-2.37810
C	2.22730	3.53840	-2.83920
C	0.50360	4.20600	3.00690

C	1.35750	3.99780	4.10360
C	0.97940	3.15630	5.15160
C	-0.25910	2.50340	5.12200
C	-1.11450	2.69990	4.03550
C	-0.73320	3.54410	2.98660
C	0.68510	5.24710	-2.14190
O	1.84780	5.86560	-2.58320
C	2.77900	4.93290	-3.01890
O	3.84280	5.28750	-3.45200
O	-0.23020	5.89920	-1.71590
C	-0.27120	3.33820	-3.43340
H	0.03070	5.19730	1.17490
H	0.49170	7.00140	2.85030
H	2.19580	6.51880	2.92310
H	1.51700	7.15360	1.40940
H	1.47450	-0.53230	1.18460
H	0.85420	0.24730	-0.27980
H	3.60570	-1.13000	-0.11280
H	2.13280	-1.95120	-0.60870
H	1.86140	-0.35190	-2.51700
H	3.34810	0.46830	-2.05050
H	3.76160	-1.16090	-3.91810
H	4.66410	-1.64010	-2.46980
H	3.16920	-2.48900	-2.90520
H	2.84900	3.02410	-2.09850
H	2.30830	2.98450	-3.77890
H	2.32690	4.48810	4.13730
H	1.65240	3.00770	5.99220
H	-0.55140	1.84750	5.93840
H	-2.07870	2.19820	4.00010
H	-1.40590	3.69310	2.14480
H	-0.11160	3.90420	-4.35850
H	-0.17930	2.27190	-3.65830
H	-1.28490	3.54330	-3.07640

R radical

Final Energy = -310.248803 hartree

C	1.91730	2.35140	0.00000
C	1.79270	0.85870	0.00000
C	0.56450	0.14880	0.00000
C	0.55750	-1.27970	0.00000
C	-0.63220	-1.99580	0.00000
C	-1.86720	-1.32520	0.00000
C	-1.88800	0.07810	0.00000
C	-0.70280	0.80630	0.00000
H	2.96800	2.65630	0.00000
H	1.43830	2.80680	-0.88060
H	1.43830	2.80680	0.88060
H	2.70750	0.26960	0.00000
H	1.50890	-1.80800	0.00000
H	-0.60630	-3.08300	0.00000
H	-2.79700	-1.88780	0.00000
H	-2.84000	0.60400	0.00000
H	-0.74300	1.89200	0.00000

Z-TTC-St

Final Energy = -1700.824127 hartree

C	-2.57820	0.93740	0.23470
C	-3.11130	2.35340	-0.03840
S	-0.72080	1.04670	0.10470
C	-0.17020	-0.61430	-0.17920
S	-1.10210	-1.88470	-0.69280

S	1.56070	-0.67410	0.15630
C	2.08060	-2.33750	-0.42680
C	3.59590	-2.48260	-0.24020
C	4.09900	-3.89640	-0.58950
C	3.93890	-4.28660	-2.06490
C	-2.66730	0.96750	2.78470
C	-3.03540	0.37330	1.56630
C	-3.13770	0.45850	3.99670
C	-3.98800	-0.65340	4.01170
C	-4.36330	-1.24950	2.80530
C	-3.88760	-0.74010	1.59190
H	-2.88990	0.26910	-0.57110
H	-4.20570	2.33190	0.00740
H	-2.75810	3.07490	0.70650
H	-2.81220	2.70170	-1.03220
H	1.53620	-3.08410	0.15860
H	1.78280	-2.43260	-1.47350
H	4.11890	-1.74360	-0.86190
H	3.85720	-2.26480	0.80390
H	5.16190	-3.94900	-0.31830
H	3.58200	-4.62990	0.04600
H	4.38410	-5.27120	-2.25480
H	2.88560	-4.33960	-2.36480
H	4.43890	-3.56140	-2.72100
H	-2.00200	1.82760	2.79020
H	-2.83950	0.92940	4.93050
H	-4.35170	-1.05080	4.95610
H	-5.02170	-2.11450	2.80470
H	-4.17920	-1.21300	0.65780

Z-TTC-I

Final Energy = -1738.936962 hartree

C	-0.85520	4.69160	0.36120
C	-0.25890	5.37320	1.61710
S	-1.00810	2.83860	0.52080
C	0.60910	2.21890	0.14910
S	1.92980	3.12680	-0.28140
S	0.57560	0.45830	0.29870
C	2.27820	-0.07230	-0.14790
C	2.36790	-1.59970	-0.06570
C	3.77860	-2.09660	-0.42050
C	3.89880	-3.62370	-0.35410
C	-1.47190	5.75910	2.49790
C	-2.60180	5.87530	1.49690
C	-2.25580	5.25920	0.28420
C	-3.85110	6.48240	1.64150
C	-4.74590	6.46540	0.56460
C	-4.39760	5.84680	-0.64420
C	-3.14790	5.23470	-0.79060
H	-0.25950	4.85620	-0.53900
H	0.47530	4.75150	2.13480
H	0.25620	6.28240	1.28200
H	2.49140	0.28680	-1.15870
H	2.97540	0.40760	0.54520
H	2.10860	-1.93520	0.94750
H	1.63910	-2.05320	-0.75050
H	4.04130	-1.75080	-1.42990
H	4.50630	-1.64050	0.26550
H	4.91420	-3.95040	-0.60860
H	3.66980	-3.99520	0.65300
H	3.20570	-4.10620	-1.05490

H	-1.69260	4.97500	3.23560
H	-1.30050	6.68510	3.05780
H	-4.12670	6.96770	2.57520
H	-5.71850	6.94070	0.66490
H	-5.10010	5.84670	-1.47340
H	-2.87640	4.75470	-1.72790

Z-TTC-MAnh

Final Energy = -1770.477151 hartree

O	-2.79750	6.03040	0.81900
C	-2.49690	4.93220	0.03370
C	-1.14270	4.37180	0.45680
C	-0.79170	5.14450	1.73410
C	-1.83920	6.23150	1.81230
O	-1.93710	7.15460	2.57280
O	-3.23370	4.57370	-0.84330
S	-1.22240	2.54960	0.58380
C	0.45080	2.05980	0.18370
S	1.67550	3.07160	-0.27470
S	0.54960	0.31450	0.36250
C	2.28180	-0.08790	-0.10600
C	2.49910	-1.59860	0.02440
C	3.94000	-1.98700	-0.34480
C	4.19060	-3.49490	-0.22710
H	-0.42990	4.59250	-0.34830
H	-0.86450	4.53150	2.63920
H	0.20710	5.58710	1.70800
H	2.44120	0.25410	-1.13240
H	2.94630	0.47240	0.55730
H	2.28810	-1.91890	1.05330
H	1.79810	-2.13440	-0.62970
H	4.15190	-1.65810	-1.37140
H	4.63890	-1.44650	0.30820
H	5.22460	-3.74400	-0.49310
H	4.01370	-3.84660	0.79720
H	3.52720	-4.06000	-0.89460

Z-TTC-IAnh

Final Energy = -1809.791156 hartree

C	-2.35810	1.03000	0.02290
C	-2.82570	2.50520	-0.03990
S	-0.51610	1.14080	0.03660
C	0.09870	-0.52470	-0.05720
S	-0.81260	-1.88260	-0.31120
S	1.84570	-0.46690	0.14890
C	2.37780	-2.21220	-0.08150
C	3.90240	-2.29510	0.04400
C	4.39510	-3.74250	-0.11620
C	5.91950	-3.86020	-0.00350
C	-2.91450	0.31430	-1.21500
O	-3.96770	-0.50090	-0.83170
C	-4.07150	-0.57930	0.55210
C	-3.00180	0.27140	1.19660
O	-2.63140	0.46190	-2.37190
O	-4.92110	-1.25790	1.06220
H	-3.92020	2.54280	-0.04420
H	-2.46940	3.04680	0.84190
H	-2.45520	2.99850	-0.94190
H	1.87930	-2.81760	0.68090
H	2.03740	-2.54060	-1.06720
H	4.37430	-1.66190	-0.71890
H	4.21890	-1.90970	1.02280

H	3.92030	-4.37270	0.64880
H	4.06750	-4.13100	-1.08990
H	6.24320	-4.90140	-0.11760
H	6.42100	-3.26600	-0.77780
H	6.27310	-3.50450	0.97320
H	-2.31140	-0.39380	1.72210
H	-3.45200	0.93820	1.93780

St radical

Final Energy = -310.248803 hartree

C	1.91730	2.35140	0.00000
C	1.79270	0.85870	0.00000
C	0.56450	0.14880	0.00000
C	0.55750	-1.27970	0.00000
C	-0.63220	-1.99580	0.00000
C	-1.86720	-1.32520	0.00000
C	-1.88800	0.07810	0.00000
C	-0.70280	0.80630	0.00000
H	2.96800	2.65630	0.00000
H	1.43830	2.80680	-0.88060
H	1.43830	2.80680	0.88060
H	2.70750	0.26960	0.00000
H	1.50890	-1.80800	0.00000
H	-0.60630	-3.08300	0.00000
H	-2.79700	-1.88780	0.00000
H	-2.84000	0.60400	0.00000
H	-0.74300	1.89200	0.00000

I radical

Final Energy = -348.357096 hartree

C	-0.19360	1.50270	-0.85550
C	-0.86350	2.74150	-1.38940
C	-0.51890	3.87150	-0.61920
C	-0.91190	5.23020	-0.74520
C	-0.42100	6.16380	0.16410
C	0.45290	5.77760	1.19700
C	0.84950	4.43250	1.33030
C	0.37110	3.48890	0.43380
C	0.64680	1.99980	0.36200
H	-0.93050	0.74190	-0.55610
H	0.43780	1.02090	-1.61700
H	-1.52510	2.74930	-2.24980
H	-1.58750	5.53440	-1.54130
H	-0.71630	7.20680	0.07640
H	0.82420	6.52240	1.89630
H	1.52640	4.14310	2.13200
H	0.35470	1.49310	1.29050
H	1.71680	1.80000	0.22170

MAnh radical

Final Energy = -379.897956 hartree

C	-5.55760	-6.62650	0.01010
C	-6.31300	-7.00120	-1.20740
C	-7.63810	-7.49240	-0.64650
O	-7.61150	-7.39770	0.73130
C	-6.37110	-6.87780	1.16930
O	-6.15870	-6.72010	2.35420
O	-8.60470	-7.91160	-1.22780
H	-4.55430	-6.22550	0.06350
H	-6.48210	-6.16260	-1.89830
H	-5.83410	-7.79580	-1.79760

IAnh radical

Final Energy = -419.225259 hartree

C	-0.09030	-0.53690	-0.94710
C	1.28090	-0.20290	-0.47260
C	1.03480	0.51380	0.84220
O	-0.32140	0.57920	1.07550
C	-1.03560	-0.04280	0.02100
O	-2.25040	-0.08380	0.05380
O	1.82850	0.98190	1.61840
C	-0.44800	-1.25730	-2.18920
H	1.91500	-1.08570	-0.30730
H	1.83480	0.45260	-1.16010
H	-1.53210	-1.32710	-2.31130
H	-0.01990	-0.75190	-3.06690
H	-0.02700	-2.27440	-2.17990

MAnh-Z-TTC-St radical

Final Energy = -2080.726972 hartree

O	-1.32940	3.45230	2.61720
C	-1.18230	3.36440	1.23440
C	-0.19620	4.40870	0.76270
C	0.03330	5.28970	1.99320
C	-0.63510	4.54170	3.12570
O	-0.63730	4.77640	4.30440
O	-1.78270	2.53250	0.60650
S	1.41140	3.58770	0.23450
C	1.03160	2.92440	-1.34050
S	0.53430	3.94970	-2.68210
S	1.18010	1.22310	-1.73210
C	1.31590	0.33770	-0.12180
C	1.31520	-1.17360	-0.38250
C	1.56690	-1.99610	0.89500
C	0.47480	-1.86640	1.96470
C	2.07360	4.98070	-3.05850
C	1.61680	6.13710	-3.95570
C	3.18480	4.13450	-3.63620
C	4.33370	3.87890	-2.87250
C	5.37940	3.10190	-3.38470
C	5.28930	2.56670	-4.67190
C	4.14630	2.81390	-5.44290
C	3.10460	3.58830	-4.92920
H	-0.58540	4.93970	-0.10790
H	1.08430	5.47050	2.23920
H	-0.45020	6.26790	1.88900
H	2.24450	0.64570	0.36730
H	0.47200	0.64310	0.50130
H	0.35540	-1.47000	-0.82690
H	2.09520	-1.41640	-1.11580
H	1.65760	-3.05030	0.60150
H	2.53840	-1.71000	1.32220
H	0.67840	-2.53490	2.80960
H	0.40680	-0.84690	2.36260
H	-0.50930	-2.13250	1.55720
H	2.39070	5.38080	-2.09160
H	2.47670	6.77440	-4.19050
H	1.19150	5.78400	-4.90120
H	0.86330	6.74820	-3.44780
H	4.41280	4.29360	-1.86990
H	6.26090	2.91630	-2.77630
H	6.09890	1.96210	-5.07230
H	4.06560	2.40040	-6.44520
H	2.21910	3.75960	-5.53650

MAnh-Z-TTC-I radical

Final Energy = -2118.835314 hartree

O	-2.48910	4.99210	1.43310
C	-1.92440	4.19710	0.43710
C	-0.65560	3.56590	0.95460
C	-0.38530	4.29440	2.27210
C	-1.65590	5.06930	2.54160
O	-1.98270	5.69570	3.51380
O	-2.46460	4.07900	-0.63210
S	-0.93830	1.72100	1.26500
C	-0.73810	0.98420	-0.30240
S	-2.00820	0.14270	-1.18200
S	0.77170	1.09890	-1.21220
C	2.03900	0.45060	-0.02450
C	3.41430	0.45040	-0.69930
C	4.55540	0.07270	0.26450
C	4.48190	-1.35770	0.81480
C	-3.60680	0.54420	-0.30100
C	-3.90340	-0.39100	0.89880
C	-4.74830	0.25840	-1.25270
C	-5.17580	1.01110	-2.34940
C	-6.28050	0.56560	-3.08380
C	-6.93720	-0.62040	-2.72610
C	-6.50100	-1.37560	-1.63040
C	-5.40190	-0.93040	-0.89280
C	-4.74670	-1.55410	0.32190
H	0.14580	3.64090	0.21760
H	-0.15820	3.64210	3.12070
H	0.44150	5.00800	2.17740
H	2.04010	1.09450	0.86010
H	1.72780	-0.55480	0.27050
H	3.40760	-0.24520	-1.54980
H	3.61640	1.45010	-1.10760
H	5.50460	0.20160	-0.27290
H	4.57380	0.78870	1.09880
H	5.36120	-1.58170	1.43090
H	3.59500	-1.51230	1.44050
H	4.44890	-2.09270	-0.00040
H	-3.53390	1.59620	-0.01990
H	-3.00140	-0.72680	1.41620
H	-4.50680	0.17780	1.61800
H	-4.66550	1.93120	-2.62500
H	-6.63450	1.14500	-3.93270
H	-7.79660	-0.95400	-3.30240
H	-7.01820	-2.29240	-1.35640
H	-4.10810	-2.39700	0.02290
H	-5.47040	-1.94240	1.04650

IAnh-Z-TTC-St radical

Final Energy = -2120.037838 hartree

O	-0.84040	6.47590	2.18180
C	-0.35510	6.23690	0.90890
C	0.06240	4.76690	0.77000
C	1.58990	4.71140	0.59670
C	-0.87410	5.30870	2.94000
O	-1.24040	5.33720	4.08360
O	-0.27380	7.12610	0.10510
S	-0.84790	4.14340	-0.75290
C	-0.03650	2.64070	-1.20660
S	-0.05340	2.24920	-2.92650
S	0.03000	1.33380	-0.02380
C	1.49350	0.33630	-0.55780

C	1.85970	-0.66990	0.53670
C	3.01690	-1.58380	0.10170
C	3.43040	-2.57690	1.19420
C	1.03930	3.54180	-3.73720
C	0.69810	3.50850	-5.23540
C	2.51510	3.33890	-3.46010
C	3.17440	2.14180	-3.78600
C	4.54550	1.99900	-3.56360
C	5.28510	3.05200	-3.01050
C	4.64060	4.24810	-2.68560
C	3.26590	4.38760	-2.90960
C	-0.42390	4.14280	2.09370
H	2.08040	5.12230	1.48690
H	1.91220	3.67480	0.47440
H	1.90240	5.28760	-0.27610
H	1.24070	-0.17450	-1.49060
H	2.31700	1.02950	-0.74960
H	2.14060	-0.13250	1.45240
H	0.98510	-1.28740	0.78470
H	2.72150	-2.13450	-0.80290
H	3.88190	-0.96600	-0.17780
H	4.24780	-3.22270	0.85120
H	3.77300	-2.05340	2.09590
H	2.59070	-3.22310	1.48130
H	0.72270	4.50120	-3.31970
H	1.29610	4.26360	-5.75740
H	0.92450	2.53320	-5.68110
H	-0.36130	3.72940	-5.40170
H	2.61170	1.31200	-4.20710
H	5.03810	1.06420	-3.82050
H	6.35190	2.93840	-2.83560
H	5.20320	5.07360	-2.25690
H	2.77330	5.32450	-2.65990
H	-1.28010	3.47390	1.96460
H	0.35430	3.58260	2.61880

IAnh-Z-TTC-I radical

Final Energy = -2158.146159 hartree

O	-1.37670	3.84780	-1.83110
C	-0.22190	3.46530	-1.16820
C	-0.27100	3.93820	0.28280
C	-2.23640	4.55370	-0.99370
O	-3.28730	4.96300	-1.40810
O	0.64740	2.86930	-1.74620
S	-0.07960	2.48430	1.45940
C	-1.04260	1.14570	0.82230
S	-2.80170	1.30200	0.89890
S	-0.33240	-0.47020	0.89060
C	1.24560	-0.31670	-0.07300
C	2.49810	-0.37780	0.80620
C	3.80680	-0.25720	0.00220
C	4.09420	-1.43730	-0.93740
C	-3.43750	0.10010	-0.36700
C	-3.18060	0.49720	-1.84130
C	-4.95020	-0.01410	-0.28410
C	-5.77740	-0.07560	0.84010
C	-7.15930	-0.21930	0.65860
C	-7.69980	-0.30960	-0.63010
C	-6.86550	-0.26260	-1.75490
C	-5.48870	-0.11280	-1.57700
C	-4.39080	-0.07710	-2.62010

C	-1.61860	4.68020	0.37610
C	0.93840	4.84290	0.58600
H	1.21640	-1.14250	-0.79100
H	1.19030	0.62170	-0.63150
H	2.45220	0.43470	1.54170
H	2.50380	-1.32000	1.37310
H	3.79160	0.67900	-0.57460
H	4.63470	-0.16340	0.71880
H	5.07170	-1.31990	-1.42050
H	4.10720	-2.38710	-0.38480
H	3.34370	-1.52450	-1.73320
H	-2.96960	-0.86220	-0.13150
H	-3.17860	1.58870	-1.92880
H	-2.21710	0.12700	-2.20480
H	-5.36300	-0.00720	1.84270
H	-7.81590	-0.25790	1.52470
H	-8.77480	-0.41580	-0.75830
H	-7.28850	-0.33870	-2.75420
H	-4.64840	0.52570	-3.49780
H	-4.17830	-1.09500	-2.97930
H	-2.30600	4.26890	1.11830
H	-1.48980	5.74390	0.60410
H	0.88790	5.74940	-0.02670
H	0.92320	5.14250	1.63870
H	1.87760	4.32590	0.37540

Styrene

Final Energy = -309.665050 hartree

C	0.94900	2.86980	0.00000
C	-0.11090	2.04440	0.00000
C	-0.10240	0.56920	0.00000
C	1.08130	-0.19590	0.00000
C	1.03100	-1.58940	0.00000
C	-0.20170	-2.25550	0.00000
C	-1.38440	-1.51140	0.00000
C	-1.33280	-0.11500	0.00000
H	0.81090	3.94750	0.00000
H	1.97650	2.51420	0.00000
H	-1.10630	2.48930	0.00000
H	2.04870	0.29860	0.00000
H	1.95640	-2.16010	0.00000
H	-0.23640	-3.34190	0.00000
H	-2.34760	-2.01570	0.00000
H	-2.25840	0.45700	0.00000

Indene

Final Energy = -347.779297 hartree

C	-0.47640	3.87970	-0.62870
C	0.35640	3.48660	0.44500
C	0.79080	4.41960	1.38110
C	0.38870	5.75760	1.24170
C	-0.43660	6.14810	0.17800
C	-0.87700	5.21310	-0.76720
C	0.62050	2.00090	0.33570
C	-0.15090	1.61520	-0.90610
C	-0.76730	2.69180	-1.44160
H	1.43150	4.12410	2.20940
H	0.72050	6.49770	1.96560
H	-0.73780	7.18890	0.08650
H	-1.51730	5.52080	-1.59090
H	1.69260	1.77460	0.23820
H	0.27240	1.44960	1.22170

H	-0.18580	0.60150	-1.29190
H	-1.38610	2.69940	-2.33390

Maleic anhydride

Final Energy = -379.318244 hartree

C	0.00000	0.66900	1.30400
C	0.00000	1.12920	-0.10870
O	0.00000	0.00000	-0.92750
C	0.00000	-1.12920	-0.10870
C	0.00000	-0.66900	1.30400
O	0.00000	-2.24090	-0.56770
O	0.00000	2.24090	-0.56770
H	0.00000	1.35940	2.13740
H	0.00000	-1.35940	2.13740

Itaconic anhydride

Final Energy = -418.638660 hartree

C	0.14220	-0.09960	-1.39660
C	0.56390	-1.21530	-0.46480
O	0.30890	-0.84610	0.84980
C	-0.25380	0.43170	0.91740
C	-0.38490	0.95730	-0.46300
O	-0.54220	0.91740	1.98190
O	1.05020	-2.28530	-0.71780
C	-0.89350	2.16480	-0.72790
H	1.00750	0.22540	-1.98550
H	-0.60860	-0.48060	-2.09850
H	-1.23300	2.81100	0.07660
H	-0.98280	2.53470	-1.74530

Styrene radical

Final Energy = -310.248803 hartree

C	1.91750	2.35120	0.00000
C	1.79280	0.85850	0.00000
C	0.56450	0.14870	0.00000
C	0.55740	-1.27980	0.00000
C	-0.63240	-1.99570	0.00000
C	-1.86730	-1.32510	0.00000
C	-1.88800	0.07820	0.00000
C	-0.70270	0.80640	0.00000
H	2.96820	2.65610	0.00000
H	1.43850	2.80670	-0.88060
H	1.43850	2.80670	0.88060
H	2.70760	0.26940	0.00000
H	1.50870	-1.80810	0.00000
H	-0.60650	-3.08290	0.00000
H	-2.79720	-1.88760	0.00000
H	-2.84000	0.60420	0.00000
H	-0.74280	1.89210	0.00000

Indene radical

Final Energy = -348.357097 hartree

C	-0.45060	3.88760	-0.66650
C	0.34090	3.48190	0.45440
C	0.72000	4.40230	1.41980
C	0.31880	5.74640	1.29030
C	-0.46040	6.15470	0.19230
C	-0.85050	5.24470	-0.78710
C	0.63830	1.99780	0.36710
C	-0.05630	1.53460	-0.95150
C	-0.70160	2.77930	-1.50190
H	1.32220	4.09550	2.27290
H	0.61260	6.47310	2.04350
H	-0.76130	7.19650	0.10890

H	-1.45250	5.56620	-1.63390
H	1.71870	1.80670	0.34500
H	0.24510	1.46130	1.24020
H	0.66660	1.10580	-1.66210
H	-0.79590	0.74110	-0.76550
H	-1.27730	2.80680	-2.42200

Maleic anhydride radical

Final Energy = -379.897946 hartree

C	-5.49170	-6.64900	-0.02320
C	-6.39670	-6.87970	1.17680
O	-7.61310	-7.36870	0.74110
C	-7.62220	-7.49330	-0.66760
C	-6.34270	-7.06160	-1.16280
O	-8.61000	-7.90880	-1.23830
O	-6.17670	-6.69680	2.34550
H	-5.17770	-5.59600	-0.06400
H	-4.57100	-7.24180	0.07820
H	-6.08240	-7.05630	-2.21290

Itaconic anhydride radical

Final Energy = -419.225254 hartree

C	0.13850	-0.09480	-1.37020
C	0.56900	-1.22900	-0.45860
O	0.32190	-0.87660	0.85060
C	-0.24770	0.41890	0.91500
C	-0.37590	0.93360	-0.42390
O	-0.53640	0.90160	1.99340
O	1.05480	-2.29450	-0.74090
C	-0.93090	2.26080	-0.77200
H	0.99230	0.25030	-1.97110
H	-0.61850	-0.45220	-2.08320
H	-1.24020	2.81000	0.12080
H	-0.18770	2.85990	-1.31790
H	-1.79650	2.15430	-1.44200

Styrene-styrene radical

Final Energy = -619.936778 hartree

C	0.02200	-0.02040	-0.02030
C	1.51590	-0.15130	-0.03860
C	2.22390	-1.38030	-0.04270
C	3.65220	-1.38680	-0.06890
C	4.36880	-2.57620	-0.07440
C	3.69920	-3.81170	-0.05430
C	2.29610	-3.83310	-0.02820
C	1.56710	-2.64830	-0.02220
C	-0.48130	1.44020	0.03740
C	-2.01690	1.48760	-0.08510
C	-0.00070	2.18060	1.28030
C	0.72170	3.37740	1.16090
C	1.15380	4.07970	2.29180
C	0.86850	3.59340	3.57030
C	0.14760	2.40150	3.70570
C	-0.28200	1.70500	2.57290
H	-0.40850	-0.49410	-0.91850
H	-0.40230	-0.58460	0.82590
H	2.10610	0.76360	-0.06090
H	4.17990	-0.43520	-0.08390
H	5.45590	-2.54940	-0.09420
H	4.26230	-4.74110	-0.05900
H	1.77050	-4.78530	-0.01290
H	0.48170	-2.69020	-0.00280
H	-0.06310	1.96320	-0.83360

H	-2.37920	2.52200	-0.08280
H	-2.34570	1.01300	-1.01790
H	-2.49700	0.96100	0.74890
H	0.95070	3.76500	0.16990
H	1.71360	5.00420	2.17140
H	1.20390	4.13480	4.45150
H	-0.08000	2.01260	4.69550
H	-0.84080	0.78060	2.70150

Styrene-styrene intermediate

Final Energy = -619.913194 hartree

C	0.07160	0.03330	0.39170
C	1.56560	-0.06430	0.35500
C	2.30280	-1.27030	0.47360
C	3.72930	-1.25200	0.40360
C	4.47200	-2.42060	0.50850
C	3.83110	-3.65810	0.68860
C	2.43050	-3.70300	0.76220
C	1.67580	-2.53950	0.65830
C	0.61800	-4.54390	-3.34360
C	1.99910	-4.43050	-3.52230
C	2.58060	-3.17320	-3.70530
C	1.79860	-2.00260	-3.71260
C	0.40730	-2.13400	-3.52940
C	-0.17410	-3.38830	-3.34880
C	2.46880	-0.70310	-3.90650
C	1.90400	0.51540	-3.93170
H	-0.25260	1.07840	0.38250
H	-0.39540	-0.46460	-0.47340
H	-0.35450	-0.44200	1.28740
H	2.13280	0.85130	0.20190
H	4.23450	-0.29880	0.26170
H	5.55690	-2.37630	0.44840
H	4.41440	-4.57180	0.76690
H	1.92710	-4.65770	0.89700
H	0.59230	-2.59940	0.71020
H	0.16140	-5.51990	-3.19990
H	2.62560	-5.31890	-3.51620
H	3.65740	-3.09360	-3.83930
H	-0.22640	-1.25170	-3.52750
H	-1.24960	-3.46650	-3.20940
H	3.54910	-0.76940	-4.03920
H	2.51200	1.40340	-4.08110
H	0.83610	0.67620	-3.80490

Styrene-maleic anhydride radical

Final Energy = -689.584151 hartree

C	0.04300	-0.06530	-0.00980
C	1.52440	0.00960	-0.06520
C	-0.62030	0.80630	1.13010
C	-0.18350	2.27790	0.99960
C	-2.13600	0.67170	1.14590
C	-2.78150	0.17240	2.28590
C	-4.17610	0.07960	2.34000
C	-4.94820	0.48440	1.24810
C	-4.31520	0.98560	0.10500
C	-2.92230	1.07990	0.05620
C	-0.18450	-1.56730	0.17570
O	1.03460	-2.20860	0.31730
C	2.09220	-1.29020	0.16510
O	3.24570	-1.66570	0.23290
O	-1.21250	-2.19100	0.20790

H	-0.40700	0.24060	-0.96530
H	2.12950	0.88450	-0.25930
H	-0.23790	0.42330	2.08330
H	-0.67930	2.87570	1.77130
H	0.89770	2.38920	1.13240
H	-0.45520	2.69470	0.02270
H	-2.18860	-0.15020	3.13900
H	-4.65570	-0.31200	3.23340
H	-6.03200	0.41020	1.28480
H	-4.90640	1.30380	-0.75020
H	-2.45230	1.47550	-0.84180

Styrene-maleic anhydride intermediate

Final Energy = -689.563749 hartree

C	-5.94310	-6.89810	0.92540
C	-7.09710	-7.58430	1.63840
O	-8.01830	-8.01430	0.70330
C	-7.58460	-7.69290	-0.60470
C	-6.31800	-7.01980	-0.50210
O	-8.26570	-7.99270	-1.56440
O	-7.26770	-7.76790	2.81590
C	-5.76870	-2.33700	-1.31740
C	-5.97420	-2.37520	-2.64450
C	-6.65430	-2.85020	-0.25490
C	-7.88880	-3.47860	-0.51580
C	-8.69060	-3.94090	0.52760
C	-8.28120	-3.78880	1.85880
C	-7.05870	-3.17000	2.13460
C	-6.25580	-2.70710	1.08810
H	-5.86060	-5.85530	1.26760
H	-4.99150	-7.38630	1.18060
H	-5.76170	-6.66540	-1.35950
H	-4.84910	-1.87660	-0.95460
H	-6.86190	-2.81300	-3.09440
H	-5.24120	-1.95800	-3.32930
H	-8.22890	-3.60560	-1.53950
H	-9.63940	-4.42140	0.30290
H	-8.90900	-4.14990	2.66930
H	-6.72940	-3.04510	3.16340
H	-5.30710	-2.22390	1.31260

Maleic anhydride-styrene radical

Final Energy = -689.598109 hartree

C	-0.01500	-0.05320	-0.12130
C	1.47830	-0.16590	-0.20270
C	2.21130	-1.37390	-0.08070
C	3.63480	-1.35590	-0.20210
C	4.38270	-2.52050	-0.09190
C	3.75030	-3.75360	0.14180
C	2.35280	-3.79890	0.26250
C	1.59230	-2.63930	0.15480
C	-0.47860	1.39200	0.13580
C	-0.12060	1.98880	1.50690
C	-1.38990	2.65690	1.98010
O	-2.43830	2.31710	1.13000
C	-1.99080	1.53170	0.07390
O	-2.77050	1.08860	-0.72830
O	-1.58310	3.36920	2.92970
H	-0.48040	-0.39840	-1.05830
H	-0.41590	-0.70270	0.66950
H	2.04070	0.73990	-0.42390
H	4.13330	-0.40570	-0.38400

H	5.46490	-2.47590	-0.18810
H	4.33760	-4.66400	0.22670
H	1.85600	-4.75010	0.44010
H	0.51190	-2.70330	0.24680
H	-0.08930	2.03520	-0.66590
H	0.14610	1.21560	2.23850
H	0.69420	2.71660	1.48580

Maleic anhydride-styrene intermediate

Final Energy = -689.567182 hartree

C	-0.01320	0.33300	-1.11560
C	1.42480	0.12440	-0.75310
C	2.01980	-1.13420	-0.48020
C	3.40760	-1.21680	-0.15180
C	4.01400	-2.43570	0.12150
C	3.26930	-3.62690	0.07940
C	1.90440	-3.57370	-0.24350
C	1.28580	-2.35840	-0.51920
C	0.81070	-0.07920	3.55520
C	2.06490	-0.79710	3.90200
O	1.78040	-2.16170	3.94390
C	0.42970	-2.33300	3.64220
C	-0.15830	-0.98950	3.40100
O	-0.07670	-3.42400	3.61130
O	3.16930	-0.37560	4.12510
H	-0.26690	1.39760	-1.11370
H	-0.24460	-0.05720	-2.12010
H	-0.69650	-0.17780	-0.42210
H	2.07240	0.99820	-0.71660
H	3.99220	-0.29990	-0.11600
H	5.07200	-2.46650	0.37100
H	3.74520	-4.57960	0.29560
H	1.32170	-4.49120	-0.27880
H	0.22870	-2.34260	-0.76970
H	0.76910	0.99820	3.45800
H	-1.20060	-0.85200	3.14310

Styrene-itaconic anhydride radical

Final Energy = -728.912680 hartree

C	0.06320	0.03200	-0.03850
C	1.54480	0.08610	0.02570
C	-0.52200	-1.42350	-0.09820
C	-2.05580	-1.36010	0.01900
C	-0.06270	-2.18530	-1.33340
C	2.30080	-0.00520	1.24940
O	3.68150	0.06170	0.93820
C	3.86080	0.19080	-0.42190
C	2.50630	0.20990	-1.10440
O	1.94580	-0.11710	2.40710
O	4.96220	0.26850	-0.90470
C	0.76610	-3.31000	-1.20310
C	1.19760	-4.02390	-2.32680
C	0.80500	-3.62160	-3.60610
C	-0.02230	-2.50210	-3.75100
C	-0.45090	-1.79260	-2.62590
H	-0.34890	0.51150	0.85750
H	-0.28760	0.59210	-0.91320
H	-0.14030	-1.95560	0.78120
H	-2.48170	-2.36950	0.00270
H	-2.35090	-0.87880	0.95870
H	-2.49980	-0.79170	-0.80640
H	2.43940	-0.61390	-1.82890

H	2.38610	1.13860	-1.68040
H	1.07660	-3.63290	-0.21130
H	1.83920	-4.89250	-2.20000
H	1.13820	-4.17350	-4.48140
H	-0.33520	-2.18100	-4.74160
H	-1.09420	-0.92590	-2.76140

Styrene-itaconic anhydride intermediate

Final Energy = -728.887919 hartree

C	0.00230	0.31840	-2.36570
C	1.31890	0.38720	-1.65520
C	1.90790	-0.68160	-0.93220
C	3.17650	-0.50910	-0.29790
C	3.77420	-1.54050	0.41440
C	3.13870	-2.78840	0.52900
C	1.89210	-2.98420	-0.08570
C	1.28370	-1.95900	-0.80230
C	1.62940	-0.77240	4.04840
C	2.43770	-1.97800	4.47620
O	1.61050	-3.09160	4.54970
C	0.29050	-2.76370	4.22910
C	0.23160	-1.31490	3.91880
O	-0.56850	-3.60900	4.24150
O	3.60890	-2.06770	4.73280
H	-0.29280	1.30450	-2.73790
H	0.03630	-0.36400	-3.23040
H	-0.80400	-0.04950	-1.71410
H	1.87930	1.31850	-1.70970
H	3.67720	0.45330	-0.38160
H	4.74100	-1.37980	0.88560
H	3.60860	-3.59430	1.08600
H	1.39470	-3.94770	-0.00280
H	0.31970	-2.13450	-1.27160
H	2.03690	-0.38750	3.10620
C	-0.90730	-0.69290	3.59750
H	-1.84310	-1.24170	3.55060
H	-0.93280	0.37030	3.37580
H	1.72960	0.01900	4.79970

Itaconic anhydride-Styrene radical

Final Energy = -728.911868 hartree

C	0.01540	-0.04840	0.57370
C	1.49840	-0.24310	0.66910
C	2.21240	-1.41660	0.31440
C	3.62830	-1.46020	0.50910
C	4.36920	-2.58740	0.18160
C	3.73810	-3.72430	-0.35190
C	2.34880	-3.70950	-0.55090
C	1.59560	-2.58570	-0.22820
C	-0.43680	1.38500	0.18800
C	-1.98240	1.45230	0.15720
C	0.18220	1.90930	-1.12430
C	0.71130	3.28300	-0.79580
O	0.64360	3.48960	0.57900
C	0.04840	2.40730	1.21590
O	-0.05040	2.38810	2.41540
O	1.15760	4.13600	-1.51690
H	-0.42700	-0.73020	-0.16030
H	-0.45900	-0.29030	1.53840
H	2.07950	0.55880	1.12290
H	4.12630	-0.58570	0.92340
H	5.44490	-2.58860	0.34090

H	4.31930	-4.60660	-0.60630
H	1.85180	-4.58640	-0.96020
H	0.52190	-2.60760	-0.38870
H	-2.35780	0.74980	-0.59440
H	-2.40090	1.18010	1.13080
H	-2.33540	2.45560	-0.10570
H	1.03000	1.29750	-1.45750
H	-0.52520	1.97370	-1.95590

Itaconic anhydride-Styrene intermediate

Final Energy = -728.890848 hartree

C	0.00270	-0.75300	-1.32760
C	0.10660	-1.80510	-0.23940
O	-0.35840	-1.27860	0.94590
C	-0.78300	0.06090	0.75920
C	-0.58350	0.41950	-0.62140
O	-1.22650	0.69200	1.69970
O	0.51380	-2.93760	-0.30580
C	-0.90760	1.73820	-1.21010
C	2.46230	4.08140	1.07930
C	3.08890	3.48620	0.05050
C	3.45090	2.06200	-0.08200
C	4.06410	1.62700	-1.27260
C	4.42580	0.28900	-1.45370
C	4.18250	-0.64480	-0.44260
C	3.57520	-0.22710	0.74920
C	3.21390	1.10790	0.92830
H	0.99840	-0.55480	-1.75080
H	-0.61910	-1.12420	-2.15460
H	-1.37980	2.39670	-0.47710
H	0.00380	2.22650	-1.58580
H	-1.57700	1.62260	-2.07370
H	2.25210	5.14700	1.05610
H	2.13860	3.54380	1.96730
H	3.37400	4.10360	-0.80210
H	4.25890	2.34800	-2.06410
H	4.89880	-0.02180	-2.38250
H	4.46260	-1.68670	-0.57790
H	3.38410	-0.94610	1.54200
H	2.74770	1.40870	1.86210

Indene-indene radical

Final Energy = -696.153984 hartree

C	-0.60200	3.99430	-0.54740
C	0.24240	3.67930	0.56350
C	0.53140	4.63630	1.52450
C	-0.01990	5.92720	1.40230
C	-0.86130	6.24370	0.31950
C	-1.16220	5.29490	-0.65530
C	0.68820	2.23520	0.47340
C	0.15900	1.73630	-0.91110
C	-0.70810	2.87310	-1.39610
C	1.27070	1.37010	-1.93690
C	2.23100	0.27300	-1.49470
C	3.53930	0.56100	-1.91810
C	3.57350	1.86250	-2.69180
C	2.22960	2.53250	-2.31660
C	1.96380	-0.90590	-0.79370
C	3.01580	-1.78710	-0.50680
C	4.32110	-1.49280	-0.92130
C	4.58790	-0.31610	-1.63380
H	1.17910	4.39910	2.36650

H	0.20710	6.68440	2.14850
H	-1.27740	7.24550	0.24210
H	-1.80780	5.54680	-1.49340
H	1.77560	2.12820	0.56990
H	0.24900	1.64400	1.28800
H	-0.44840	0.82880	-0.77610
H	-1.28340	2.83630	-2.31670
H	0.75280	1.02860	-2.84770
H	4.44230	2.48550	-2.44790
H	3.62180	1.65830	-3.77190
H	1.82720	3.15560	-3.12100
H	2.38190	3.18280	-1.44670
H	0.95490	-1.14380	-0.46330
H	2.81770	-2.70270	0.04540
H	5.13160	-2.17910	-0.68680
H	5.60260	-0.08920	-1.95650

Indene-indene intermediate

Final Energy = -696.136228 hartree

C	1.98070	5.60330	0.93790
C	2.06270	5.05200	2.25590
C	3.15760	5.31750	3.06440
C	4.19250	6.14100	2.57960
C	4.11820	6.69270	1.28730
C	3.02740	6.43540	0.46040
C	0.82500	4.22670	2.54790
C	0.00610	4.26440	1.22040
C	0.78850	5.17880	0.31490
C	1.63790	9.47920	4.35410
C	0.41040	8.92540	4.00410
C	-0.25910	8.04650	4.88750
C	0.30270	7.71790	6.12590
C	1.53920	8.27720	6.47230
C	2.20140	9.14950	5.59730
C	-1.51680	7.63090	4.25430
C	-1.62770	8.21510	3.04090
C	-0.42770	9.08950	2.75450
H	3.22100	4.89960	4.06730
H	5.05310	6.35430	3.20840
H	4.92570	7.32780	0.93030
H	2.97670	6.86270	-0.53810
H	1.07820	3.20230	2.84690
H	0.25370	4.66400	3.37690
H	-0.09590	3.25960	0.78170
H	-1.02030	4.62420	1.38230
H	0.47650	5.45020	-0.68870
H	2.15900	10.15510	3.67960
H	-0.20780	7.04210	6.80860
H	1.99080	8.03250	7.43080
H	3.16060	9.57390	5.88330
H	-2.23440	6.95400	4.70820
H	-2.45130	8.09020	2.34530
H	-0.71610	10.13630	2.57990
H	0.10700	8.76490	1.84990

Indene-maleic anhydride radical

Final Energy = -727.695505 hartree

C	-0.56710	4.00070	-0.61430
C	0.12510	3.61950	0.67780
C	0.78970	2.26500	0.33470
C	-0.09760	1.65520	-0.78420
C	-0.69550	2.88380	-1.45510

C	0.63410	0.68330	-1.75330
C	1.14200	-0.58020	-1.05970
O	2.47530	-0.77240	-1.36160
C	2.94830	0.27290	-2.18890
C	1.85930	1.18040	-2.42820
O	0.54510	-1.34670	-0.34850
O	4.10380	0.28020	-2.56160
C	-1.33960	2.99510	-2.68910
C	-1.84600	4.24080	-3.08300
C	-1.71290	5.35650	-2.24740
C	-1.07510	5.24050	-1.00550
H	0.84730	4.36940	1.01860
H	-0.61510	3.49760	1.48200
H	1.79850	2.44960	-0.05680
H	0.88370	1.60300	1.20090
H	-0.90640	1.06520	-0.33040
H	-0.10430	0.35320	-2.50310
H	1.95700	2.07460	-3.02970
H	-1.45100	2.13630	-3.34770
H	-2.34200	4.34100	-4.04510
H	-2.10460	6.31950	-2.56600
H	-0.97530	6.10890	-0.35780

Indene-maleic anhydride intermediate

Final Energy = -727.678253 hartree

C	-5.88130	-6.81160	1.25100
C	-7.06370	-7.68180	1.64350
O	-7.74040	-8.07040	0.50400
C	-7.11090	-7.54520	-0.64950
C	-5.97150	-6.77860	-0.22610
O	-7.56360	-7.78150	-1.75150
O	-7.43050	-8.02630	2.73700
C	-5.88370	-2.69360	-1.44020
C	-6.66690	-3.09550	-2.46540
C	-6.55240	-2.98820	-0.16680
C	-7.79630	-3.60000	-0.45260
C	-8.65000	-3.98240	0.57830
C	-8.25650	-3.75010	1.90560
C	-7.02420	-3.14400	2.18990
C	-6.16040	-2.75770	1.15650
H	-5.97950	-5.81690	1.71370
H	-4.94550	-7.24210	1.63300
H	-5.31110	-6.26590	-0.91180
H	-4.90960	-2.22130	-1.52280
H	-9.60820	-4.45160	0.36560
H	-8.91370	-4.04180	2.72140
H	-6.73830	-2.96890	3.22470
H	-5.20750	-2.28450	1.38240
C	-7.95200	-3.70480	-1.95360
H	-6.43320	-3.00440	-3.52080
H	-8.07700	-4.74340	-2.28980
H	-8.83570	-3.15890	-2.31710

Maleic anhydride-indene radical

Final Energy = -727.705880 hartree

C	-0.37570	4.17210	-0.65450
C	0.42200	3.71870	0.44090
C	0.66040	4.54090	1.53130
C	0.11230	5.83800	1.54720
C	-0.66560	6.29860	0.46870
C	-0.91660	5.48410	-0.63240
C	0.92520	2.31930	0.16050

C	0.16170	1.87920	-1.13320
C	-0.49810	3.14940	-1.61730
C	1.09330	1.18140	-2.15400
C	0.38080	0.69280	-3.40820
O	0.79980	-0.59860	-3.71830
C	1.66490	-1.09230	-2.75060
C	1.79550	-0.08600	-1.63380
O	-0.41600	1.24950	-4.11590
O	2.16490	-2.17910	-2.87560
H	1.26590	4.19600	2.36690
H	0.29290	6.48950	2.39820
H	-1.07850	7.30400	0.49930
H	-1.52280	5.84180	-1.46110
H	2.01000	2.33730	-0.01650
H	0.75460	1.63190	0.99560
H	-0.61640	1.14640	-0.86060
H	-1.06260	3.21680	-2.53960
H	1.83990	1.90960	-2.50020
H	2.84930	0.05320	-1.38040
H	1.29570	-0.50370	-0.75120

Maleic anhydride-indene intermediate

Final Energy = -727.675633 hartree

C	1.43470	6.26140	2.07040
C	2.09910	5.00960	1.87300
C	3.32330	4.95580	1.22310
C	3.91270	6.14730	0.75640
C	3.26790	7.38340	0.94720
C	2.03840	7.45680	1.59800
C	1.27170	3.88620	2.46640
C	-0.00090	4.59120	3.03160
C	0.21400	6.05450	2.74680
C	1.35430	6.55270	-2.84040
O	2.16470	5.42530	-2.97430
C	1.49400	4.33980	-2.41130
C	0.18730	4.82650	-1.89840
C	0.10380	6.13720	-2.15350
O	1.97750	3.23840	-2.39690
O	1.70130	7.63030	-3.24640
H	3.82960	4.00440	1.07160
H	4.87140	6.11190	0.24550
H	3.73780	8.29310	0.58080
H	1.54480	8.41490	1.74240
H	1.01770	3.13150	1.71140
H	1.82470	3.36140	3.25580
H	-0.91850	4.21690	2.55170
H	-0.13000	4.39940	4.10750
H	-0.48940	6.83460	3.02130
H	-0.52380	4.17200	-1.41140
H	-0.69340	6.83400	-1.92900

Indene-itaconic anhydride radical

Final Energy = -767.021142 hartree

C	-0.04030	0.04460	0.03880
C	1.43810	0.08870	-0.04480
C	-0.82670	-1.16260	0.00620
O	-2.19690	-0.81630	0.12110
C	-2.34010	0.54880	0.22940
C	-0.96970	1.19970	0.19420
O	-0.50480	-2.33100	-0.08950
O	-3.42630	1.06080	0.33280
C	2.00620	0.74650	-1.35050

C	1.69420	-0.05330	-2.60520
C	2.81330	-0.80210	-3.00530
C	3.98150	-0.55400	-2.07320
C	3.56090	0.73830	-1.32950
C	0.50540	-0.11460	-3.33660
C	0.44030	-0.93860	-4.46790
C	1.55320	-1.69290	-4.85960
C	2.74720	-1.62690	-4.12990
H	1.81670	0.68210	0.80050
H	1.83730	-0.92650	0.05310
H	-0.80200	1.77010	1.11960
H	-0.92260	1.92690	-0.62830
H	1.61580	1.76880	-1.40930
H	4.10420	-1.39500	-1.37510
H	4.93390	-0.44180	-2.60330
H	3.92480	1.61050	-1.88540
H	3.96820	0.79980	-0.31460
H	-0.36080	0.47750	-3.04940
H	-0.47770	-0.98720	-5.04820
H	1.49310	-2.32610	-5.74140
H	3.61340	-2.20550	-4.44440

Indene-itaconic anhydride intermediate

Final Energy = -767.005182 hartree

C	0.10890	-0.63770	-1.41810
C	0.24240	-1.71130	-0.35470
O	-0.23610	-1.22500	0.84260
C	-0.70110	0.10440	0.68570
C	-0.51670	0.49840	-0.68690
O	-1.16050	0.70190	1.64080
O	0.67970	-2.83060	-0.44710
C	-0.89370	1.81450	-1.24910
C	2.51090	3.60280	1.29900
C	2.93980	3.53150	0.01940
C	3.37580	2.16090	-0.27670
C	3.89710	1.58960	-1.44290
C	4.23370	0.22970	-1.43290
C	4.05250	-0.54460	-0.27810
C	3.53010	0.02790	0.89260
C	3.19420	1.37840	0.88830
H	1.10100	-0.39660	-1.82800
H	-0.49560	-1.00860	-2.25810
H	-1.34710	2.45720	-0.49060
H	-0.01160	2.32370	-1.66390
H	-1.60160	1.69030	-2.08130
H	2.96800	4.34910	-0.69470
H	4.04220	2.18690	-2.34040
H	4.64240	-0.23070	-2.32950
H	4.31840	-1.59890	-0.28920
H	3.39230	-0.57950	1.78480
C	2.62650	2.25820	1.98020
H	2.13050	4.48880	1.79680
H	1.65330	1.89780	2.34350
H	3.28310	2.30180	2.86190

Itaconic anhydride-indene radical

Final Energy = -767.018615 hartree

C	-0.46620	4.11300	-0.58850
C	0.34710	3.67330	0.50050
C	0.62040	4.51750	1.56640
C	0.08600	5.82040	1.56730
C	-0.71860	6.26310	0.50050

C	-1.00250	5.42760	-0.57700
C	0.79500	2.24660	0.26530
C	0.13970	1.83960	-1.10030
C	-0.59720	3.08170	-1.54050
C	1.17640	1.27040	-2.13150
C	2.16040	2.35160	-2.63480
C	0.45230	0.70010	-3.35340
O	0.86580	-0.60590	-3.60170
C	1.76120	-1.03830	-2.63390
C	1.91760	0.02980	-1.58090
O	-0.34950	1.22050	-4.08370
O	2.26570	-2.12780	-2.71150
H	1.23990	4.18340	2.39640
H	0.29580	6.48940	2.39820
H	-1.12310	7.27230	0.52040
H	-1.62490	5.77320	-1.39880
H	1.88950	2.17400	0.23940
H	0.46290	1.58190	1.07240
H	-0.58440	1.02880	-0.92050
H	-1.17750	3.14030	-2.45390
H	2.70990	2.77770	-1.78930
H	2.89180	1.92630	-3.33150
H	1.62440	3.15780	-3.14240
H	2.97950	0.19820	-1.38150
H	1.46860	-0.35290	-0.65620

Itaconic anhydride-indene intermediate

Final Energy = -766.996008 hartree

C	1.61810	6.03180	2.12610
C	2.32300	4.79580	1.97400
C	3.56340	4.76300	1.35430
C	4.12840	5.96000	0.87220
C	3.44340	7.18060	1.01740
C	2.19740	7.23290	1.63780
C	1.51250	3.66160	2.57020
C	0.21770	4.34510	3.11060
C	0.39040	5.80530	2.78320
C	1.14890	6.76070	-2.73340
O	2.01250	5.67470	-2.90410
C	1.49450	4.52320	-2.32470
C	0.16280	4.83560	-1.67720
C	-0.04250	6.29500	-1.98310
O	2.09520	3.48320	-2.38480
O	1.43710	7.84580	-3.17250
H	4.10020	3.82360	1.23730
H	5.09960	5.94100	0.38450
H	3.89500	8.09490	0.63930
H	1.67290	8.17910	1.74730
H	1.28320	2.89660	1.81750
H	2.06560	3.15400	3.37040
H	-0.68770	3.92830	2.64350
H	0.09380	4.18380	4.19220
H	-0.34070	6.57080	3.02450
H	0.22890	4.62420	-0.60330
H	-0.60930	4.18100	-2.09680
C	-1.06640	7.10000	-1.68250
H	-1.93170	6.73840	-1.13430
H	-1.05750	8.14400	-1.98260

Itaconic anhydride-itaconic anhydride radical

Final Energy = -837.882628 hartree

C	0.08880	-0.07740	-0.00440

C	1.57530	-0.01780	0.01550
C	-0.51530	-1.51370	-0.11180
C	-0.02780	-2.41750	1.04480
C	-0.33550	-2.19050	-1.48700
C	-1.70820	-2.69970	-1.85770
O	-2.64980	-2.16530	-0.98500
C	-2.03910	-1.40360	-0.00010
O	-2.69790	-0.80140	0.80450
O	-2.04720	-3.42840	-2.75040
C	2.34530	0.31740	1.19230
O	3.71290	0.35050	0.84560
C	3.87920	0.06150	-0.49280
C	2.52180	-0.20010	-1.12100
O	1.99780	0.55540	2.33130
O	4.97050	0.04010	-0.99920
H	-0.29400	0.37940	0.91260
H	-0.27690	0.51700	-0.85310
H	1.05260	-2.57330	0.96090
H	-0.24230	-1.95660	2.01300
H	-0.51290	-3.39890	1.01080
H	-0.03330	-1.48470	-2.26980
H	0.38090	-3.01630	-1.49090
H	2.51100	-1.20780	-1.56030
H	2.34680	0.50110	-1.94980

Itaconic anhydride-itaconic anhydride intermediate

Final Energy = -837.865749 hartree

C	-0.18910	0.96850	-0.23130
C	0.47760	1.29780	-1.55330
O	1.80170	1.59530	-1.33360
C	2.10690	1.50200	0.04980
C	0.91250	1.12190	0.75870
O	3.23650	1.73290	0.43560
O	0.00500	1.32140	-2.66290
C	0.82080	0.92540	2.22240
C	-2.97480	1.75160	-4.25070
C	-3.39190	1.58020	-2.83850
O	-3.11890	0.26610	-2.45500
C	-2.52440	-0.44550	-3.48930
C	-2.39370	0.44080	-4.70750
O	-2.20760	-1.59570	-3.33550
O	-3.89180	2.35250	-2.05790
C	-3.13180	2.90180	-4.91360
H	-1.03630	1.64660	-0.05560
H	-0.60860	-0.04740	-0.26430
H	1.78900	1.07420	2.70670
H	0.09370	1.62540	2.65990
H	0.45610	-0.08560	2.45410
H	-1.33770	0.50620	-4.99040
H	-2.93540	-0.01310	-5.54510
H	-2.82140	3.00850	-5.94900
H	-3.57700	3.76520	-4.42740

Bibliography

1. J. B. McLeary, F.M. Calitz, J.M. McKenzie, M.P. Tonge, R.D. Sanderson, B. Klumperman, *Macromolecules*, 2005, **38**, 3151-3161.

2. J. Gardiner, I. Martinez-Botella, J. Tsanaktsidis and G. Moad, *Polym. Chem.*, 2016, **7**, 481-492.

3. A. A. A. Autzen, S. Beuermann, M. Drache, C. M. Fellows, S. Harrisson, A. M. van Herk, R. A. Hutchinson, A, Kajiwara, D. J. Keddie, B. Klumperman, G. T. Russell, *Polym. Chem.,* 2024, **15**, 1851–1861.

4. E. T. A. Van Den Dungen, J. Rinquest, N. O. Pretorius, J. M. McKenzie, J. B. McLeary, R. D. Sanderson and B. Klumperman, *Aust. J. Chem.*, 2006, **59**, 742–748.

5. A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang and R. A. Friesner, *Int. J. Quant. Chem.*, 2013, **113**, 2110-2142.

6. Schrödinger, Maestro, 2021-4.

7. S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 12.

8. P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 5.

9. A. D. Becke, J. Chem. Phys., 1993, **98**, 5648-5652.

10. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B.*, 1988, **37**, 785-789.

11. T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, *J. Comput. Chem.*, 1983, **4**, 294-301.

12. R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724-728.

13. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.

14. P. C. Hariharan and J. A. Pople, Theor. *Chim. Acta*, 1973, **28**, 213-222.

15. M. Cossi, N. Rega, G. Scalmani and V. Barone, *J. Comp. Chem.*, 2003, **24**, 669-681.

16. A. Klamt and G. Schüürmann, *J. Chem. Soc., Perkin Trans.* 1993, **2**, 799-805.

17. M. Cossi and V. Barone, *J. Phys. Chem.*, 1998, **102**, 11, 1995-2001.

18. B. P. Pritchard, D. Altarawy, B. Didier, T. D. Gibsom and T. L. Windus, *J. Chem. Inf. Model.*, 2019, **59**, 4814-4820.

19. K. L. Schuchardt, B. T. Didier, T. Elsethagen, L. Sun, V. Gurumoorthi, J. Chase, J. Li and T. L. Windus, *J. Chem. Inf. Model.*, 2007, **47**, 1045-1052.

20. D. Feller, *J. Comput. Chem.*, 1996, **17**, 1571-1586.