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Direct Synthesis of Polyethylene Containing Two Kinds of Heteroatoms by Scandium Complexes

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Experimental Procedures

General Methods and Materials.

All manipulations were conducted under dry and oxygen-free argon atmosphere employing standard high-vacuum Schlenk techniques or within MBRAUN glovebox. Solvents were purified using a MBRAUN SPS 5 solvent purification system. $[Ph_3C][B(C_6F_5)_4]$ (97%, Strem Chemical Corporation) and triisobutylaluminum (0.5M in toluene, Aldrich) were used without further purification. Scandium complexes (**Sc-1**[1] and **Sc-2**[2]), and polar α-olefins (**1a-1p**)[3-9] were prepared following literature procedures. The ^1H and ^{13}C NMR spectra were acquired on a Bruker AV 400 spectrometer (FT, 400 MHz for ^1H and 100 MHz for ^{13}C) or an AV 500 spectrometer (FT, 500 MHz for ^1H and 125 MHz for ^{13}C). Number-averaged molecular weights (M_n) and molecular weight distributions of copolymers were determined by PL-GPC 220-type in 1,2,4-trichlorobenzene at 150°C relative to polystyrene standards. DSC analysis was conducted on a METTLER-TOLEDO Instrument (Switzerland) with a heating rate of 10 °C min^{-1} under a nitrogen atmosphere. To eliminate thermal history differences in the polymers, samples were first heated to 150 °C, and cooled to -100 °C at a rate of 10 °C min^{-1}, and then recorded the second DSC scan. WAXD tests were performed on a 1 mm thick film at ambient temperature. WAXD experiments were conducted with a Rigaku X-ray diffractometer (D8) with Cu Kα radiation at 40 kV and 200 mA with the wavelength of 0.154 nm. AFM was used to study the surface topography of the spin-coated film. Images were obtained using a SPI3800N AFM (Seiko Instruments Inc., Japan) with a Si tip with a spring constant of 40 N m^{-1}. The cantilevers were operated slightly below their resonance frequency of around 200-400 kHz. The image acquisition was performed under ambient conditions. Water contact angles on polymer films were measured by the sessile drop angle measurement using a contact angle goniometer (DSA 100, Kruss GmbH, Hamburg, Germany) at 25 °C. The refractive index of thin film sample was measured using an Abbe refractometer (DR-M4, Atago Co. Ltd., Tokyo, Japan) at 20 °C without using the contact liquid.

General procedure for the copolymerization of polar olefins with ethylene.

The detailed polymerization procedure is as follows (Table 2, entry 23). In a glovebox, a toluene solution (1 mL) of **Sc-2** (5.9 mg, 10 μmol), one equivalent of $[Ph_3C][B(C_6F_5)_4]$ (9.2 mg, 10 μmol), and 15 equivalent of Al^iBu_3 (0.3 mL, 0.5 M in toluene, 150 μmol) were mixed together under

vigorous stirring. A solution of **1g** (0.36 g, 2 mmol) in toluene (10 mL) was charged into a pressure-resistant polymerization vessel with a magnetic stir bar under nitrogen. The vessel was degassed N_2 and refilled ethylene for three times and kept at invariable 4 bar of ethylene for 5 min. The stopcock was opened and then the catalyst solution was added quickly by using an injector, and the ethylene pressure was kept at 4 bar. Polymerization was initiated and performed for 30 min. Then, the reaction was quenched by adding 300 mL acidified ethanol (HCl, 10 wt%). The resultant polymer was collected by filtration, washed with large amount of ethanol and dried to a constant weight (0.69 g) under vacuum at 40 °C.

Synthesis of polar olefin monomers

Functional polar α-olefin monomers (**1a-1p**) were prepared as following literature procedures[3-9]. Detailed experimental procedures were described as below.

Synthesis of 1a

To a solution of *o*-methylphenol (205 mg, 1.90 mmol, 1.0 equiv.) in MeCN (5 mL), K_2CO_3 (787 mg, 5.70 mmol, 3.0 equiv.) and 4-bromo-1-butene (512 mg, 3.80 mmol, 2.0 equiv.) were added at room temperature under nitrogen atmosphere. The reaction mixture was refluxing overnight. Then the reaction solution was cooled to room temperature and the solvent was removed in vacuo. The residue was extracted with ethyl acetate (3 × 10 mL). The organic layer was washed with brine, and dried over Na_2SO_4. Then the solvent was removed under vacuo. The crude product was then purified by silica gel column chromatography to afford desired product **1a**. Colorless liquid, 196 mg, 1.2 mmol, 63.1% yield, R_f = 0.60 (petroleum ether/ethyl acetate = 98/02). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.23-7.18 (m, 2 H), 6.91 (t, *J* = 7.3 Hz, 1 H), 6.87 (d, *J* = 8.5 Hz, 1 H), 6.05-5.94 (m, 1 H), 5.24 (d, *J* = 17.1 Hz, 1 H), 5.16 (d, *J* = 11.4 Hz, 1 H), 4.07 (t, *J* = 6.6 Hz, 2 H), 2.62 (q, *J* = 6.6 Hz, 2 H), 2.30 (s, 3 H); the ^{13}C NMR spectrum and Mass spectrum have been reported in literature 3.

Synthesis of 1b

A suspension of *o*-thiocresol (564 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 4-bromo-1-butene (256 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. Then the mixture was cooled to room temperature following by filtering and concentrating under vacuum. The residue was dissolved in EtOAc (20 mL) and

successively washed with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL) and brine (15 mL), and then again concentrated in vacuo. The residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1b**. Pale yellow oil, 327 mg, 1.8 mmol, 94.7% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.28 (d, *J* = 10.0 Hz, 1 H), 7.20-7.09 (m, 3 H), 5.94-5.85 (m, 1 H), 5.14 (d, *J* = 10.0 Hz, 1 H), 5.09 (d, *J* = 7.5 Hz, 1 H), 2.98 (t, *J* = 6.7 Hz, 2 H), 2.45-2.42 (m, 2 H), 2.40 (s, 3 H); the ^{13}C NMR spectrum and Mass spectrum have been reported in literature 4.

Synthesis of 1c

A suspension of *o*-methoxythiophenol (636 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 4-bromo-1-butene (256 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. After this time, the mixture was allowed to cool, filtered, and concentrated in vacuo. The residue was dissolved in EtOAc (20 mL) and washed successively with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL), and brine (15 mL), and then again concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1c**. Pale yellow oil, 311 mg, 1.6 mmol, 84.2% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.27 (d, *J* = 5.0 Hz, 1 H), 7.18 (t, *J* = 7.5 Hz, 1 H), 6.92 (t, *J* = 7.5 Hz, 1 H), 6.85 (d, *J* = 5.0 Hz, 1 H), 5.91-5.83 (m, 1 H), 5.09 (d, *J* = 10.0 Hz, 1 H), 5.04 (d, *J* = 10.0 Hz, 1 H), 3.89 (s, 3 H), 2.95 (t, *J* = 5.0 Hz, 2 H), 2.43-2.37 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 153.8, 151.8, 137.8, 124.3, 120.9, 116.0, 115.3, 114.8, 68.7, 30.0, 28.3; HRMS APCI: calcd for $C_{11}H_{15}OS$ $[M+H]^+$: 195.0765; found 195.0836.

Synthesis of 1d

A suspension of *p*-methoxythiophenol (636 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 4-bromo-1-butene (256 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. After this time, the mixture was allowed to cool, filtered, and concentrated in vacuo. The residue was dissolved in EtOAc (20 mL) and washed successively with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL), and brine (15 mL), and then again concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1d**. Pale yellow oil, 291 mg, 1.5 mmol, 78.9% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.35 (d, *J* = 5.0 Hz, 2 H), 6.85 (d, *J* = 5.0 Hz, 2 H), 5.87-5.79 (m, 1 H), 5.08-5.01 (m, 2 H), 3.79 (s, 3 H), 2.87 (t, *J* = 5.0 Hz, 2 H), 2.32 (q, *J* = 8.3 Hz, 2 H) ; the ^{13}C NMR spectrum and Mass spectrum have been reported in literature 5.

Synthesis of 1e

To a solution of *o*-fluorophenol (213 mg, 1.90 mmol, 1.0 equiv.) in MeCN (5 mL), K_2CO_3 (787 mg, 5.70 mmol, 3.0 equiv.) and 4-bromo-1-butene (256 mg, 3.80 mmol, 2.0 equiv.) were added at room temperature under nitrogen atmosphere. The reaction mixture was refluxed overnight. After completion, it was then cooled to room temperature and the solvent was removed in vacuo. The reaction mixture was extracted with ethyl acetate (3 × 10 mL). The organic layer was washed with brine, dried over Na_2SO_4, and the solvent was removed under vacuo. The crude product was then purified by silica gel column chromatography to afford desired product **1e**. Colorless liquid, 189 mg, 1.1 mmol, 57.9% yield, R_f = 0.60 (petroleum ether/ethyl acetate = 98/02); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.08-6.85 (m, 4 H), 5.95-5.86 (m, 1 H), 5.17 (d, *J* = 10.0 Hz, 1 H), 5.10 (d, *J* = 7.5 Hz, 1 H), 4.07 (t, *J* = 8.3 Hz, 2 H), 2.56 (q, *J* = 8.3 Hz, 2 H) ; the ^{13}C NMR spectrum and Mass spectrum have been reported in literature 3.

Synthesis of 1f

To a solution of *p*-fluorophenol (213 mg, 1.90 mmol, 1.0 equiv.) in MeCN (5 mL), K_2CO_3 (787 mg, 5.70 mmol, 3.0 equiv.) and 4-bromo-1-butene (512 mg, 3.80 mmol, 2.0 equiv.) were added at room temperature under nitrogen atmosphere. The reaction mixture was refluxed overnight. After completion, it was then cooled to room temperature and the solvent was removed in vacuo. The reaction mixture was extracted with ethyl acetate (3 × 10 mL). The organic layer was washed with brine, dried over Na_2SO_4, and the solvent was removed under vacuo. The crude product was then purified by silica gel column chromatography to afford desired product **1f**. Colorless liquid, 189 mg, 1.1 mmol, 57.9% yield, R_f = 0.60 (petroleum ether/ethyl acetate = 98/02); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.94 (t, *J* = 8.3 Hz, 2 H), 6.84-6.80 (m, 2 H), 5.93-5.84 (m, 1 H), 5.15 (d, *J* = 12.5 Hz, 1 H), 5.10 (d, *J* = 7.5 Hz, 1 H), 3.95 (t, *J* = 6.7 Hz, 2 H), 2.51 (q, *J* = 8.3 Hz, 2 H) ; the ^{13}C NMR spectrum and Mass spectrum have been reported in literature 3.

Synthesis of 1g

A suspension of *o*-fluorothiophenol (577 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 4-bromo-1-butene (256 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. Then the mixture was allowed to cool to room temperature, filtered, and concentrated in vacuo. The residue was dissolved in EtOAc (20 mL) and washed successively with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL), and brine (15 mL), and then

again concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1g**. Pale yellow oil, 219 mg, 1.2 mmol, 63.2% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.36 (t, *J* = 10.0 Hz, 1 H), 7.22-7.01 (m, 3 H), 5.87-5.79 (m, 1 H), 5.09-5.01 (m, 2 H), 2.95 (t, *J* = 10.0 Hz, 2 H), 2.35 (q, *J* = 11.7 Hz, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 162.5, 160.6, 136.2, 132.2, 128.2, 124.4, 123.1, 116.4, 115.5, 33.5, 32.7; HRMS APCI: calcd for $C_{10}H_{12}SF$ $[M+H]^+$: 183.0565; found 183.0636.

Synthesis of 1h

A suspension of *p*-fluorothiophenol (577 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 4-bromo-1-butene (256 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. Then the mixture was allowed to cool to room temperature, filtered, and concentrated in vacuo. The residue was dissolved in EtOAc (20 mL) and washed successively with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL), and brine (15 mL), and then again concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1h**. Pale yellow oil, 237 mg, 1.3 mmol, 68.4% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.36-7.32 (m, 2 H), 7.01-6.96 (m, 2 H), 5.86-5.78 (m, 1 H), 5.09-5.03 (m, 2 H), 2.91 (t, *J* = 5.0 Hz, 2 H), 2.38-2.30 (m, 2 H) ; the ^{13}C NMR spectrum and Mass spectrum have been reported in literature 6.

Synthesis of 1i

To a solution of *o*-methylphenol (205 mg, 1.90 mmol, 1.0 equiv.) in MeCN (5 mL), K_2CO_3 (787 mg, 5.70 mmol, 3.0 equiv.), 5-bromo-1-pentene (566 mg, 3.80 mmol, 2.0 equiv.) were added at room temperature under nitrogen atmosphere. The reaction mixture was refluxed overnight. After completion, it was then cooled to room temperature and the solvent was removed in vacuo. The reaction mixture was extracted with ethyl acetate (3 × 10 mL). The organic layer was washed with brine, dried over Na_2SO_4, and the solvent was removed under vacuo. The crude product was then purified by silica gel column chromatography to afford desired product **1i**. Colorless liquid, 194 mg, 1.1 mmol, 57.9% yield, R_f = 0.60 (petroleum ether/ethyl acetate = 98/02); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.21-7.17 (m, 2 H), 6.89 (t, *J* = 7.5 Hz, 1 H), 6.85 (d, *J* = 5.0 Hz, 1 H), 5.95-5.88 (m, 1 H), 5.12 (d, *J* = 10.0 Hz, 1 H), 5.05 (d, *J* = 7.5 Hz, 1 H), 4.02 (t, *J* = 5.0 Hz, 2 H), 2.35-2.29 (m, 6 H), 1.98-1.93 (m, 2 H) ; the ^{13}C NMR spectrum has been reported in literature 7; HRMS APCI: calcd for $C_{12}H_{17}O$ $[M+H]^+$: 177.1201; found 177.1272.

Synthesis of 1j

A suspension of *o*-thiocresol (564 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 5-bromo-1-pentene (283 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. After this time, the mixture was allowed to cool to room temperature, filtered, and concentrated in vacuo. The residue was dissolved in EtOAc (20 mL) and washed successively with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL), and brine (15 mL), and then again concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1j**. Pale yellow oil, 327 mg, 1.7 mmol, 89.5% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.24 (d, *J* = 2.5 Hz, 1 H), 7.15-7.12 (m, 2 H), 7.06 (d, *J* = 7.5 Hz, 1 H), 5.82-5.74 (m, 1 H), 5.04 (d, *J* = 10.0 Hz, 1 H), 4.98 (d, *J* = 7.5 Hz, 1 H), 2.89 (t, *J* = 5.0 Hz, 2 H), 2.36 (s, 3 H), 2.20 (q, *J* = 8.3 Hz, 2 H), 1.78-1.72 (m, 2 H) ; the ^{13}C NMR spectrum and Mass spectrum have been reported in literature 8.

Synthesis of 1k

A suspension of *o*-methoxythiophenol (636 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 5-bromo-1-pentene (283 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. After this time, the mixture was allowed to cool to room temperature, filtered, and concentrated in vacuo. The residue was dissolved in EtOAc (20 mL) and washed successively with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL), and brine (15 mL), and then again concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1k**. Pale yellow oil, 312 mg, 1.5 mmol, 78.9% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.25 (d, *J* = 5.0 Hz, 1 H), 7.17 (t, *J* = 10.0 Hz, 1 H), 6.92 (t, *J* = 7.5 Hz, 1 H), 6.85 (d, *J* = 5.0 Hz, 1 H), 5.83-5.75 (m, 1 H), 5.04 (d, *J* = 15.0 Hz, 1 H), 4.98 (d, *J* = 2.0 Hz, 1 H), 3.89 (s, 3 H), 2.89 (t, *J* = 5.0 Hz, 2 H), 2.20 (q, *J* = 8.3 Hz, 2 H), 1.78-1.72 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 157.1, 137.6, 128.9, 126.7, 124.9, 121.0, 115.1, 110.4, 55.8, 32.8, 31.3, 28.0; HRMS APCI: calcd for $C_{12}H_{17}OS$ $[M+H]^+$: 209.0922; found 209.0922.

Synthesis of 1l

A suspension of *p*-methoxythiophenol (636 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 5-bromo-1-pentene (283 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. After this time, the mixture was allowed to cool to room temperature, filtered, and concentrated in vacuo. The residue was dissolved in EtOAc (20 mL)

and washed successively with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL), and brine (15 mL), and then again concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1l**. Pale yellow oil, 333 mg, 1.6 mmol, 84.2% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.34 (d, *J* = 5.0 Hz, 2 H), 6.83 (d, *J* = 5.0 Hz, 2 H), 5.80-5.72 (m, 1 H), 5.01 (d, *J* = 10.0 Hz, 1 H), 4.96 (d, *J* = 7.5 Hz, 1 H), 3.79 (s, 3 H), 2.81 (t, *J* = 5.0 Hz, 2 H), 2.16 (q, *J* = 6.7 Hz, 2 H), 1.70-1.64 (m, 2 H) ; the ^{13}C NMR spectrum and Mass spectrum have been reported in literature 8.

Synthesis of 1m

To a solution of *o*-fluorophenol (213 mg, 1.90 mmol, 1.0 equiv.) in MeCN (5 mL), K_2CO_3 (787 mg, 5.70 mmol, 3.0 equiv.), 5-bromo-1-pentene (566 mg, 3.80 mmol, 2.0 equiv.) were added at room temperature under nitrogen atmosphere. The reaction mixture was refluxed overnight. After completion, it was then cooled to room temperature and the solvent was removed in vacuo. The reaction mixture was extracted with ethyl acetate (3 × 10 mL). The organic layer was washed with brine, dried over Na_2SO_4, and the solvent was removed under vacuo. The crude product was then purified by silica gel column chromatography to afford desired product **1m**. Colorless liquid, 216 mg, 1.2 mmol, 63.2% yield, R_f = 0.60 (petroleum ether/ethyl acetate = 98/02); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.08-6.85 (m, 4 H), 5.89-5.81 (m, 1 H), 5.06 (d, *J* = 7.5 Hz, 1 H), 5.00 (d, *J* = 7.5 Hz, 1 H), 4.03 (t, *J* = 3.3 Hz, 2 H), 2.25 (q, *J* = 8.3 Hz, 2 H), 1.94-1.89 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 153.8, 151.9, 147.0, 137.6, 124.3, 120.9, 116.2, 115.2, 114.9, 68.5, 30.0, 28.3; HRMS APCI: calcd for $C_{11}H_{14}FO$ $[M+H]^+$: 181.0950; found 181.1020.

Synthesis of 1n

To a solution of *p*-fluorophenol (213 mg, 1.90 mmol, 1.0 equiv.) in MeCN (5 mL), K_2CO_3 (787 mg, 5.70 mmol, 3.0 equiv.), 5-bromo-1-pentene (566 mg, 3.80 mmol, 2.0 equiv.) were added at room temperature under nitrogen atmosphere. The reaction mixture was refluxed overnight. After completion, it was then cooled to room temperature and the solvent was removed in vacuo. The reaction mixture was extracted with ethyl acetate (3 × 10 mL). The organic layer was washed with brine, dried over Na_2SO_4, and the solvent was removed under vacuo. The crude product was then purified by silica gel column chromatography to afford desired product **1n**. Colorless liquid, 198 mg, 1.1 mmol, 57.9% yield, R_f = 0.60 (petroleum ether/ethyl acetate = 98/02); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.95 (t, *J* = 8.3 Hz, 2 H), 6.84-6.79 (m, 2 H), 5.88-5.80 (m, 1 H), 5.05 (d, *J* = 12.5 Hz,

1 H), 5.00 (d, *J* = 7.5 Hz, 1 H), 3.91 (t, *J* = 3.3 Hz, 2 H), 2.22 (q, *J* = 8.3 Hz, 2 H), 1.89-1.83 (m, 2 H) ; the ^{13}C NMR spectrum has been reported in literature 9; HRMS APCI: calcd for $C_{11}H_{14}FO$ $[M+H]^+$: 181.0950; found 181.1020.

Synthesis of 1o

A suspension of *o*-fluorothiophenol (577 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 5-bromo-1-pentene (283 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. After this time, the mixture was allowed to cool to room temperature, filtered, and concentrated in vacuo. The residue was dissolved in EtOAc (20 mL) and washed successively with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL), and brine (15 mL), and then again concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1o**. Pale yellow oil, 236 mg, 1.2 mmol, 63.2% yield. ^1H NMR (500 MHz, $CDCl_3$): δ = 7.36 (t, *J* = 7.5 Hz, 1 H), 7.21-7.02 (m, 3 H), 5.81-5.73 (m, 1 H), 5.03 (d, *J* = 12.5 Hz, 1 H), 4.98 (d, *J* = 7.5 Hz, 1 H), 2.90 (t, *J* = 5.0 Hz, 2 H), 2.19 (q, *J* = 8.3 Hz, 2 H), 1.74-1.68 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 162.4, 160.4, 137.4, 131.9, 128.1, 124.3, 123.3, 115.6, 32.6, 28.4; HRMS APCI: calcd for $C_{11}H_{14}FS$ $[M+H]^+$: 197.0722; found 197.0791.

Synthesis of 1p

A suspension of *p*-fluorothiophenol (577 mg, 4.5 mmol, 1.0 equiv.) and K_2CO_3 (940 mg, 6.8 mmol, 1.5 equiv.) in acetone (5 mL) was treated with 5-bromo-1-pentene (283 mg, 1.9 mmol, 0.4 equiv.) and then stirred at refluxing for 21 h. After this time, the mixture was allowed to cool to room temperature, filtered, and concentrated in vacuo. The residue was dissolved in EtOAc (20 mL) and washed successively with 1.1 M aq. NaOH (2 × 10 mL), H_2O (15 mL), and brine (15 mL), and then again concentrated in vacuo. The resulting residue was purified by column chromatography (SiO_2, eluting with 10% EtOAc in hexane) to afford thioether **1p**. Pale yellow oil, 255 mg, 1.3 mmol, 68.4% yield. ^1H NMR (500 MHz, $CDCl_3$): δ = 7.35-7.31 (m, 2 H), 6.98 (t, *J* = 6.7 Hz, 2 H), 5.80-5.72 (m, 1 H), 5.02 (d, *J* = 10.0 Hz, 1 H), 4.98 (d, *J* = 10.0 Hz, 1 H), 2.86 (t, *J* = 5.0 Hz, 2 H), 2.17 (q, *J* = 8.3 Hz, 2 H), 1.72-1.66 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 162.7, 160.8, 137.4, 132.2, 131.4, 115.7, 115.3, 34.3, 32.4, 28.2; HRMS APCI: calcd for $C_{11}H_{14}FS$ $[M+H]^+$: 197.0722; found 197.0792.

Table S1. Homopolymerization of Ethylene and 1g (2S/F-*o*) catalyzed by complex **2**.

Entry[a]	Cat.	E (bar)	[M]	[M]/ [Cat.]	T (°C)	Time (min)	yield (g)	Act.[b]	M_n[c] (10^4)	M_w/ M_n[c]	T_m[d] (°C)
1	**2**	4	-	-	40	10	0.83	498	0.6	2.5	129
2	**2**	-	1g	500	40	720	n.o.	-	-	-	-

[a] General conditions: **Sc-2** 10 μmol, [**Sc-2**]/[Ph_3C][$B(C_6F_5)_4$]/[Al^{i}Bu$_3$] = 1/1/15, toluene 10 mL. [b] Given in kg mol_{Sc}^{-1} h^{-1} bar^{-1}. [c] Determined by GPC in 1,2,4-trichlorobenzene at 150 °C against a polystyrene standard. [d] Determined by DSC.

^{1}H NMR spectra of polar olefin monomers

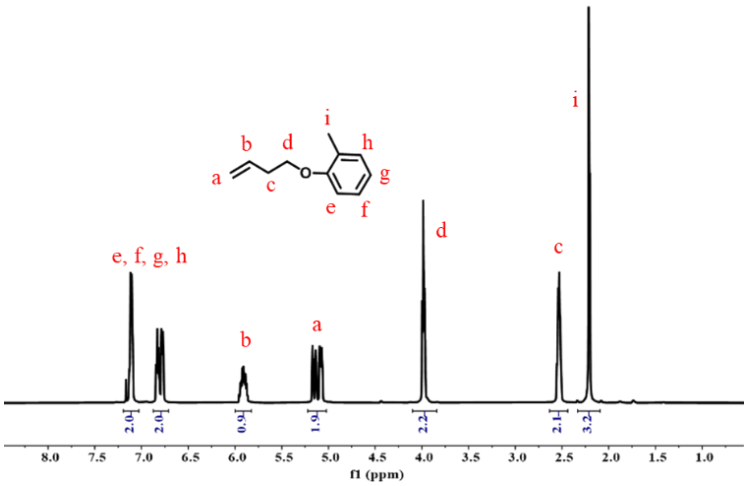


Figure S1. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 ℃) of **1a** (**2O**).

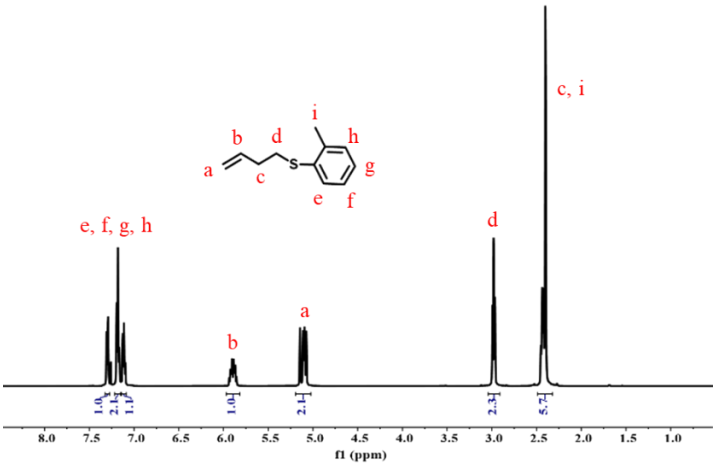


Figure S2. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 ℃) of **1b** (**2S**).

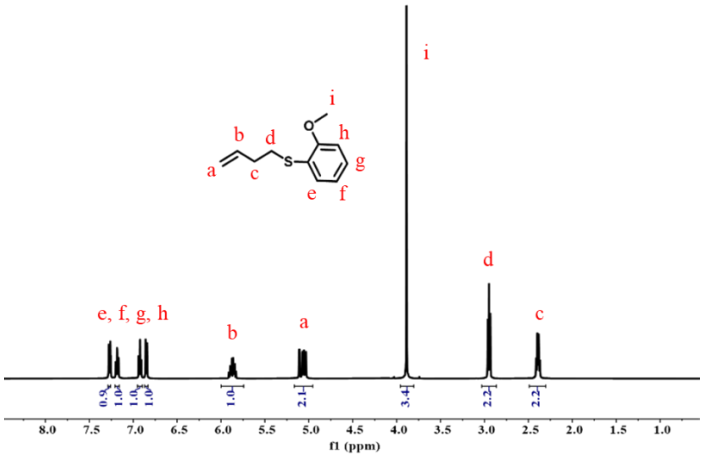


Figure S3. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 ℃) of **1c** (**2S/O-*o***).

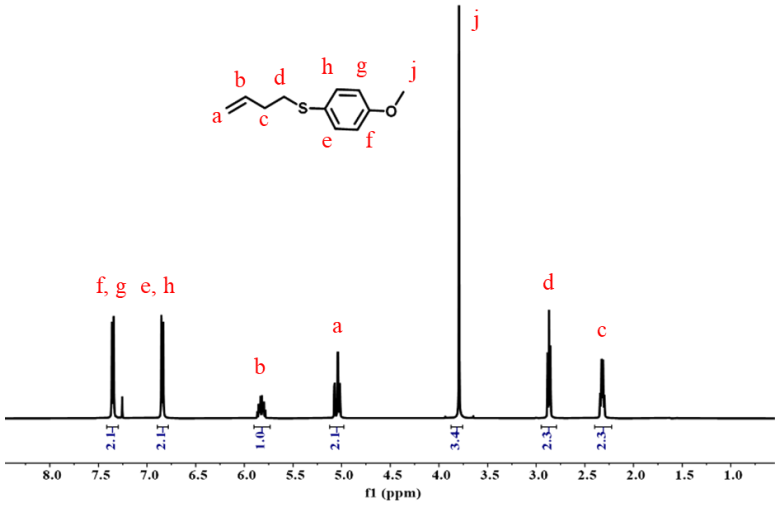


Figure S4. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1d** (**2S/O-*p***).

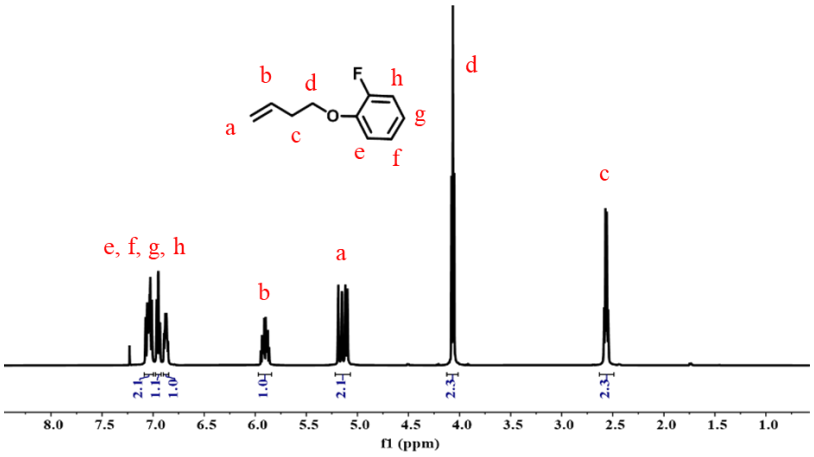


Figure S5. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1e** (**2O/F-*o***).

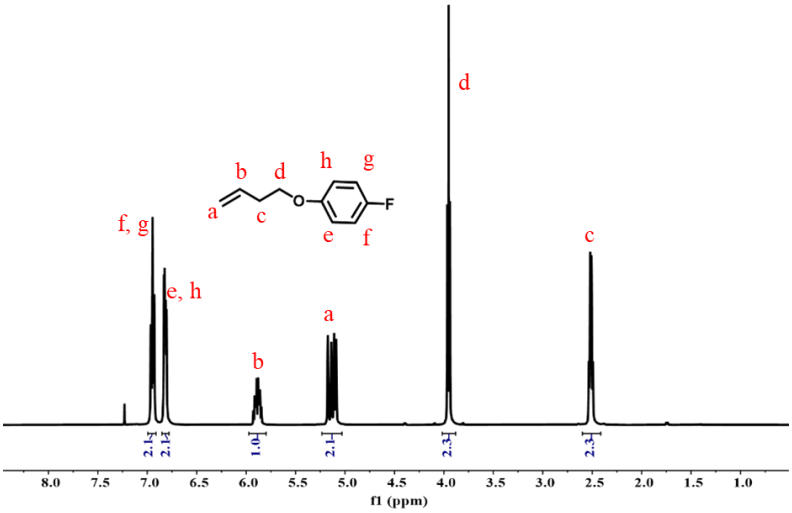


Figure S6. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1f** (**2O/F-*p***).

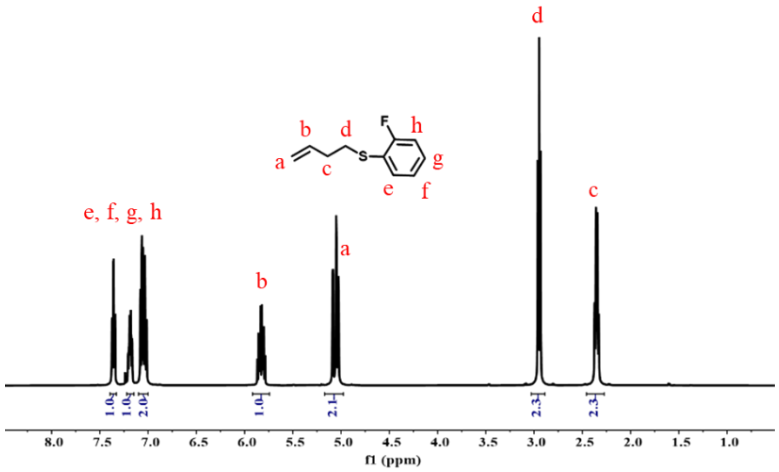


Figure S7. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1g** (**2S/F-*o***).

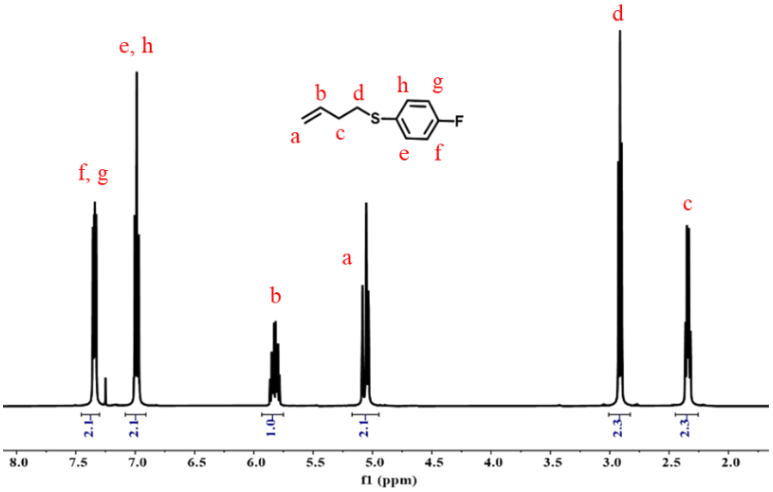


Figure S8. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1h** (**2S/F-*p***).

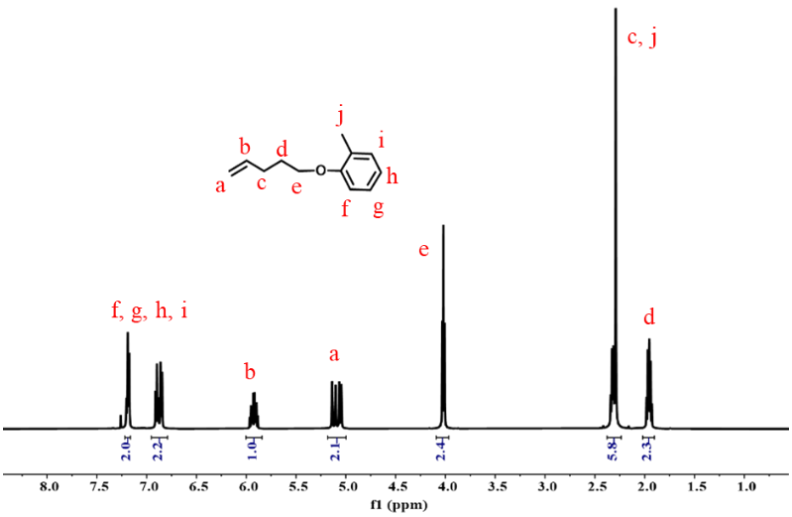


Figure S9. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1i** (**3O**).

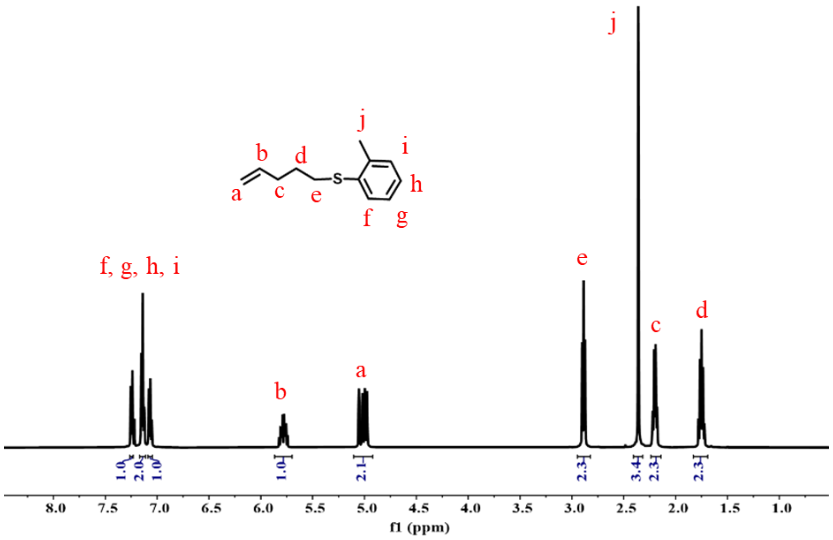


Figure S10. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1j** (**3S**).

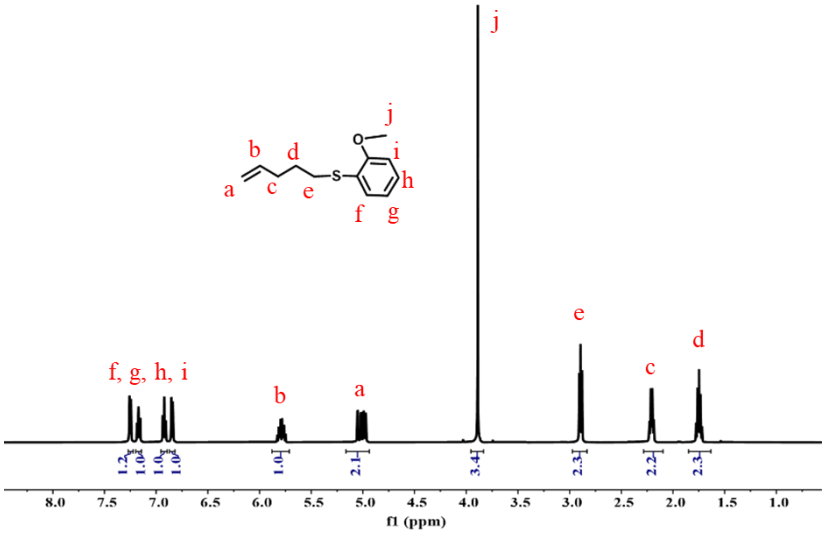


Figure S11. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1k** (**3S/O-*o***).

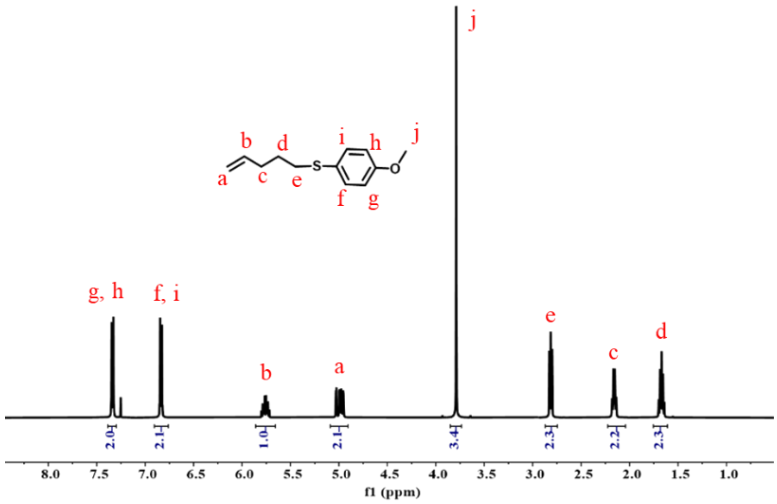


Figure S12. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1l** (**3S/O-*p***).

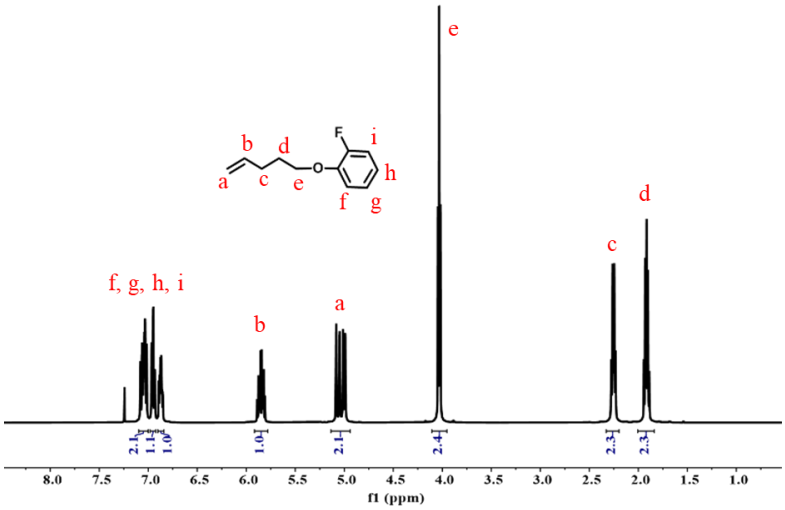


Figure S13. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1m** (**3O/F-*o***).

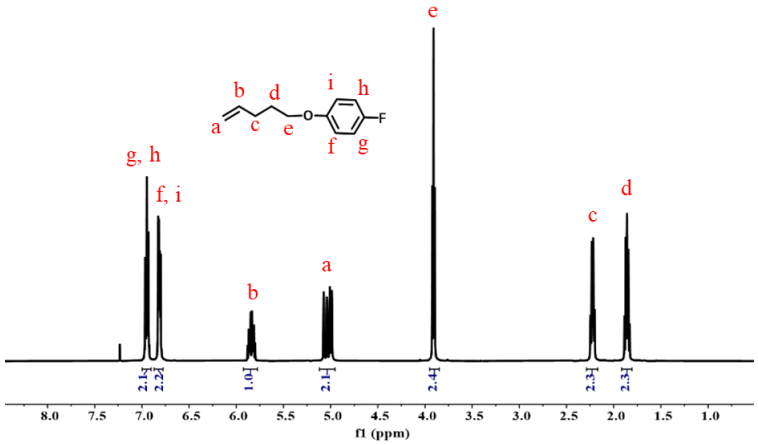


Figure S14. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1n** (**3O/F-*p***).

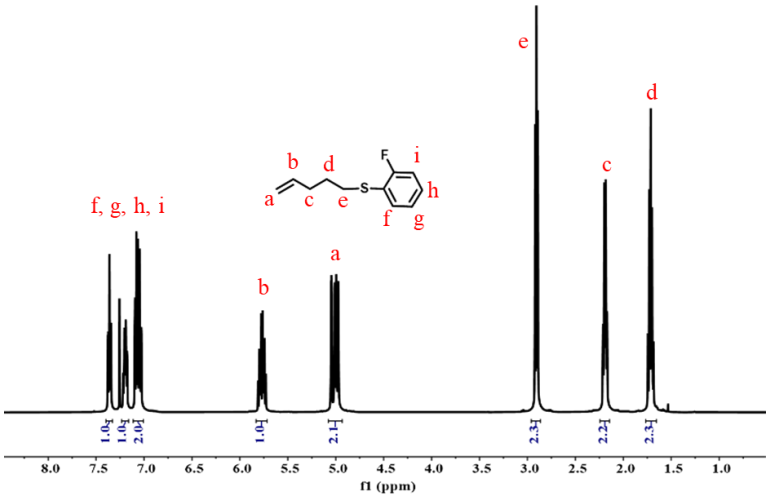


Figure S15. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1o** (**3S/F-*o***).

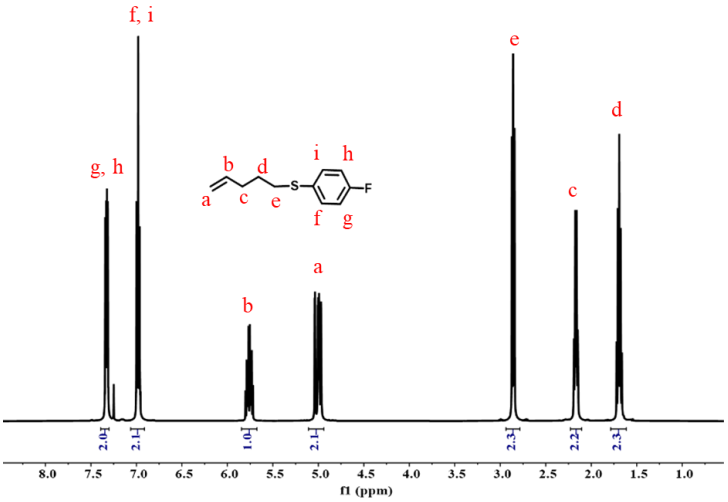


Figure S16. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of **1p** (**3S/F-*p***).

^{13}C NMR spectra of polar olefin monomers

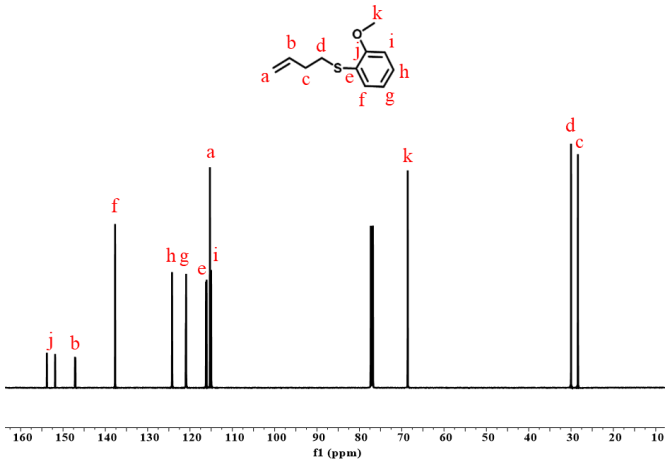


Figure S17. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 25 °C) of **1c** (**2S/O-*o***).

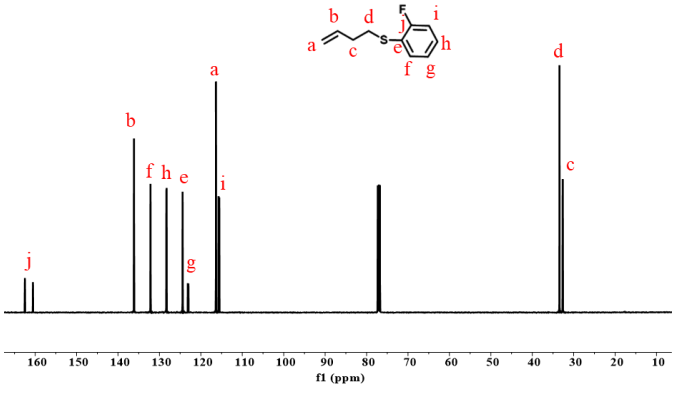


Figure S18. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 25 °C) of **1g** (**2S/F-*o***).

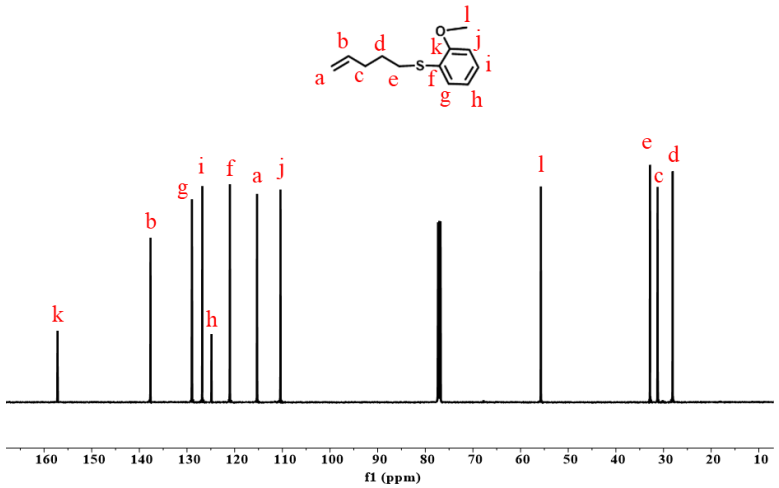


Figure S19. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 25 °C) of **1k** (**3S/O-*o***).

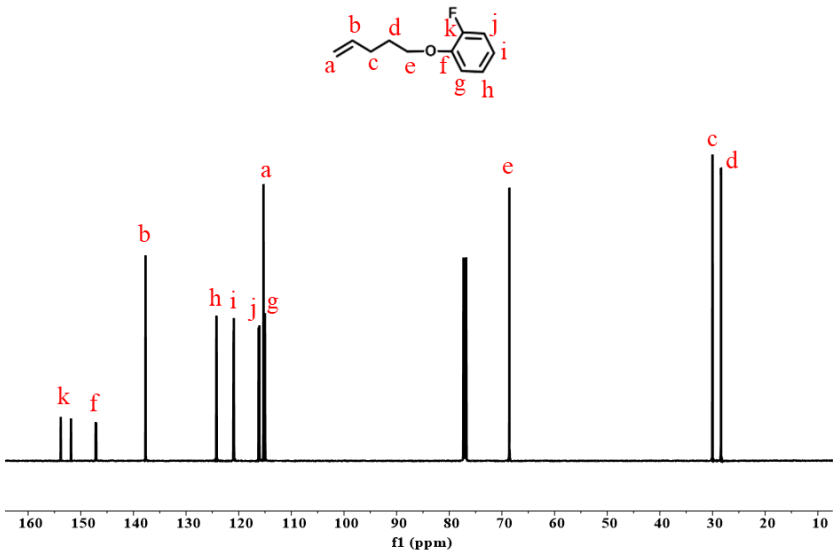


Figure S20. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 25 °C) of **1m** (**3O/F-*o***).

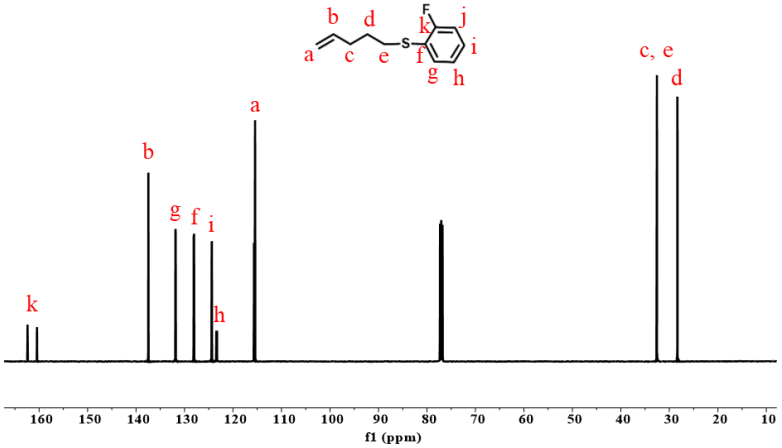


Figure S21. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 25 °C) of **1o** (**3S/F-*o***).

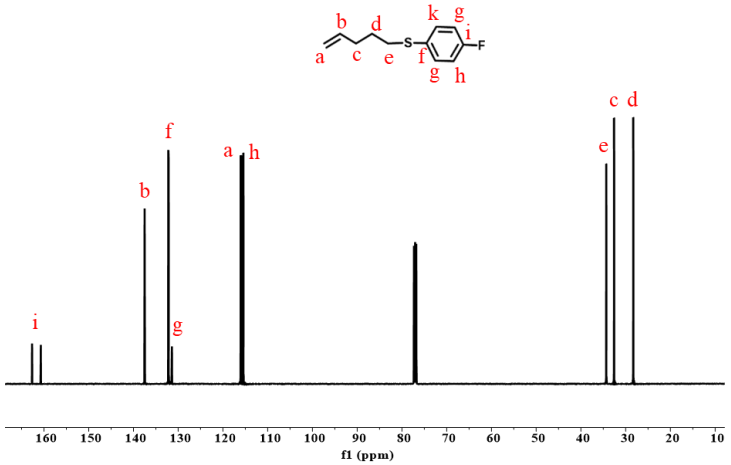


Figure S22. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 25 °C) of **1p** (**3S/F-*p***).

^{1}H NMR spectra of copolymers

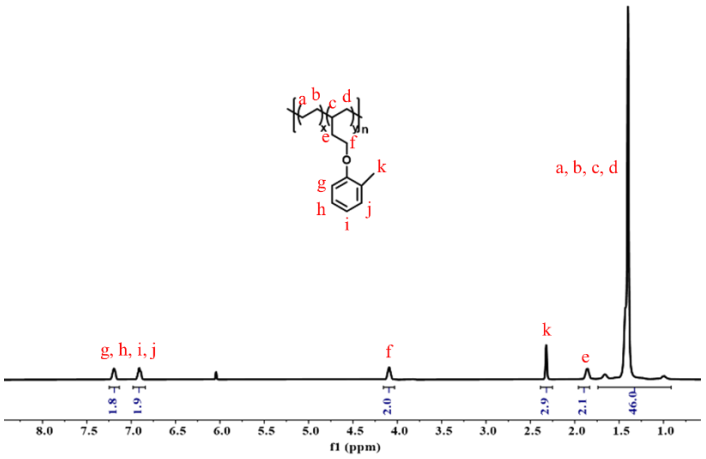


Figure S23. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2a** (Table 1, entry 1).

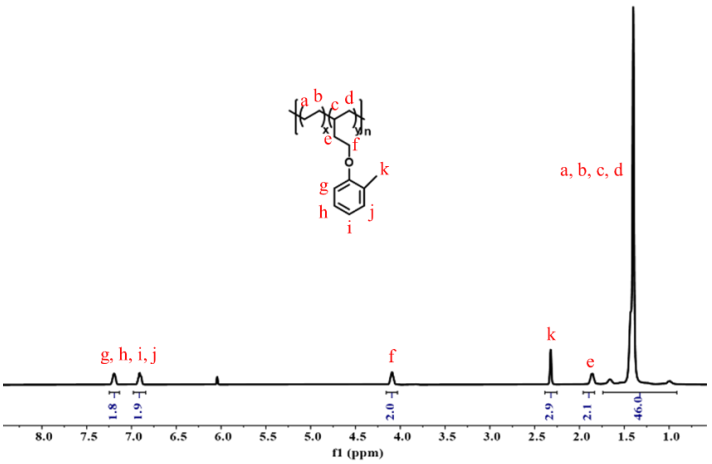


Figure S24. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2b** (Table 1, entry 2).

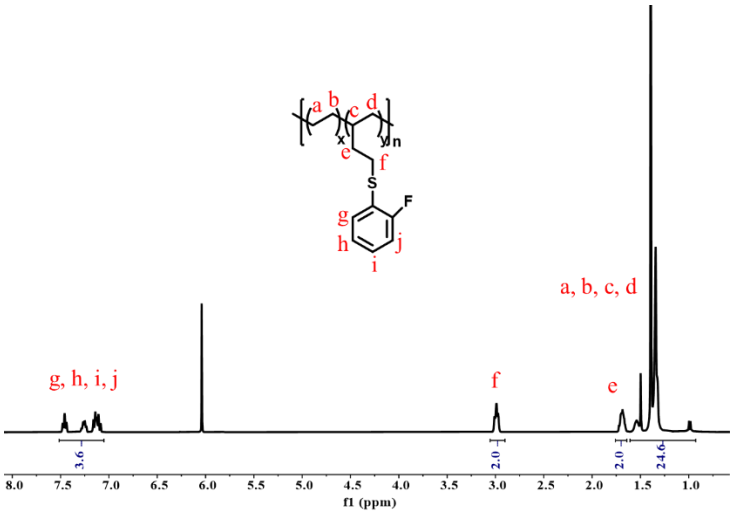


Figure S25. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2g** (Table 1, entry 7).

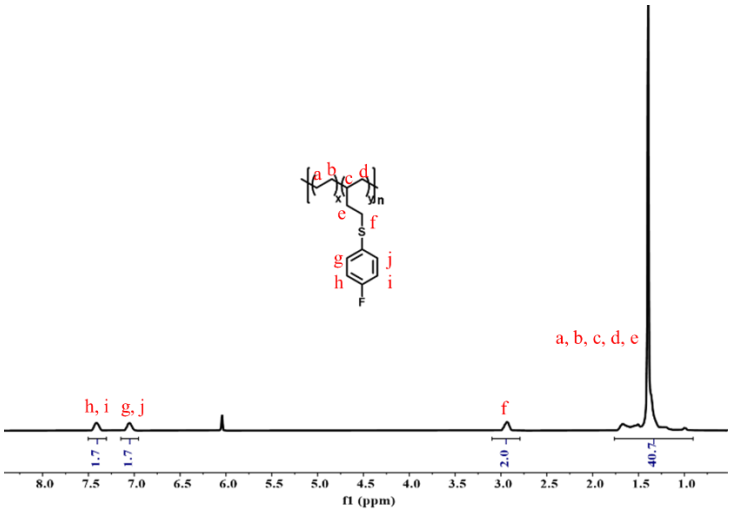


Figure S26. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2h** (Table 1, entry 8).

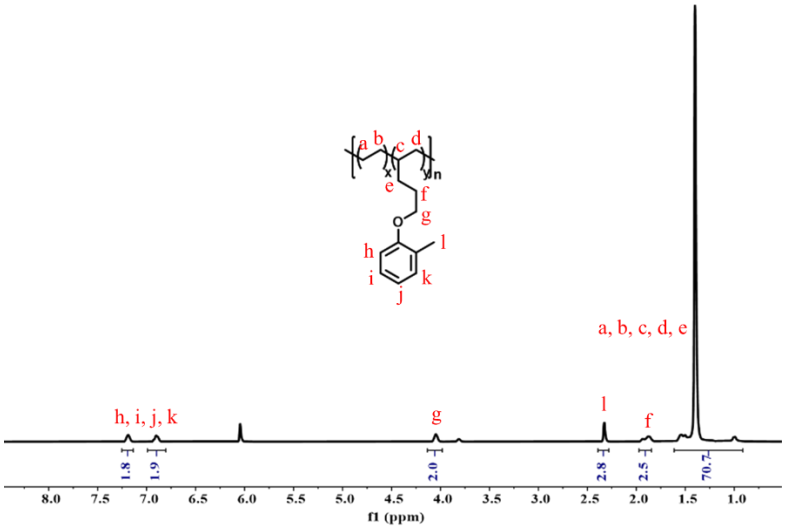


Figure S27. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2i** (Table 1, entry 9).

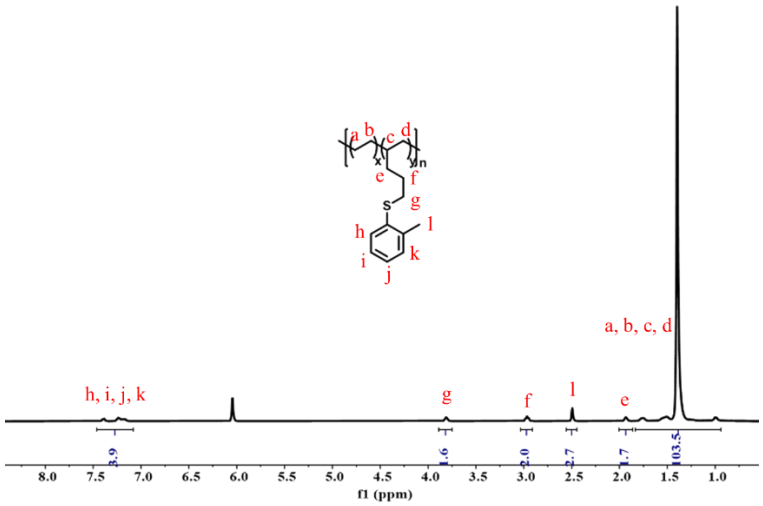


Figure S28. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2j** (Table 1, entry 10).

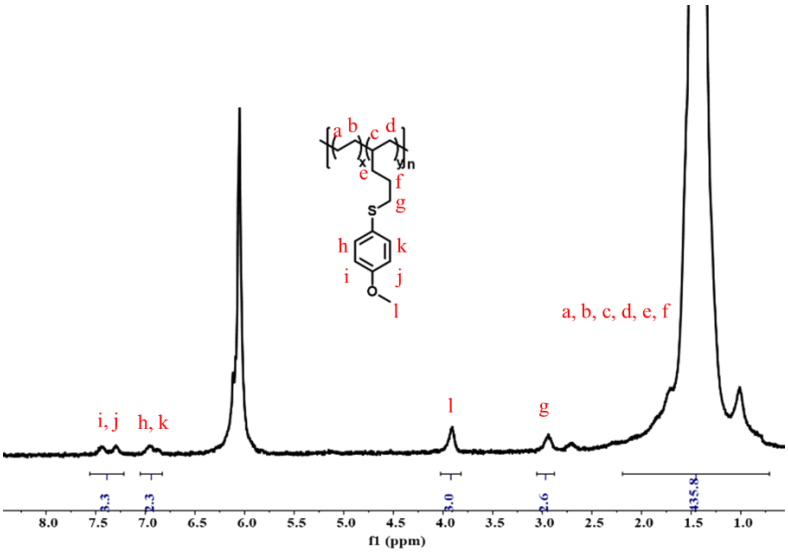


Figure S29. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2l** (Table 1, entry 12).

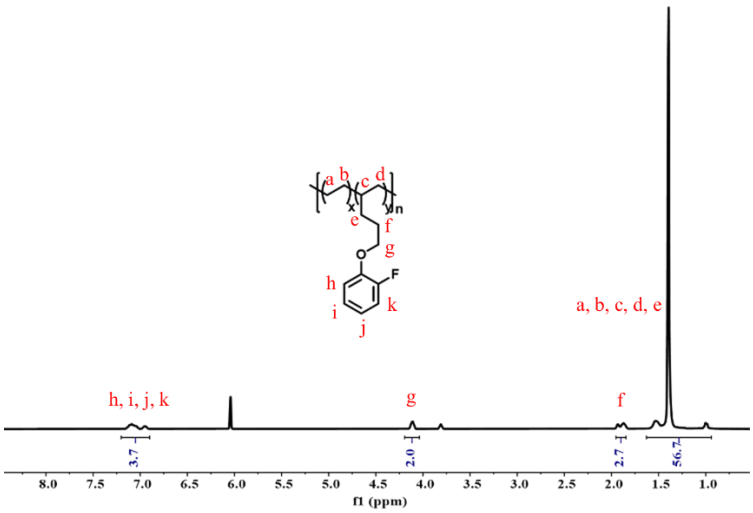


Figure S30. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2m** (Table 1, entry 13).

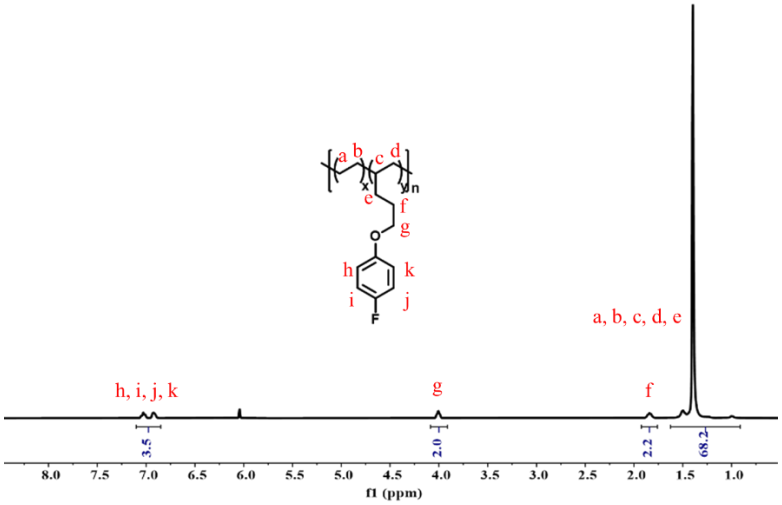


Figure S31. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2n** (Table 1, entry 14).

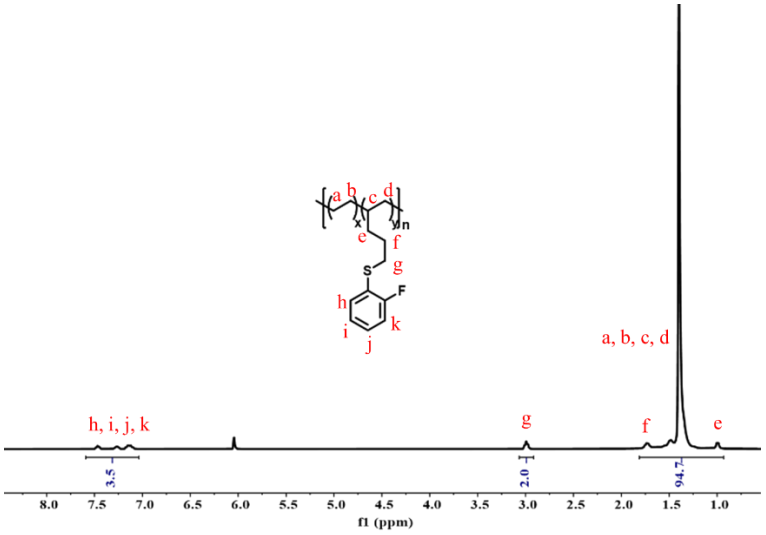


Figure S32. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2o** (Table 1, entry 15).

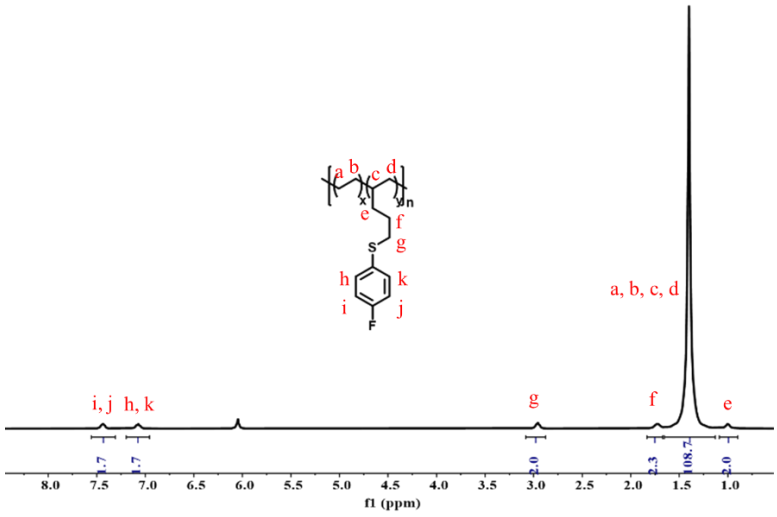


Figure S33. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2p** (Table 1, entry 16).

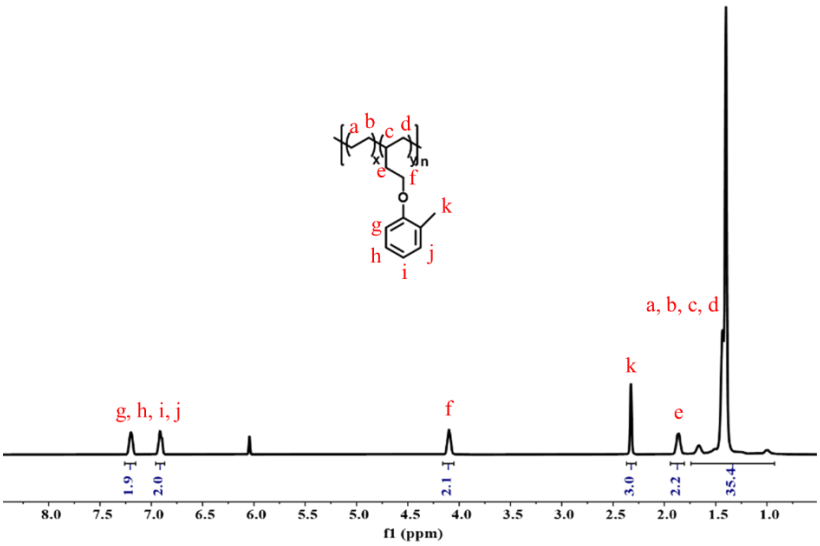


Figure S34. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2a′** (Table 2, entry 17).

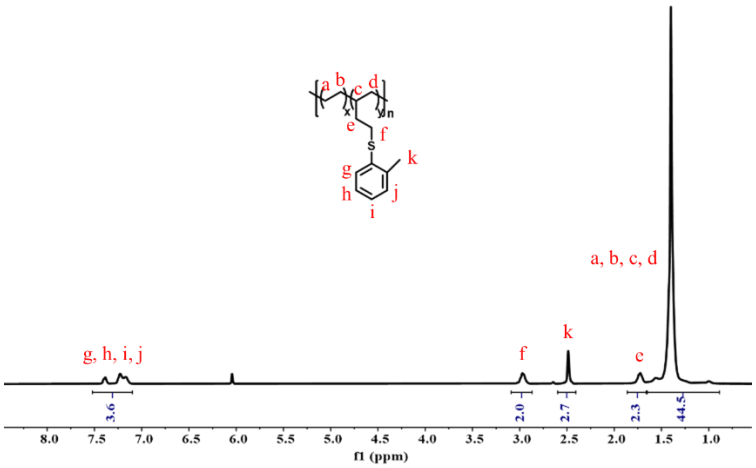


Figure S35. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2b′** (Table 2, entry 18).

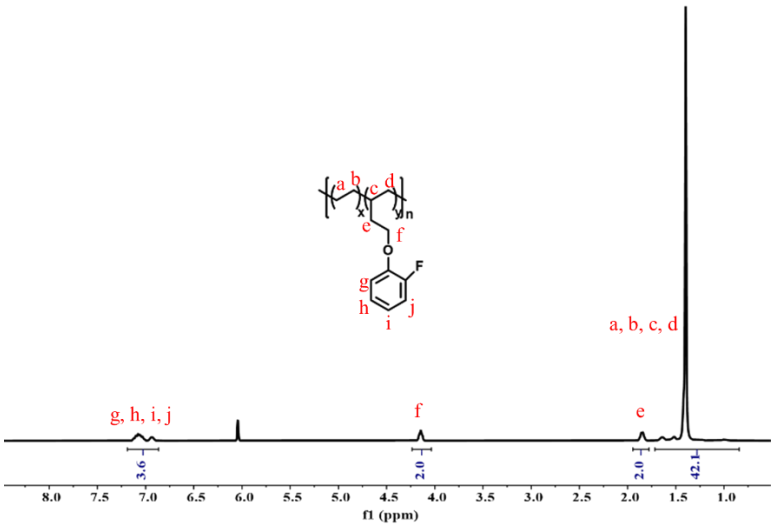


Figure S36. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2e′** (Table 2, entry 21).

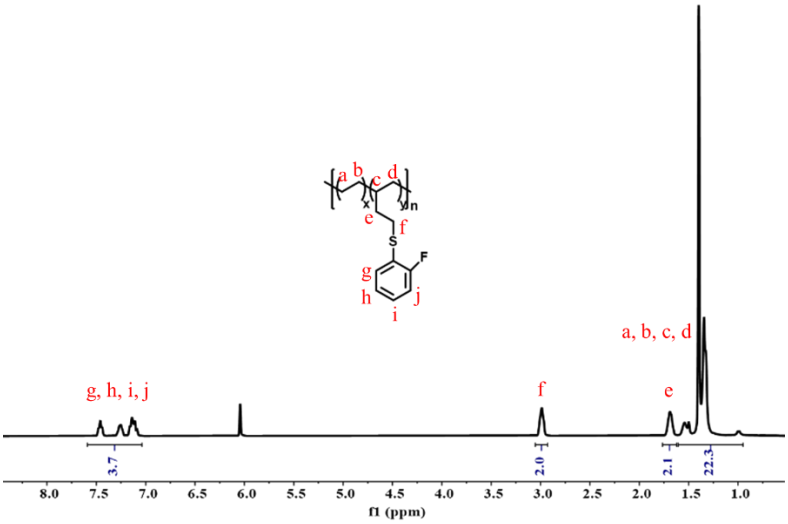


Figure S37. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2g′** (Table 2, entry 23).

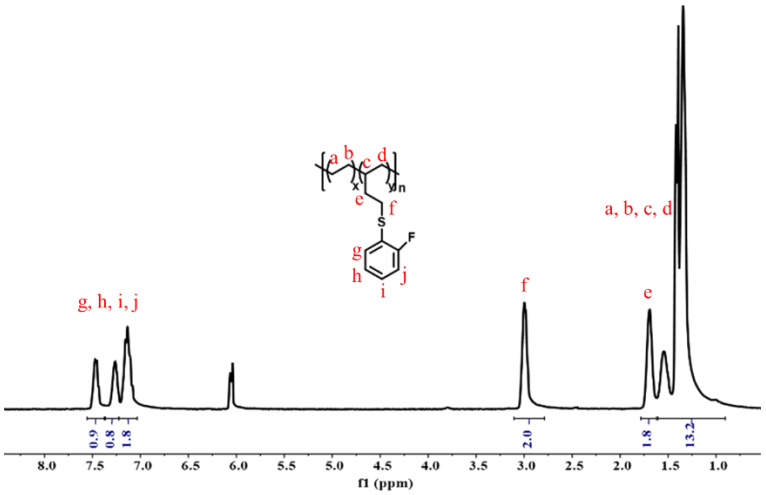


Figure S38. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2g′** (Table 2, entry 24).

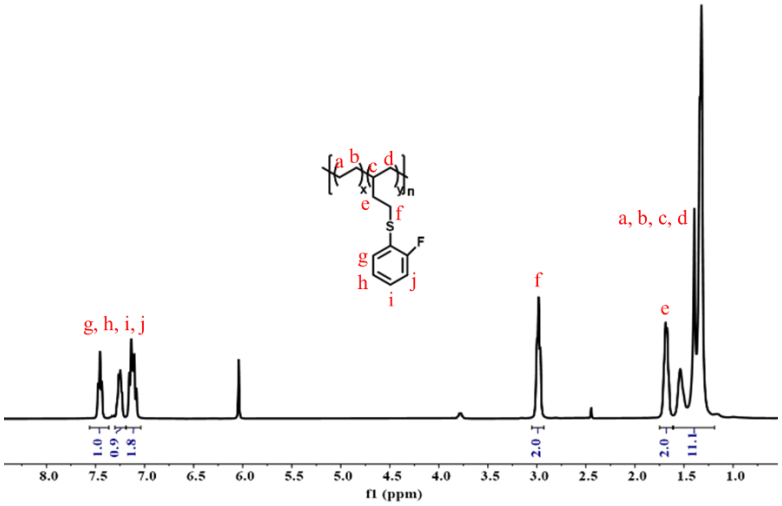


Figure S39. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2g′** (Table 2, entry 25).

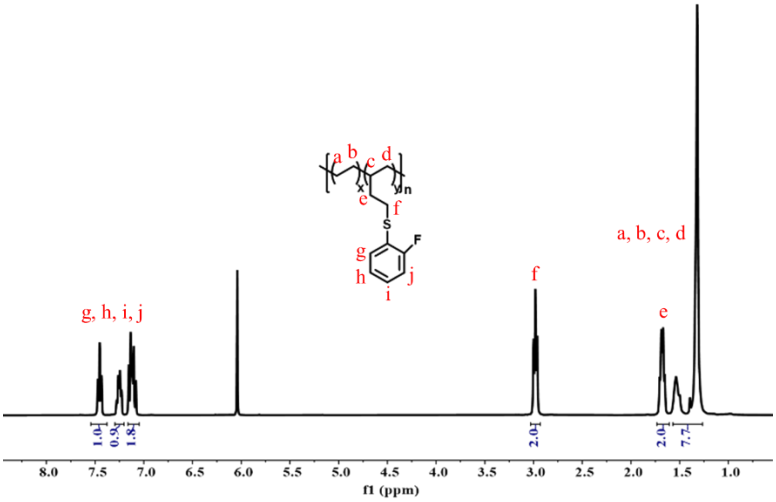


Figure S40. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2g′** (Table 2, entry 26).

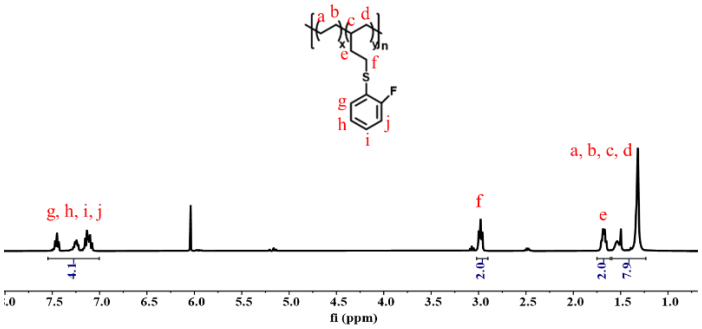


Figure S41. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2g′** (Table 2, entry 27).

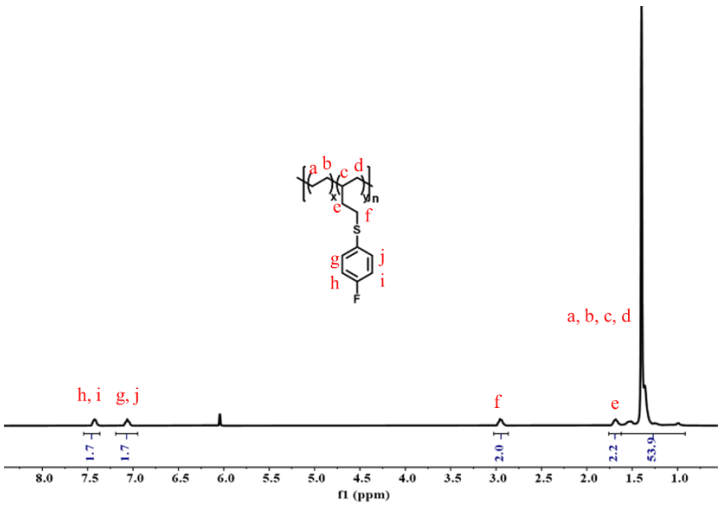


Figure S42. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2h′** (Table 2, entry 28).

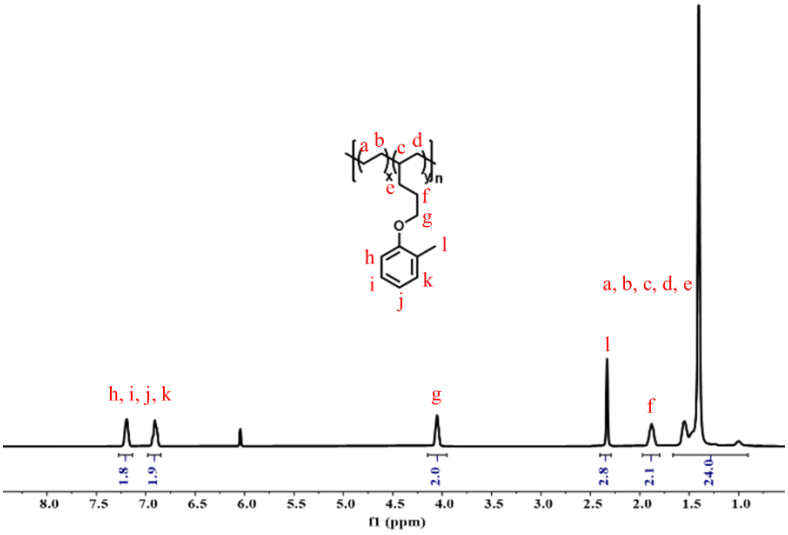


Figure S43. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2i′** (Table 2, entry 29).

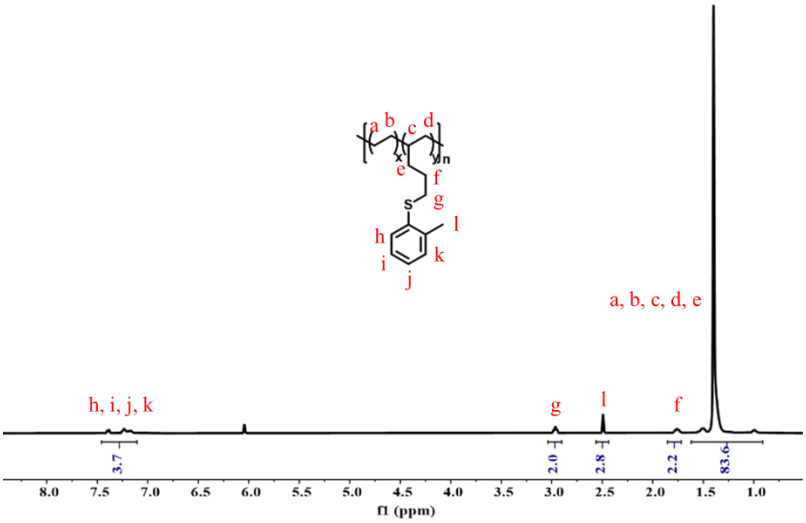


Figure S44. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2j′** (Table 2, entry 30).

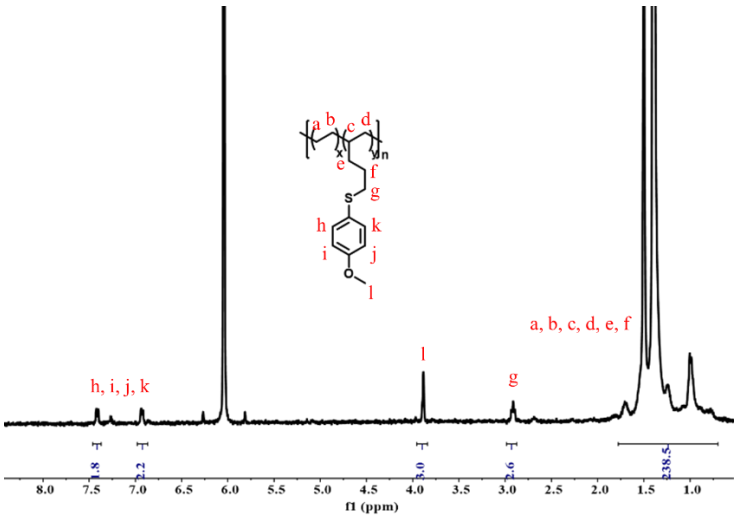


Figure S45. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2l′** (Table 2, entry 32).

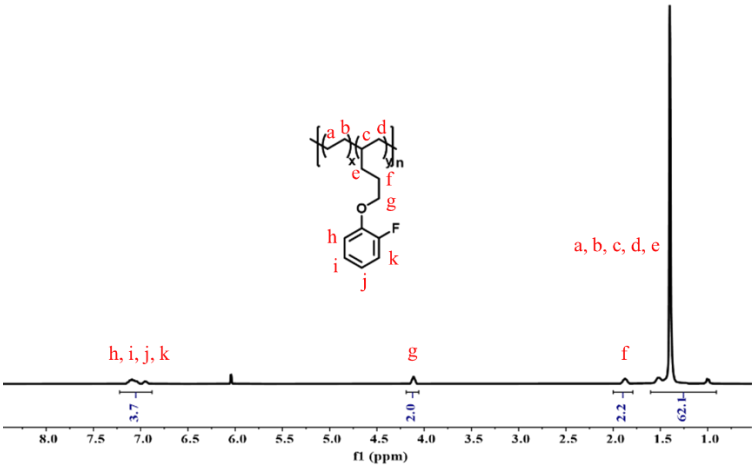


Figure S46. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2m′** (Table 2, entry 33).

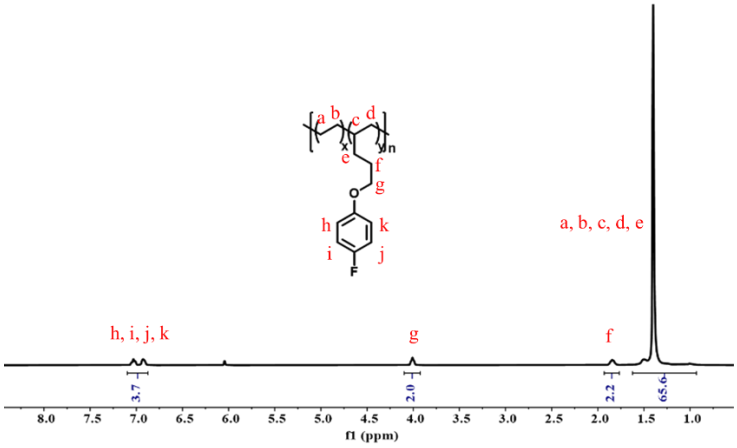


Figure S47. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2n′** (Table 2, entry 34).

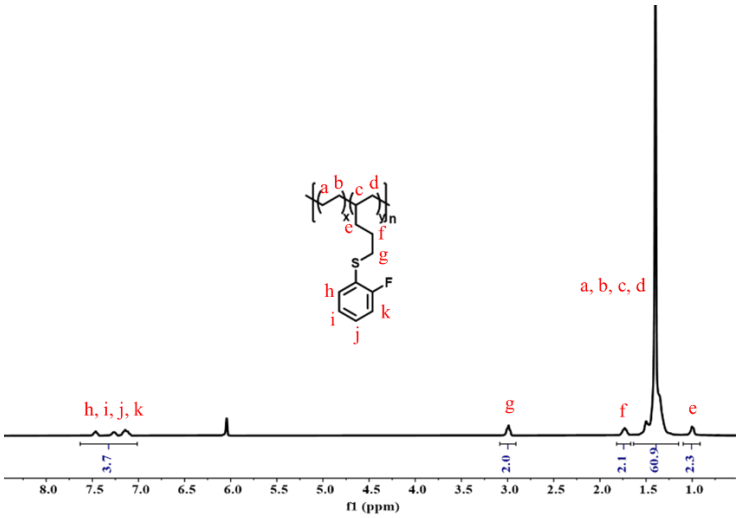


Figure S48. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2o′** (Table 2, entry 35).

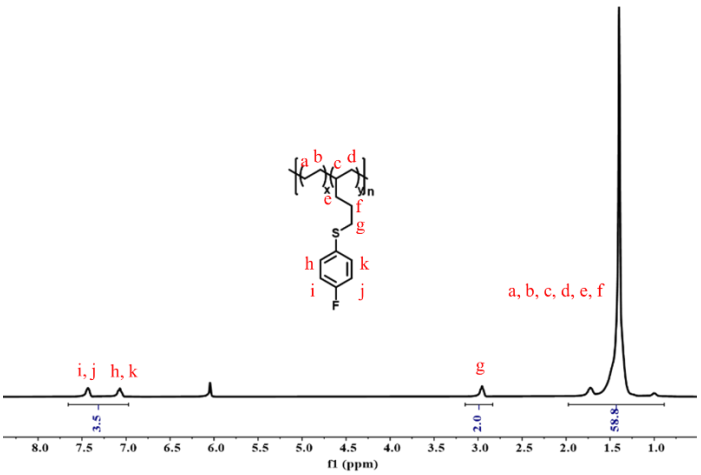


Figure S49. ^{1}H NMR spectrum (400 MHz, $C_2D_2Cl_4$, 110 °C) of **2p′** (Table 2, entry 36).

^{13}C NMR spectra of copolymers

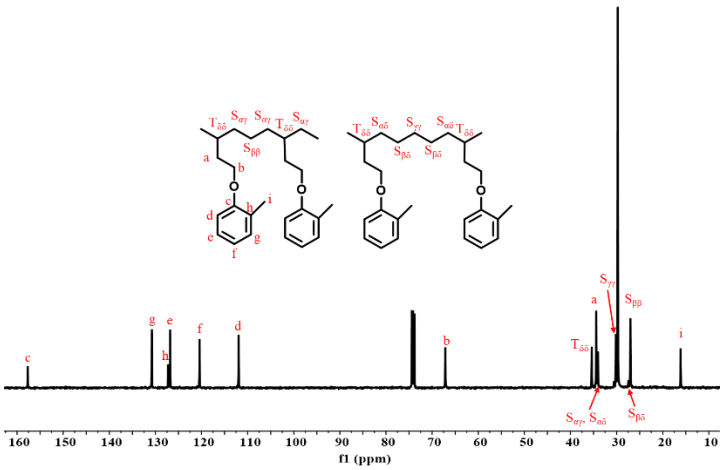


Figure S50. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2a′** (Table 2, entry 17).

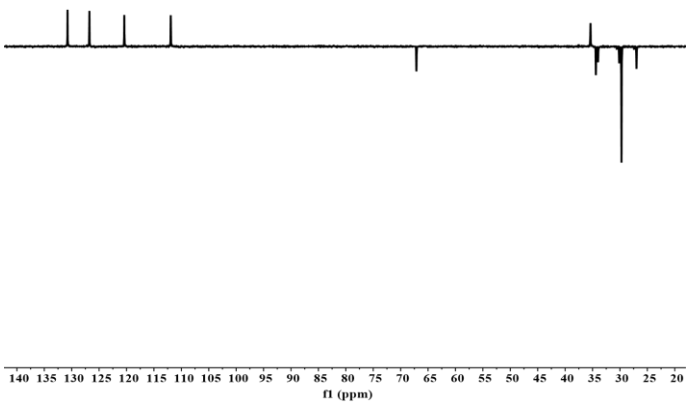


Figure S51. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2a′** (Table 2, entry 17).

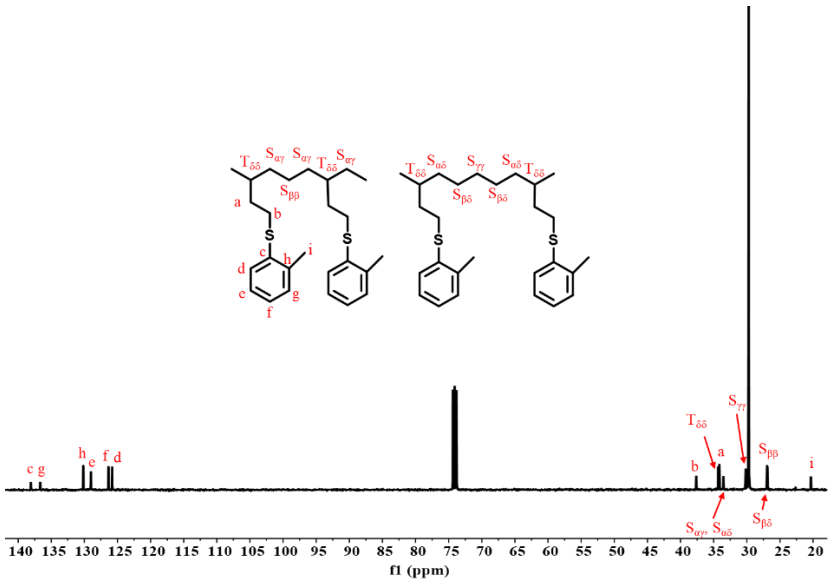


Figure S52. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2b′** (Table 2, entry 18).

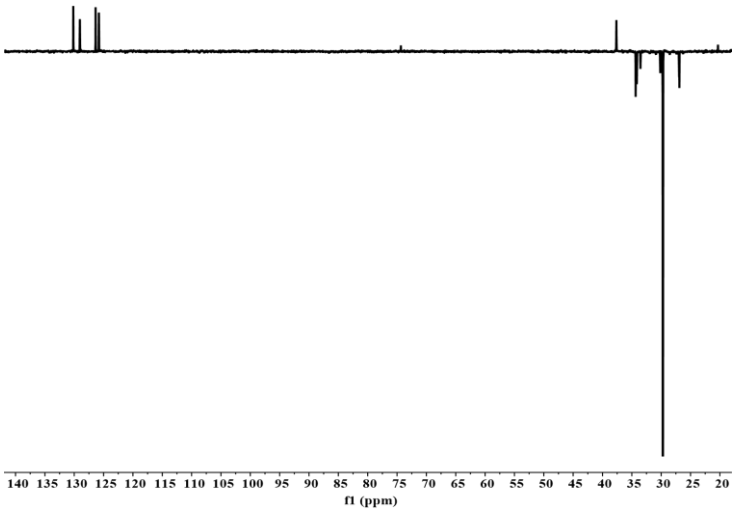


Figure S53. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2b′** (Table 2, entry 18).

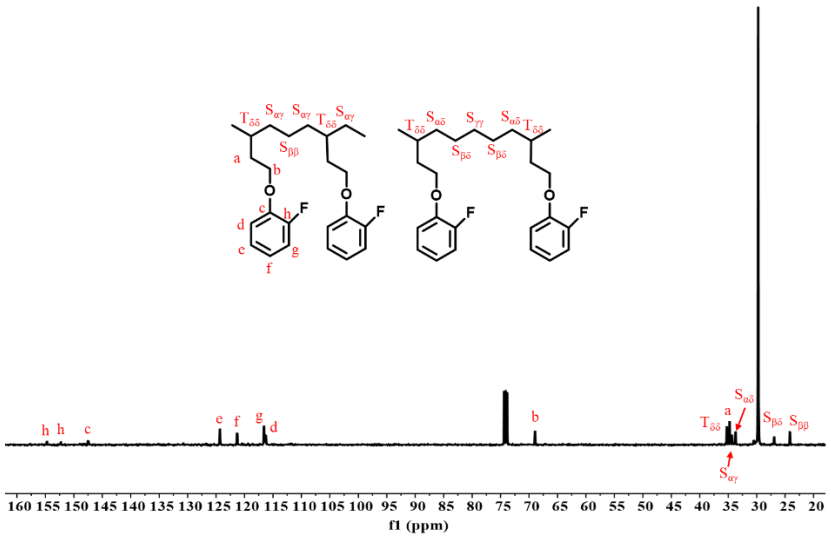


Figure S54. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2e′** (Table 2, entry 21).

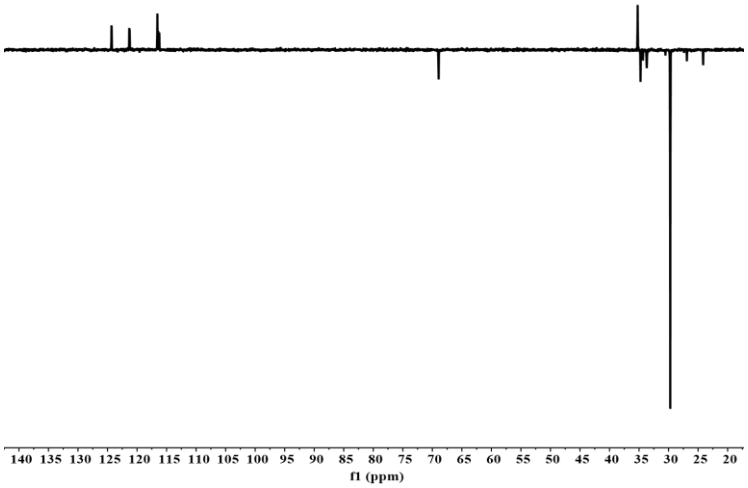


Figure S55. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2e′** (Table 2, entry 21).

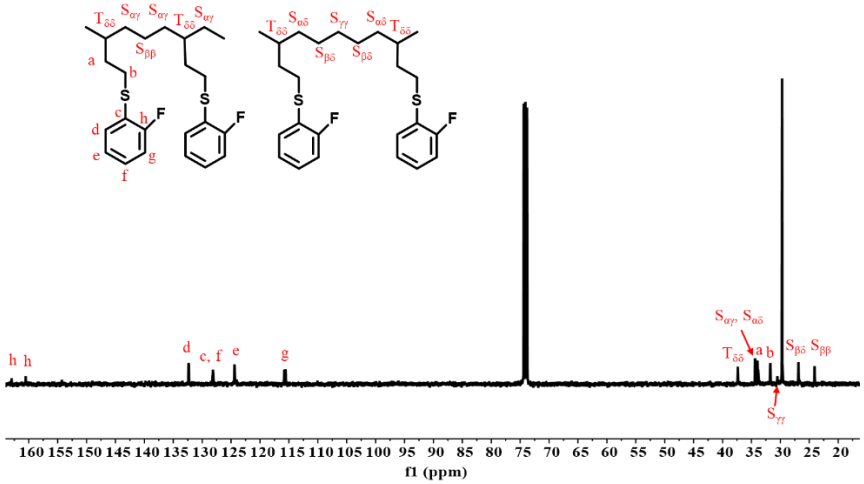


Figure S56. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2g′** (Table 2, entry 23).

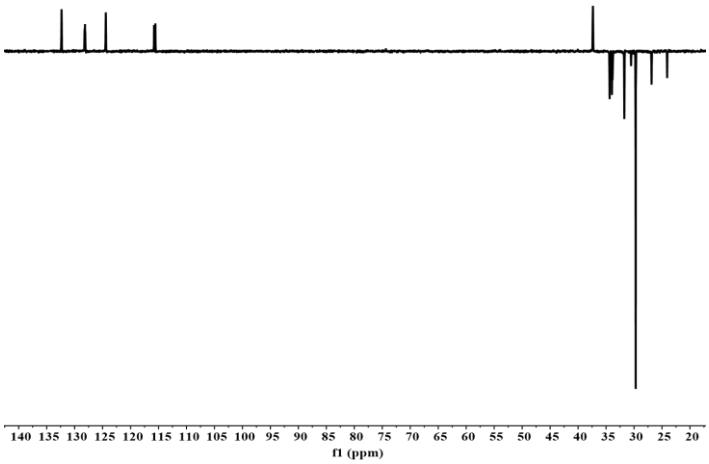


Figure S57. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2g′** (Table 2, entry 23).

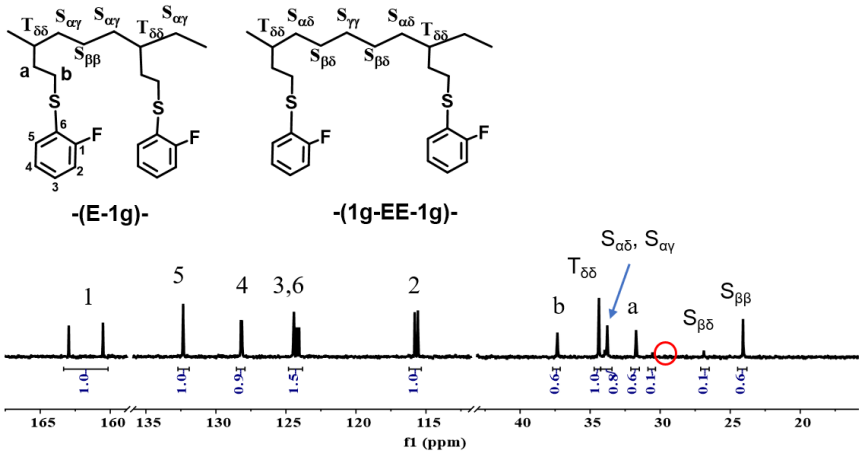


Figure S58. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2g′** (Table 2, entry 26).

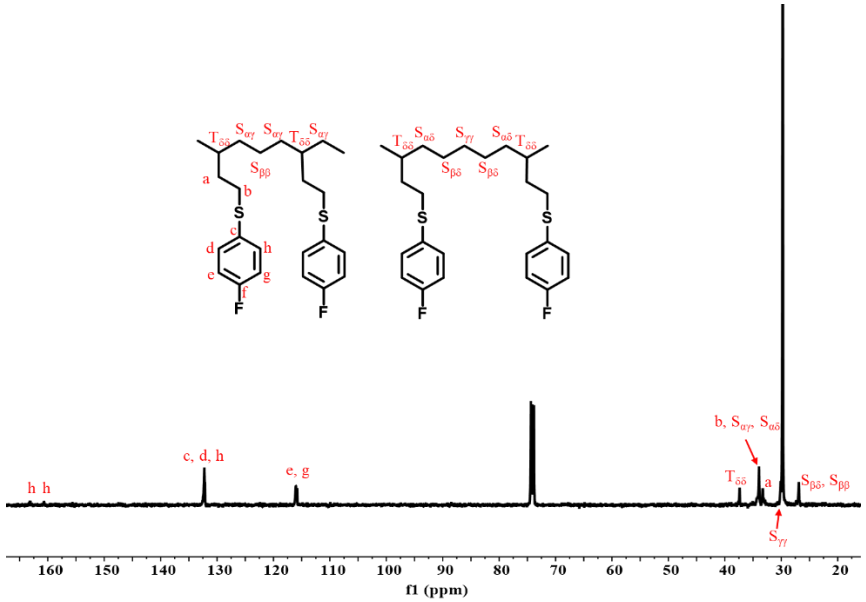


Figure S59. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2h′** (Table 2, entry 28).

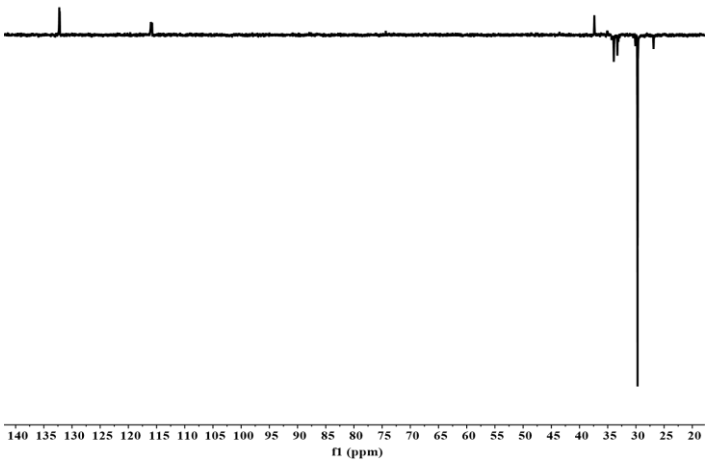


Figure S60. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2h′** (Table 2, entry 28).

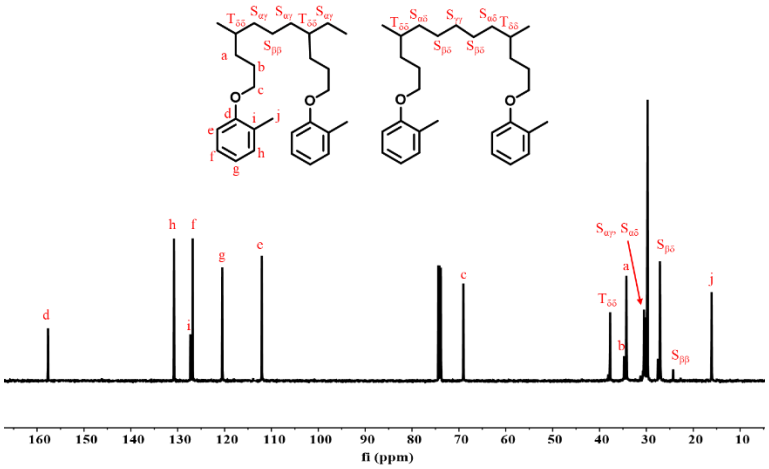


Figure S61. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2i′** (Table 2, entry 29).

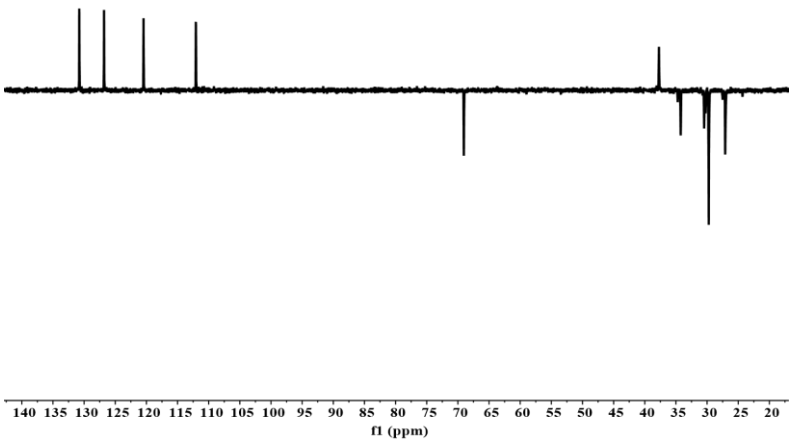


Figure S62. DEPT135 spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2i′** (Table 2, entry 29).

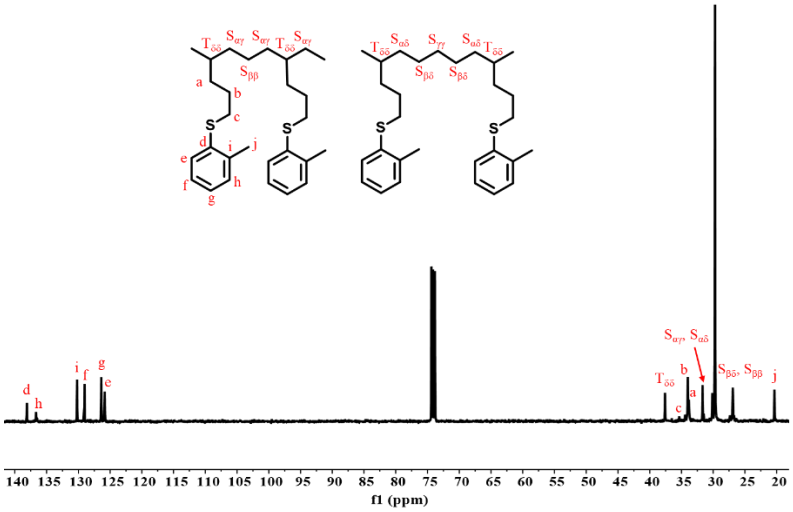


Figure S63. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2j′** (Table 2, entry 30).

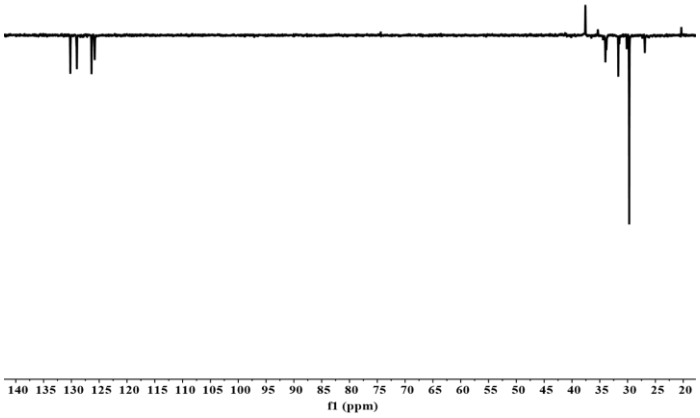


Figure S64. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2j′** (Table 2, entry 30).

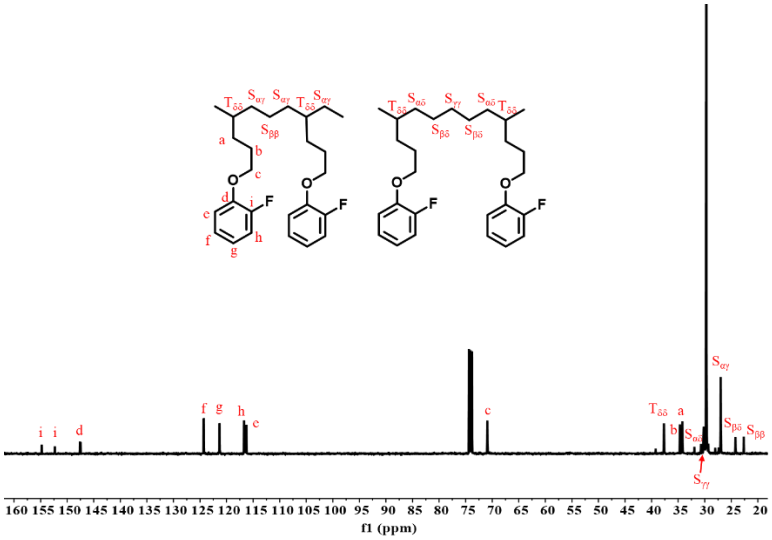


Figure S65. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2m′** (Table 2, entry 33).

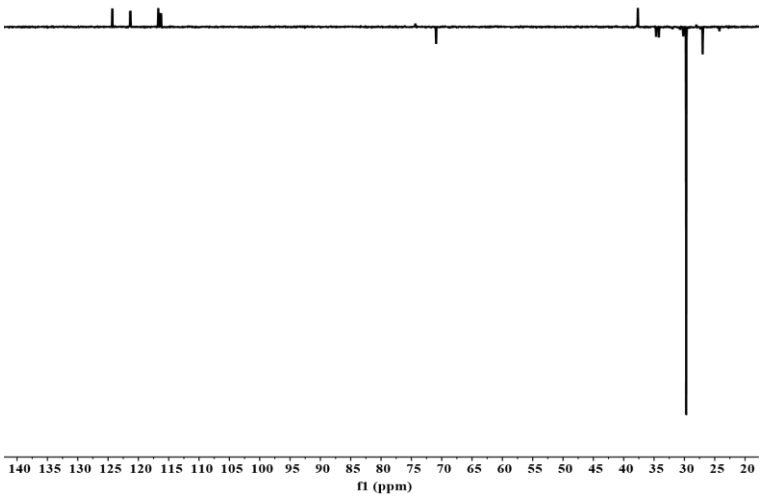


Figure S66. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2m′** (Table 2, entry 33).

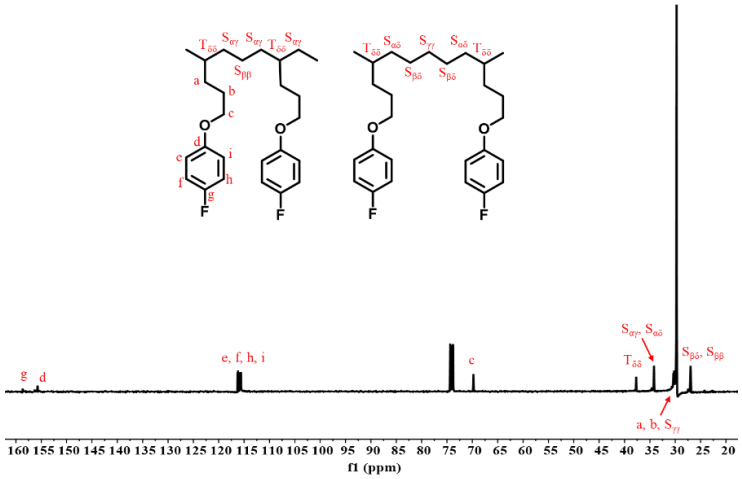


Figure S67. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2n′** (Table 2, entry 34).

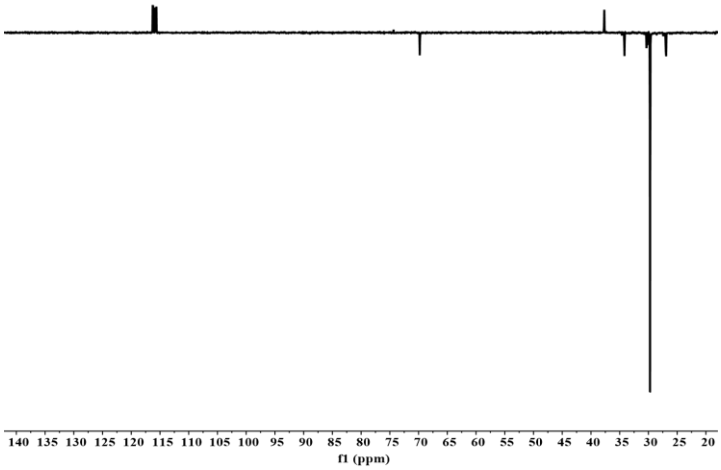


Figure S68. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2n′** (Table 2, entry 34).

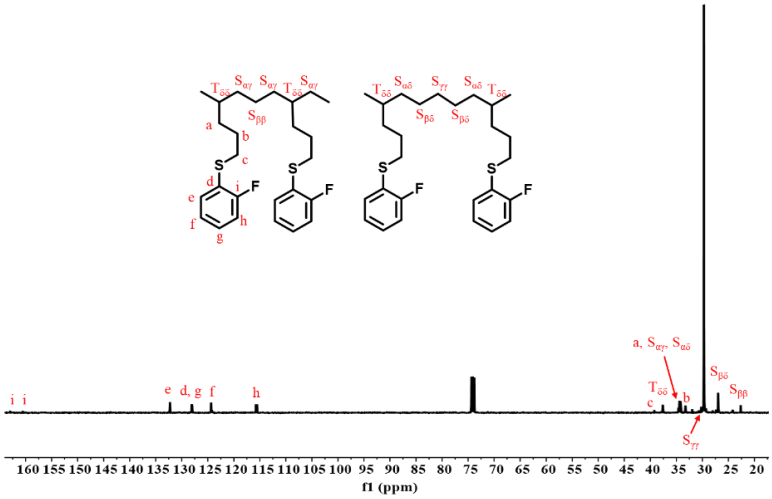


Figure S69. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2o′** (Table 2, entry 35).

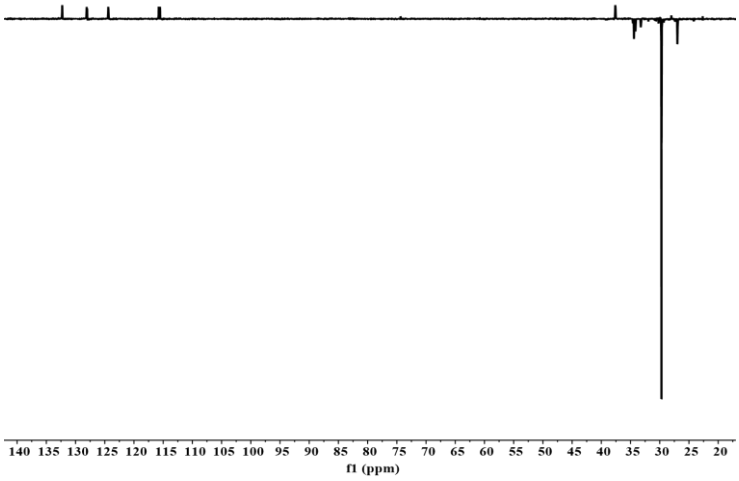


Figure S70. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2o′** (Table 2, entry 35).

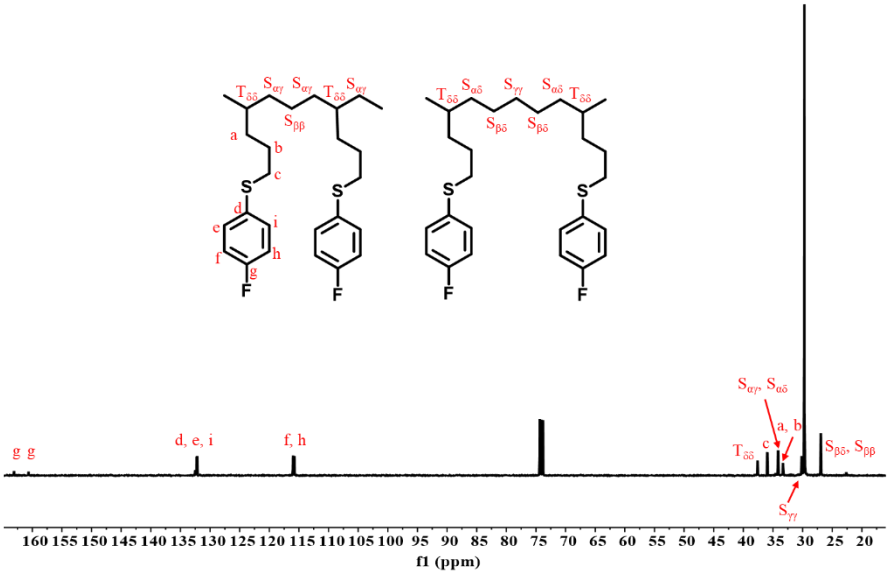


Figure S71. ^{13}C NMR spectrum (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2p′** (Table 2, entry 36).

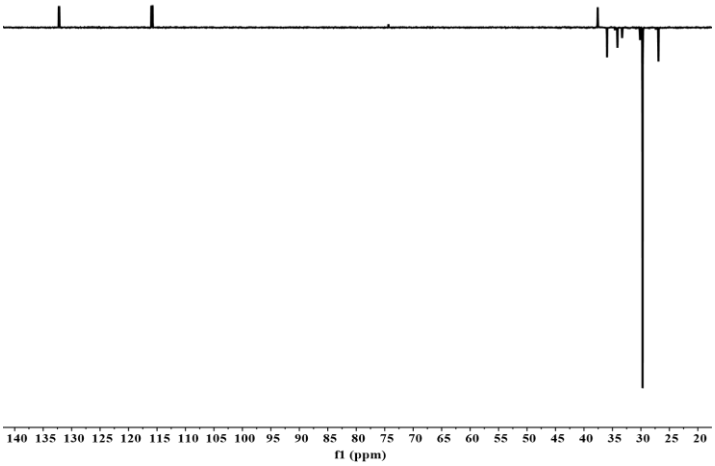


Figure S72. DEPT135 (100 MHz, $C_2D_2Cl_4$, 110 °C) of **2p′** (Table 2, entry 36).

DSC curves of copolymers

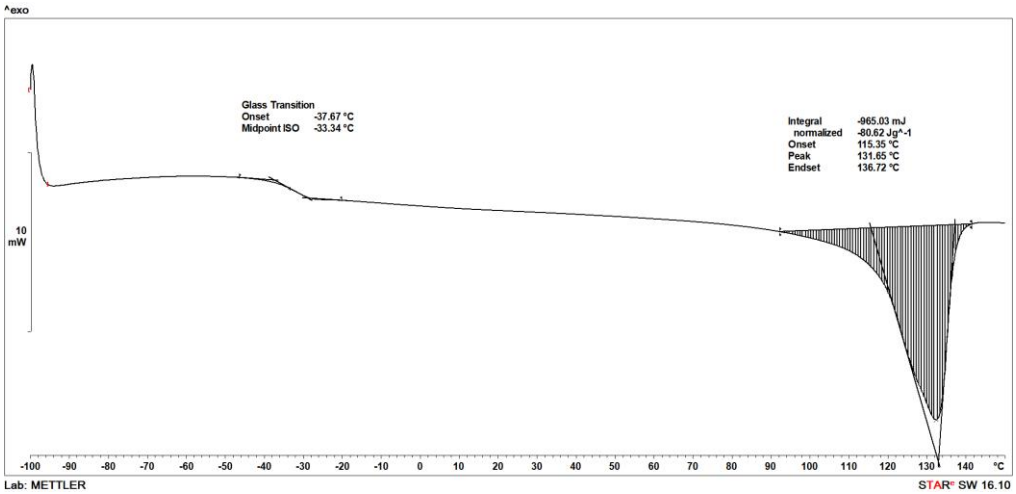


Figure S73. DSC curve of **2a** (Table 1, entry 1).

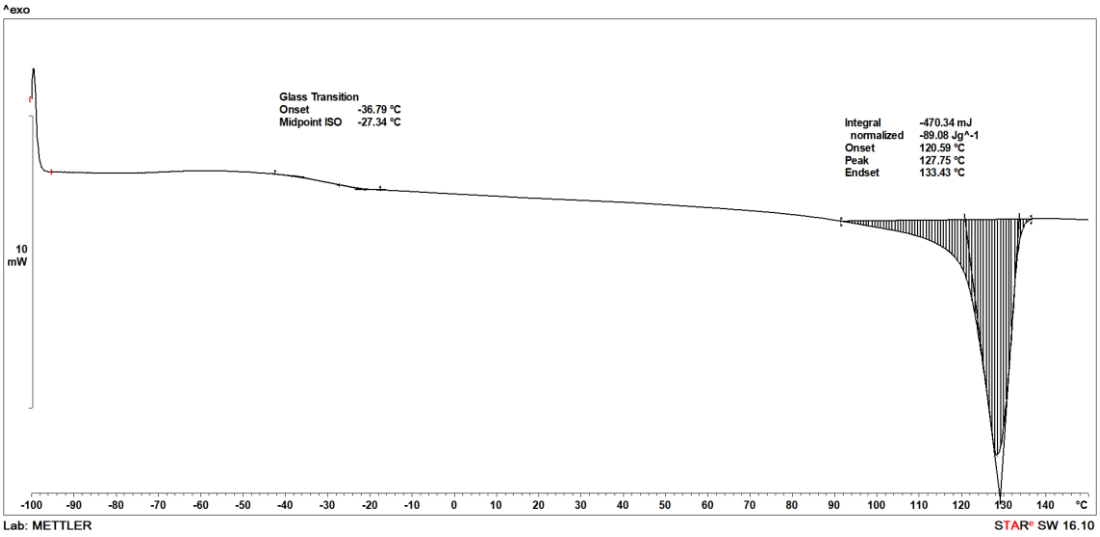


Figure S74. DSC curve of **2b** (Table 1, entry 2).

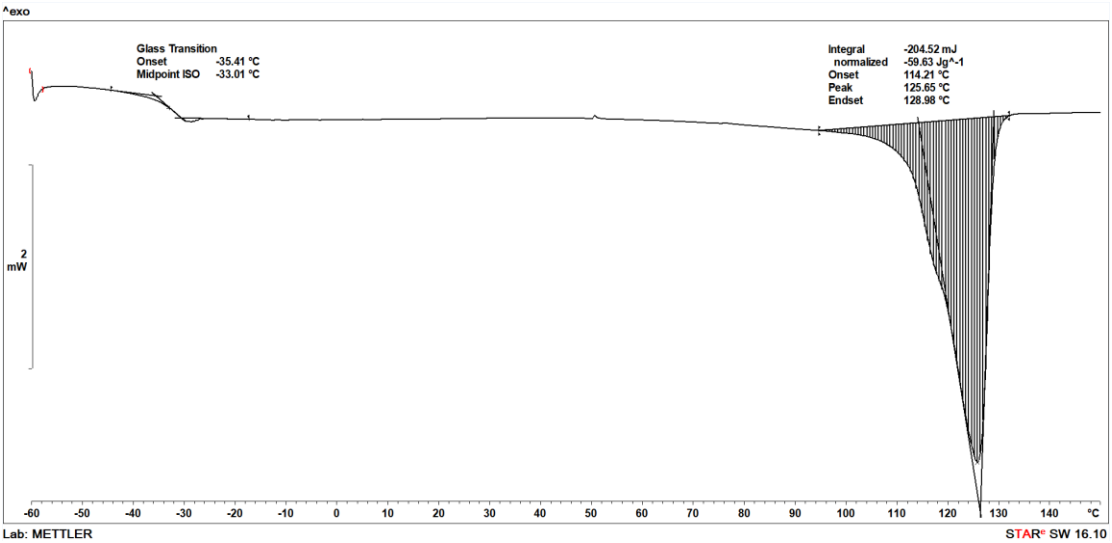


Figure S75. DSC curve of **2g** (Table 1, entry 7).

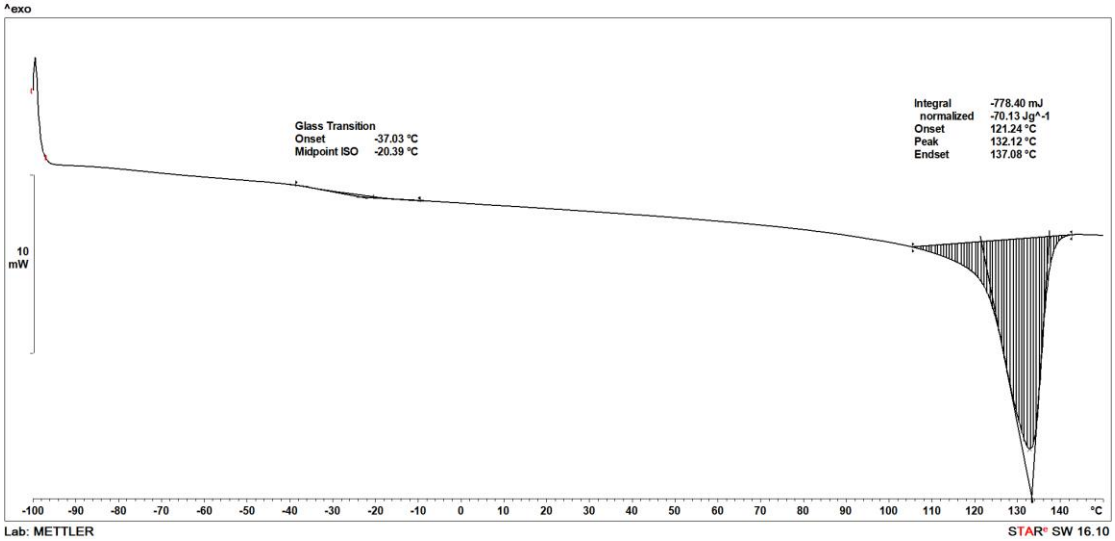


Figure S76. DSC curve of **2h** (Table 1, entry 8).

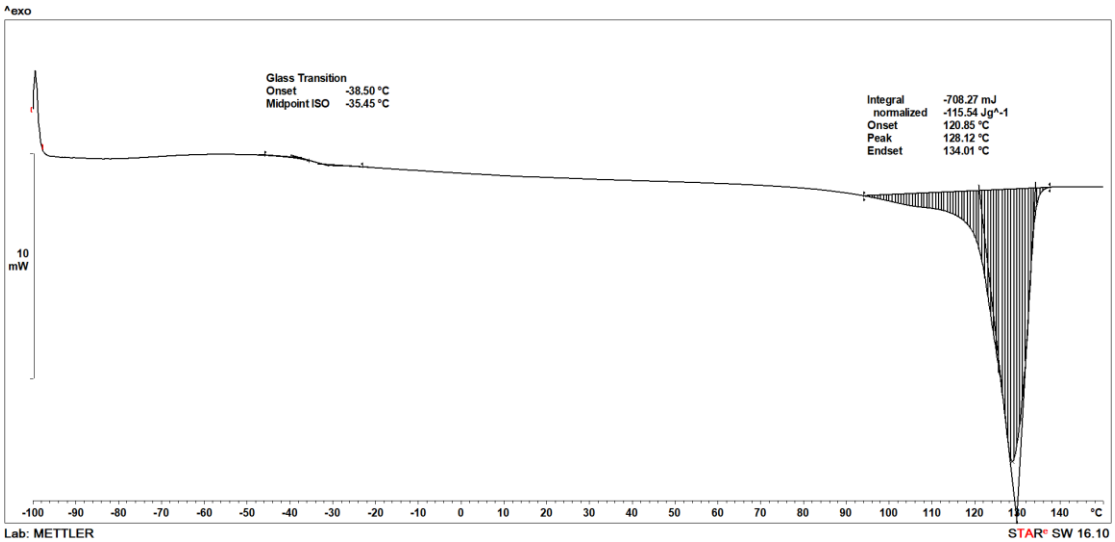


Figure S77. DSC curve of **2i** (Table 1, entry 9).

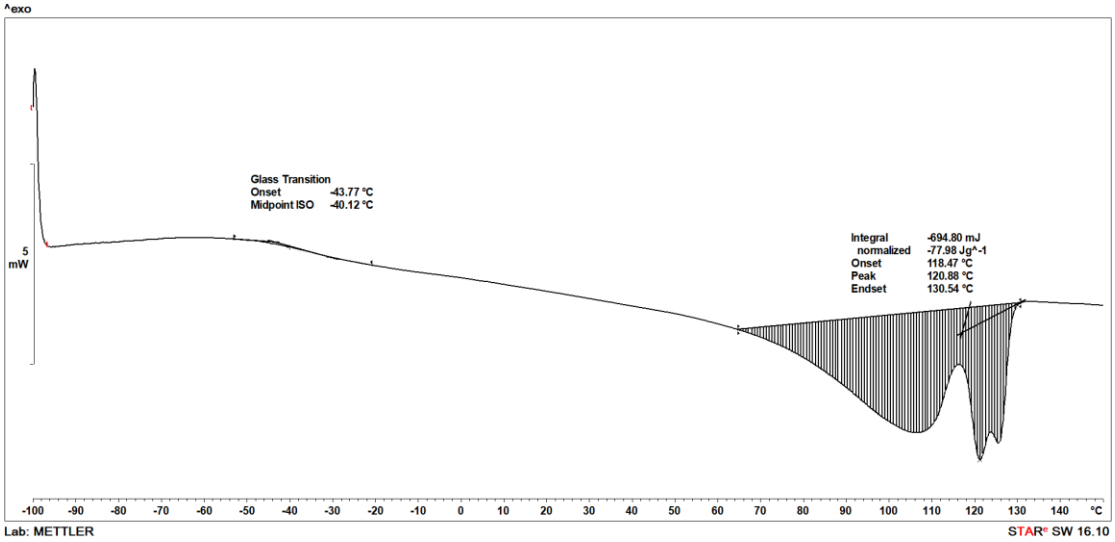


Figure S78. DSC curve of **2j** (Table 1, entry 10).

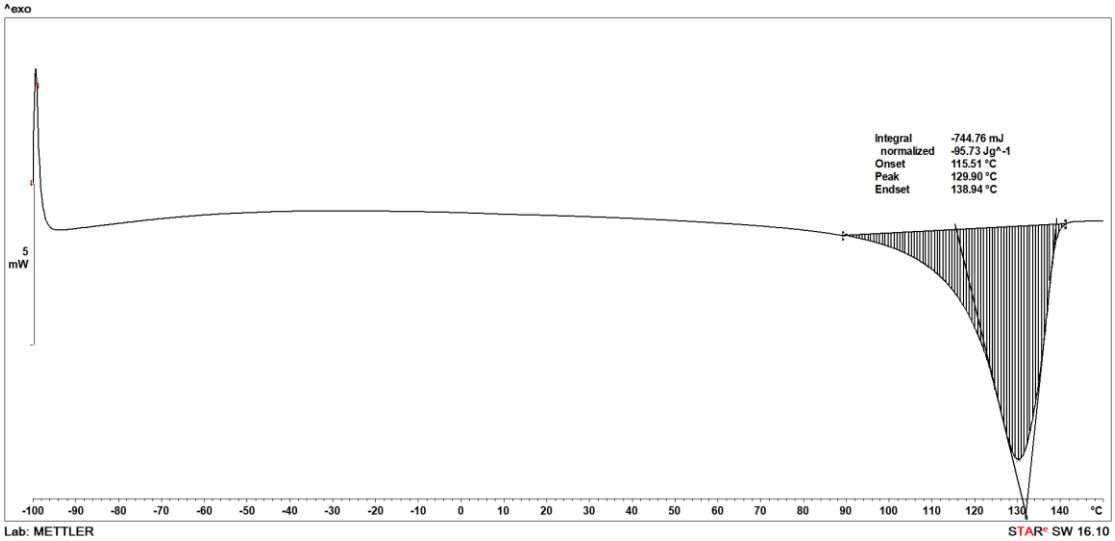


Figure S79. DSC curve of **2l** (Table 1, entry 12).

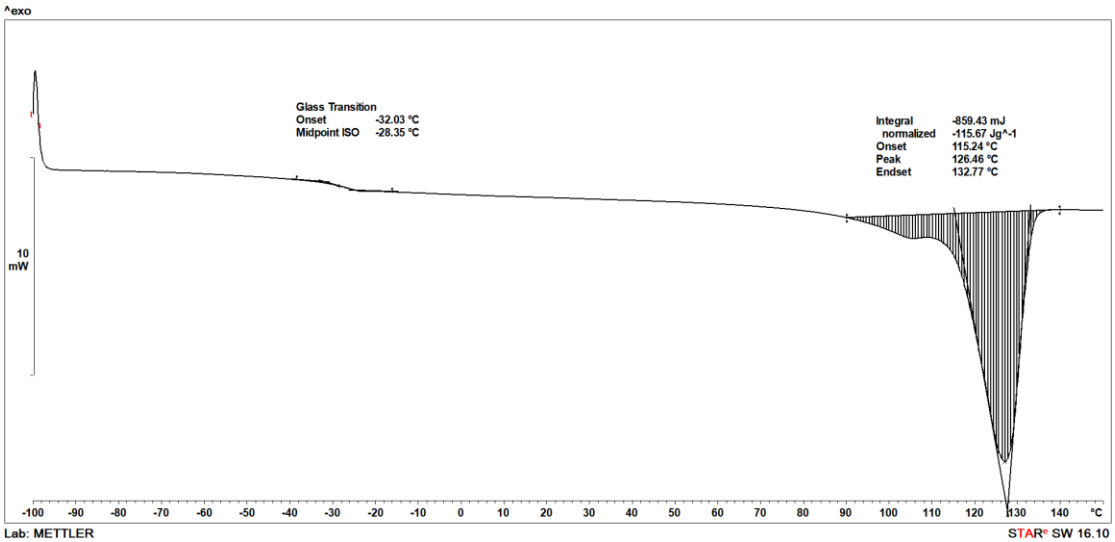


Figure S80. DSC curve of **2m** (Table 1, entry 13).

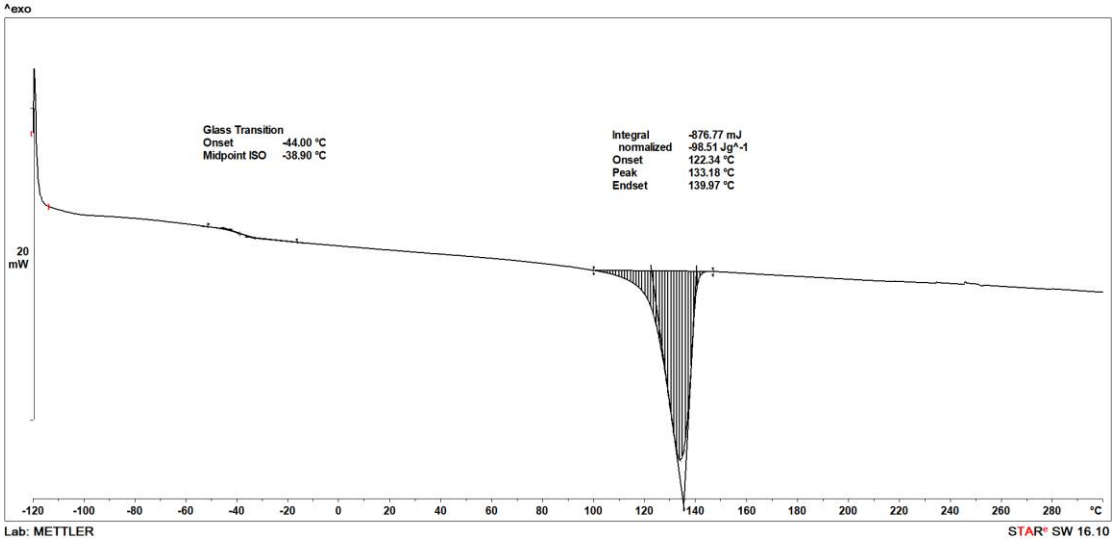


Figure S81. DSC curve of **2n** (Table 1, entry 14).

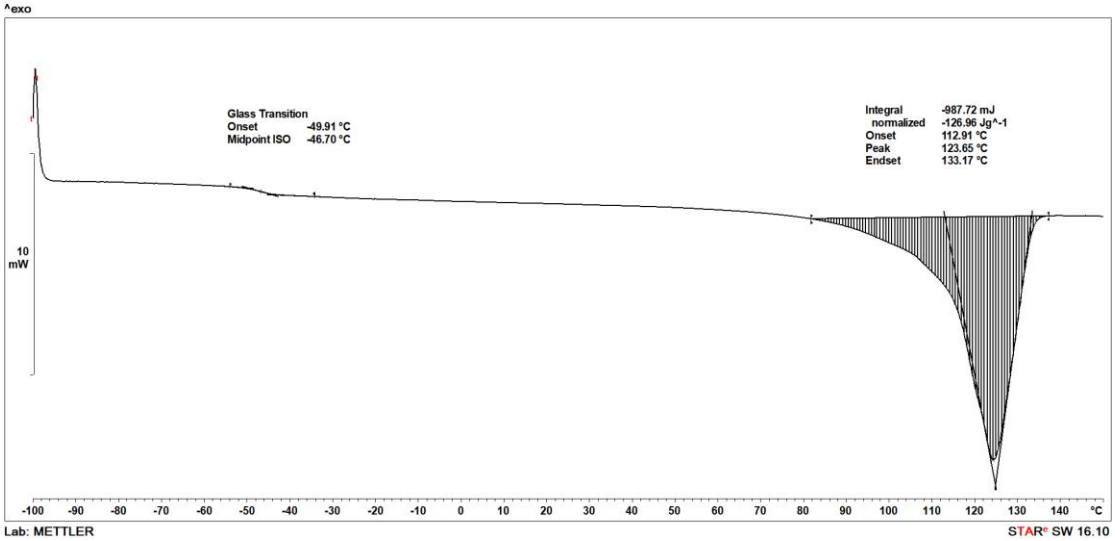


Figure S82. DSC curve of **2o** (Table 1, entry 15).

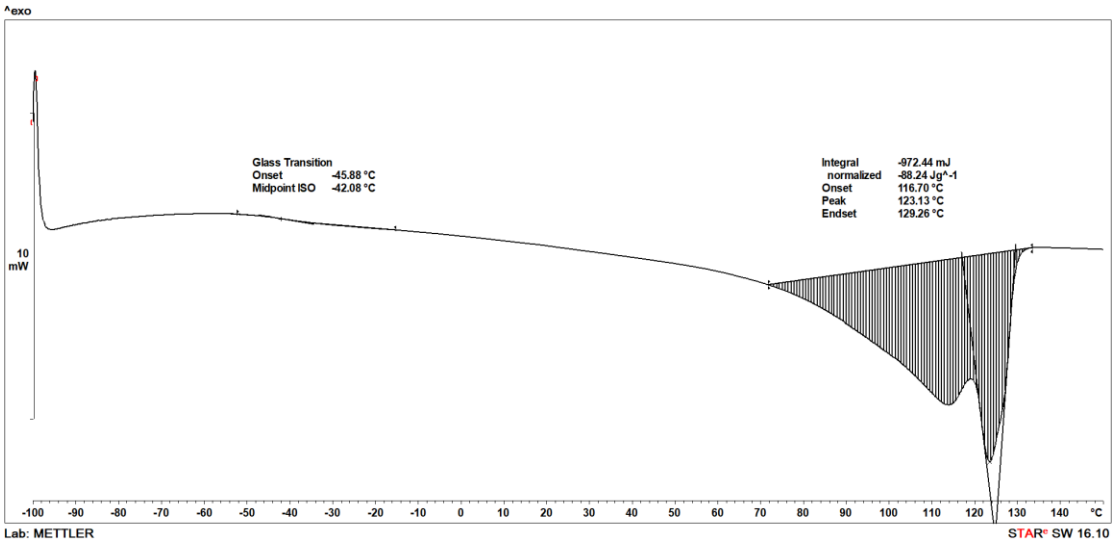


Figure S83. DSC curve of **2p** (Table 1, entry 16).

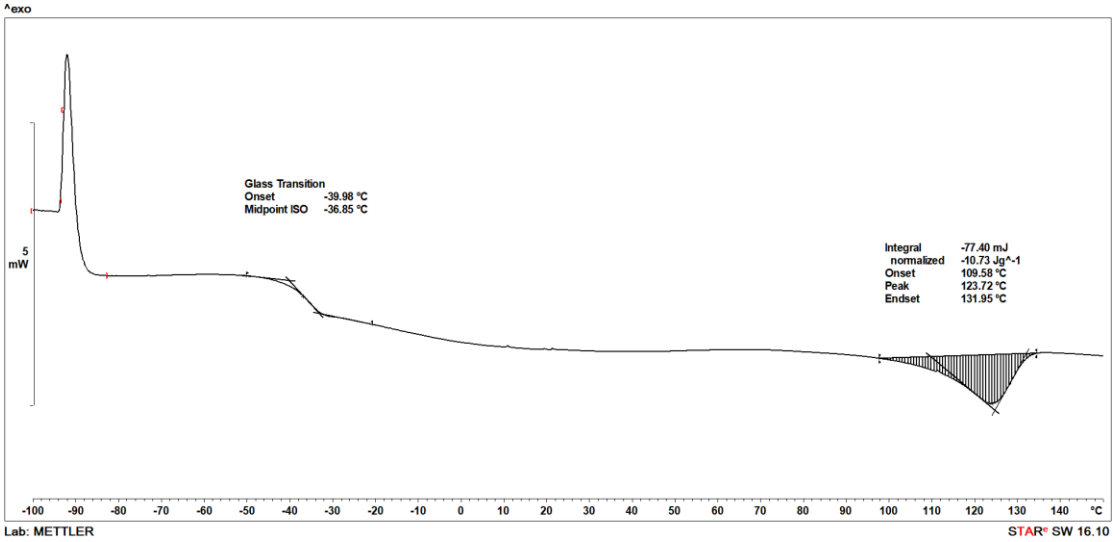


Figure S84. DSC curve of **2a′** (Table 2, entry 17).

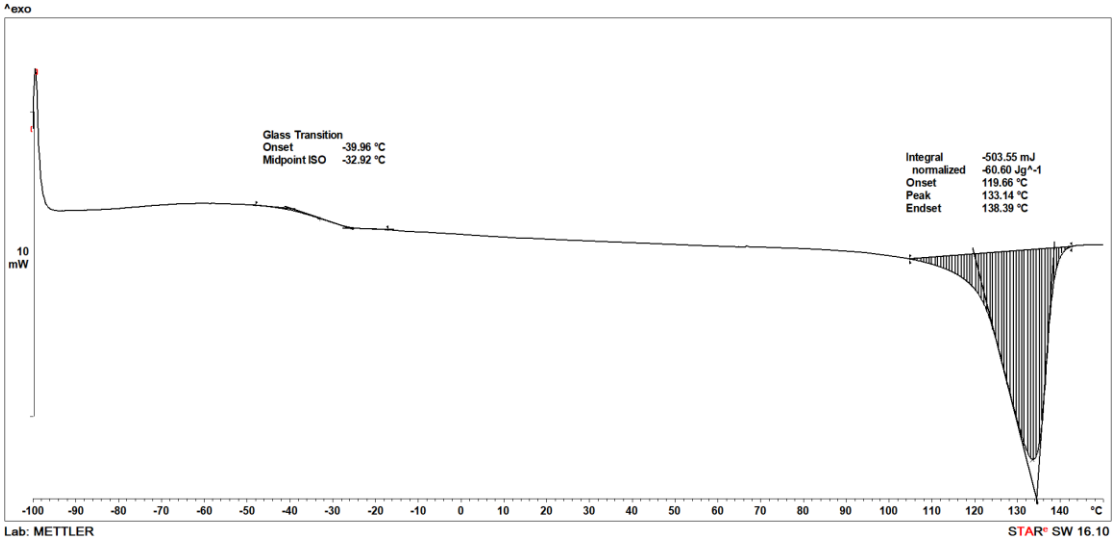


Figure S85. DSC curve of **2b′** (Table 2, entry 18).

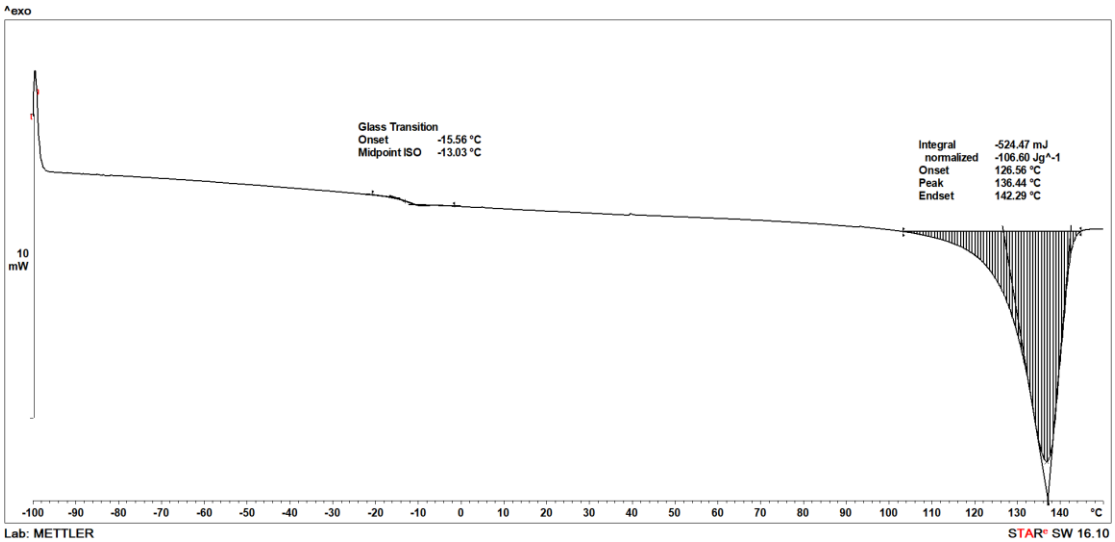


Figure S86. DSC curve of **2e′** (Table 2, entry 21).

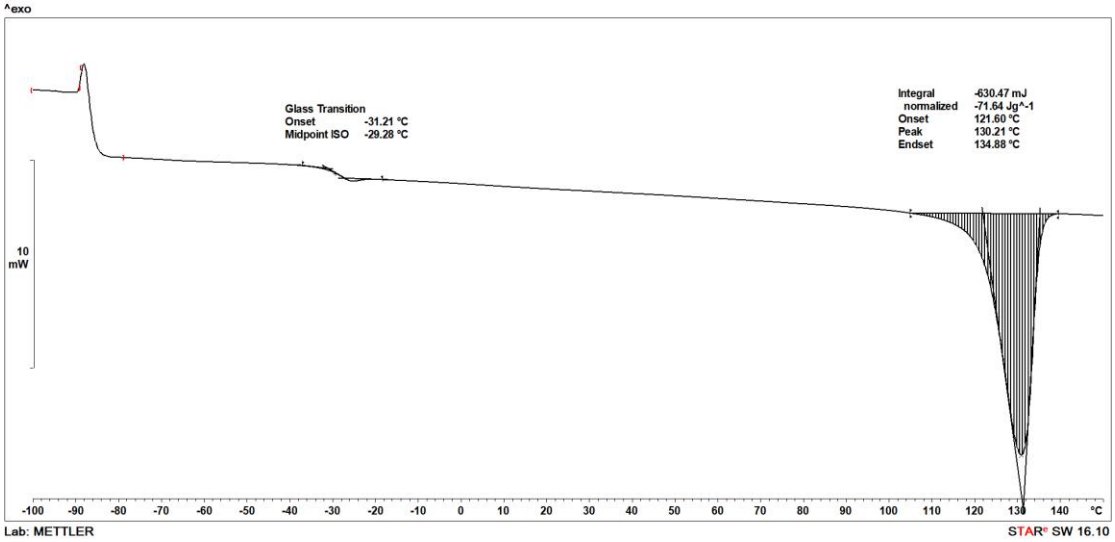


Figure S87. DSC curve of **2g′** (Table 2, entry 23).

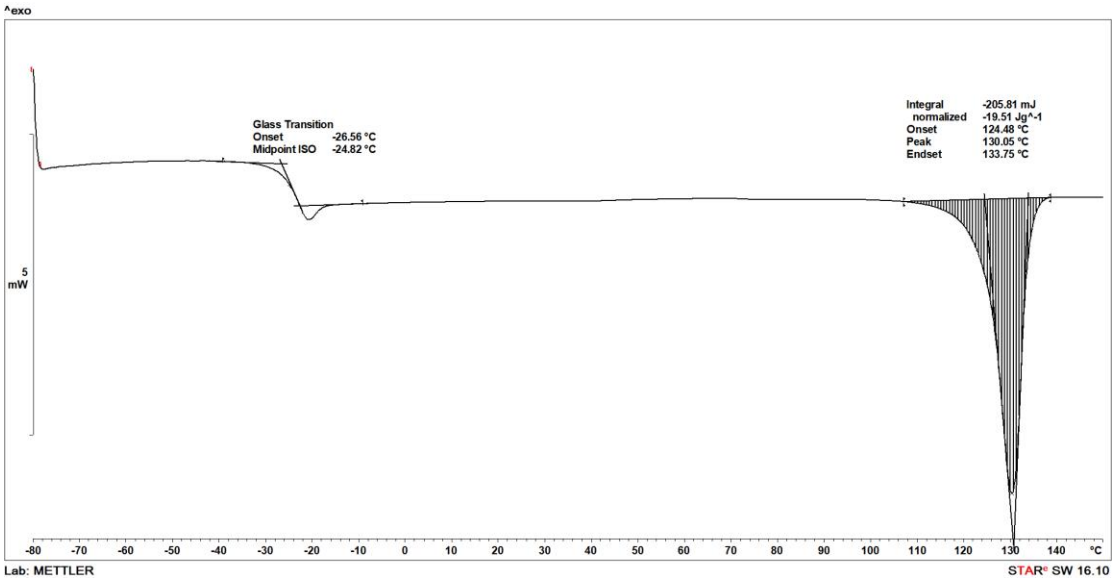


Figure S88. DSC curve of **2g′** (Table 2, entry 24).

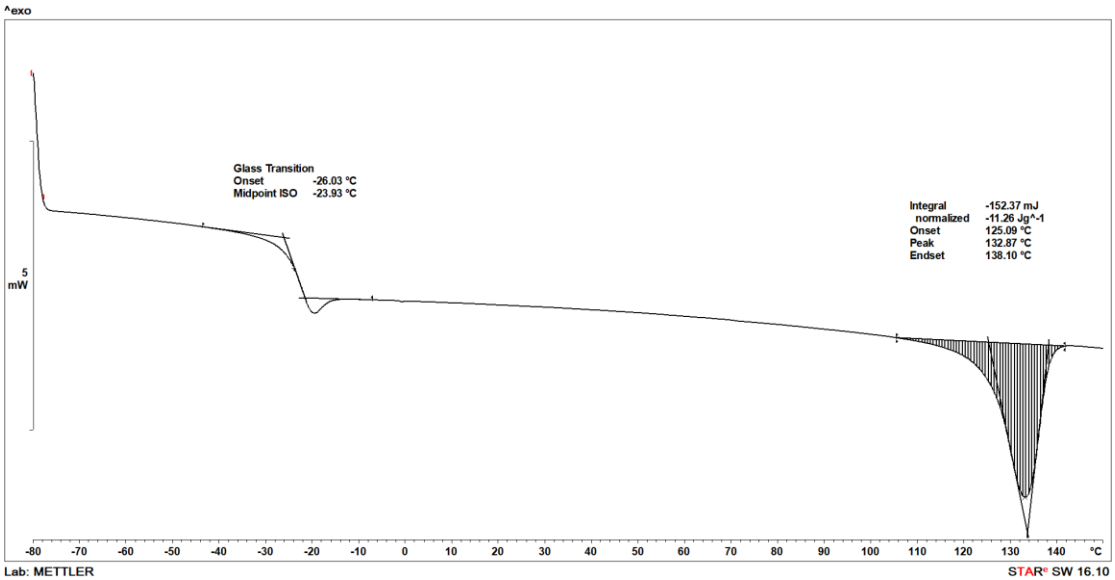


Figure S89. DSC curve of **2g′** (Table 2, entry 25).

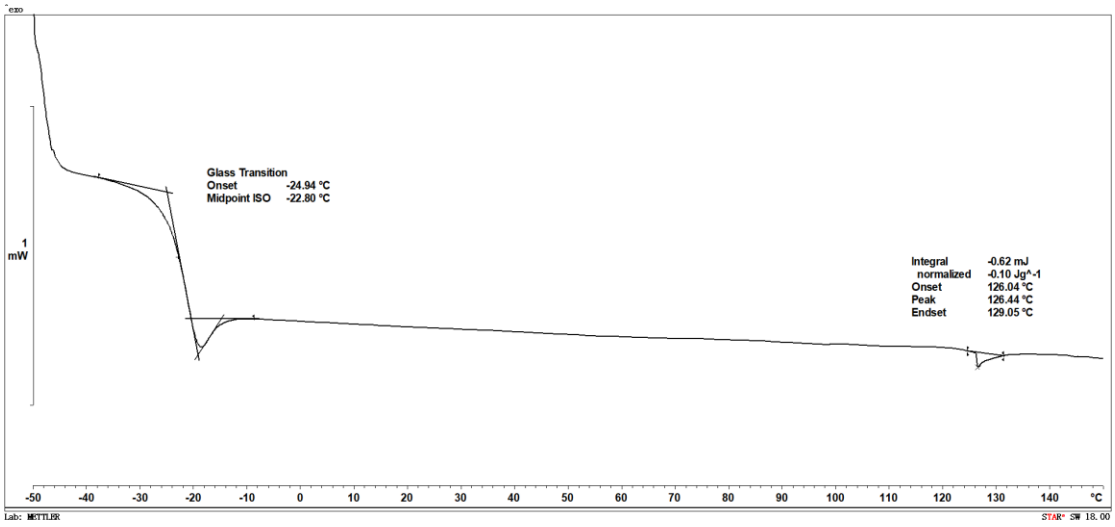


Figure S90. DSC curve of **2g′** (Table 2, entry 26).

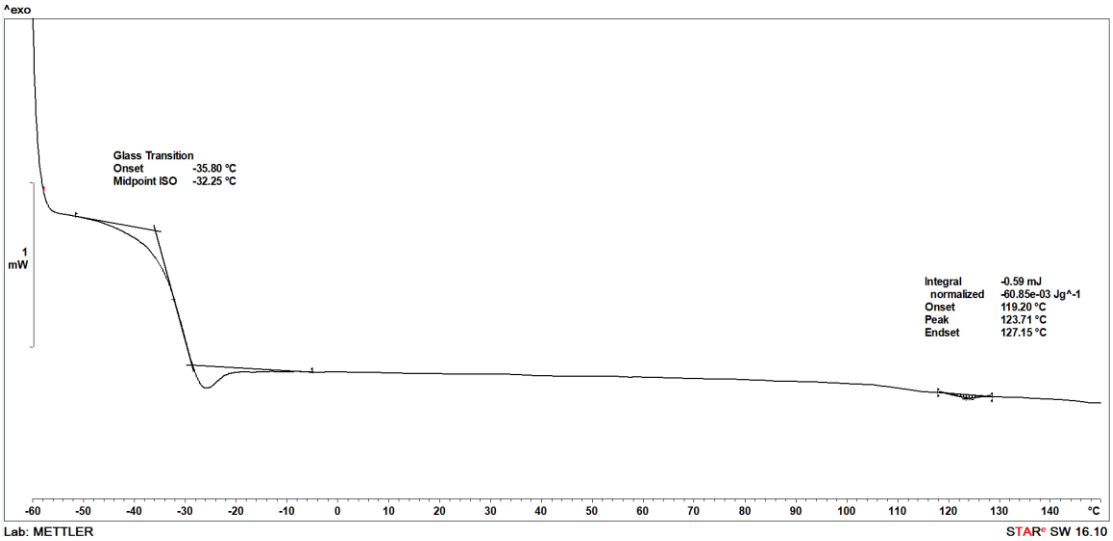


Figure S91. DSC curve of **2g′** (Table 2, entry 27).

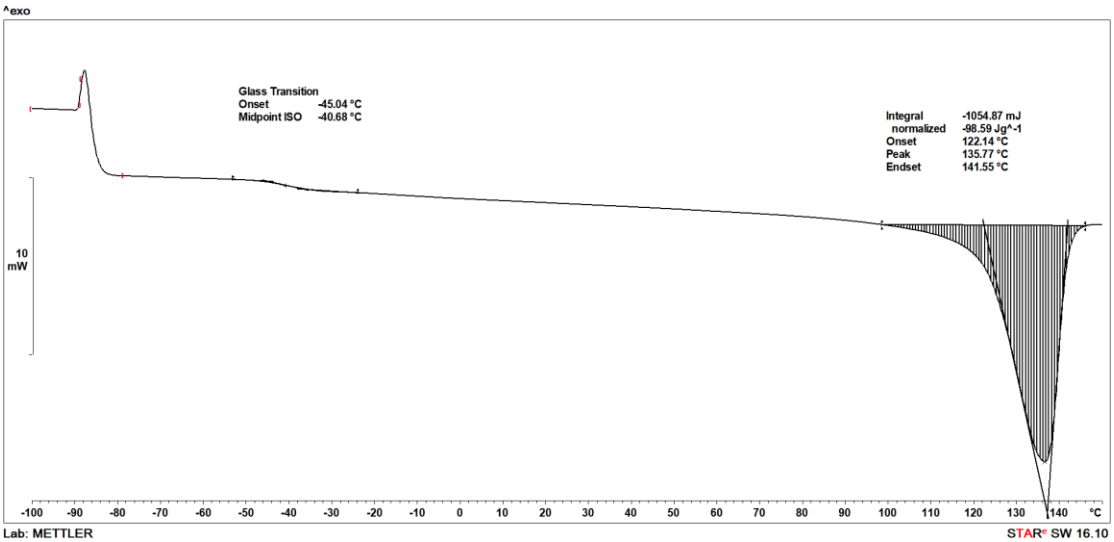


Figure S92. DSC curve of **2h′** (Table 2, entry 28).

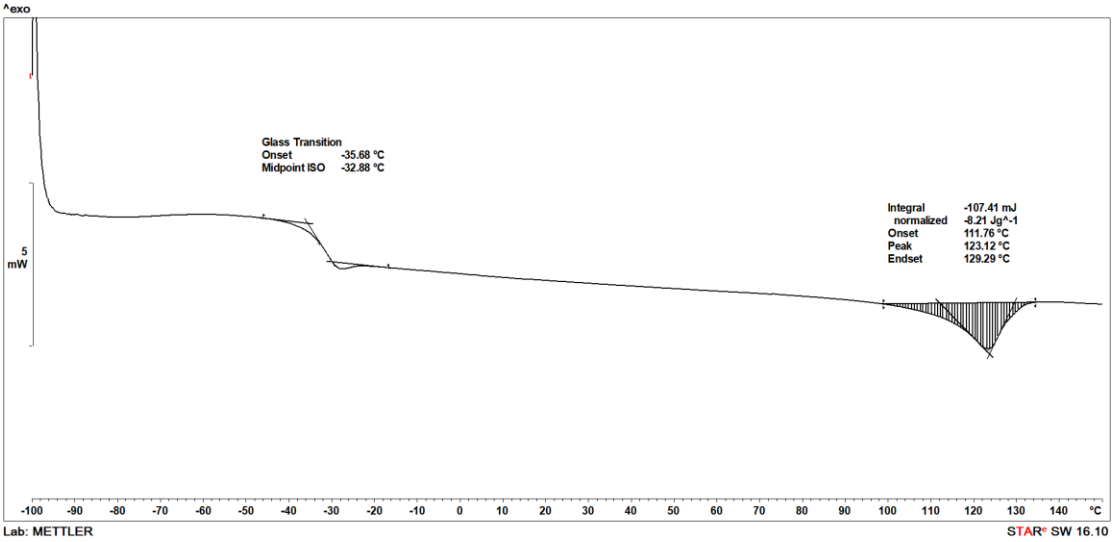


Figure S93. DSC curve of **2i′** (Table 2, entry 29).

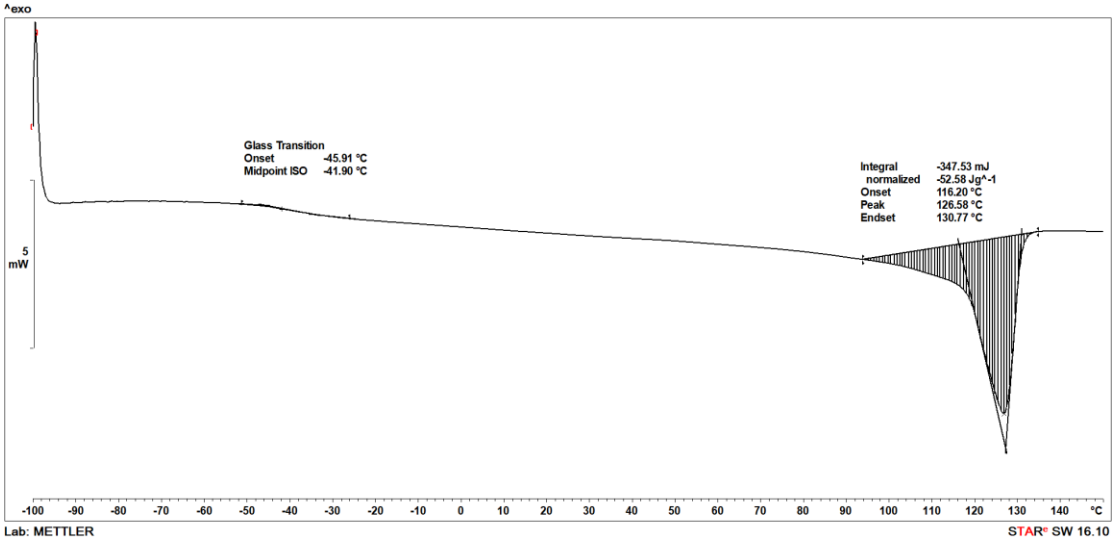


Figure S94. DSC curve of **2j′** (Table 2, entry 30).

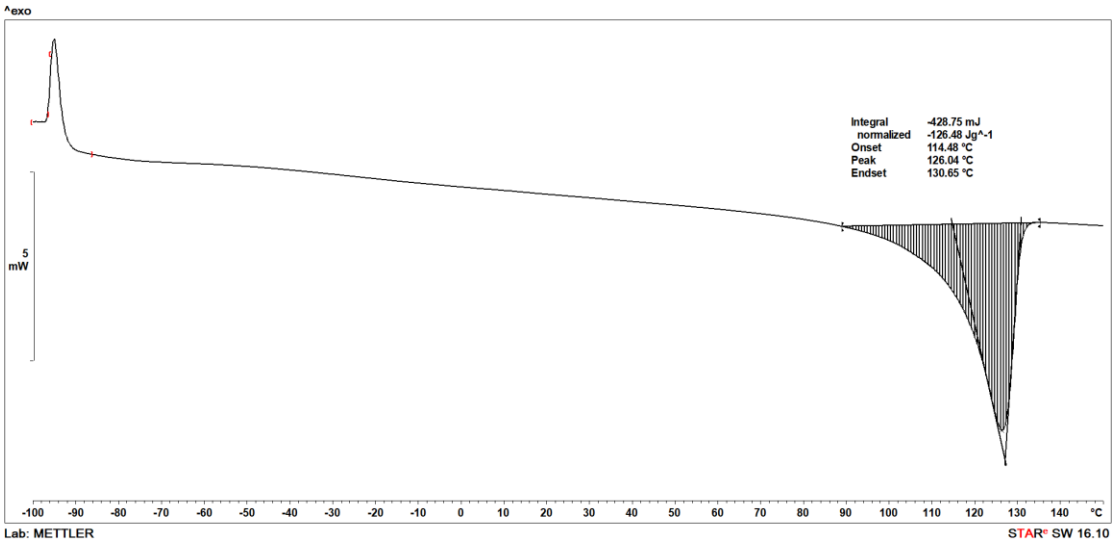


Figure S95. DSC curve of **2l′** (Table 2, entry 32).

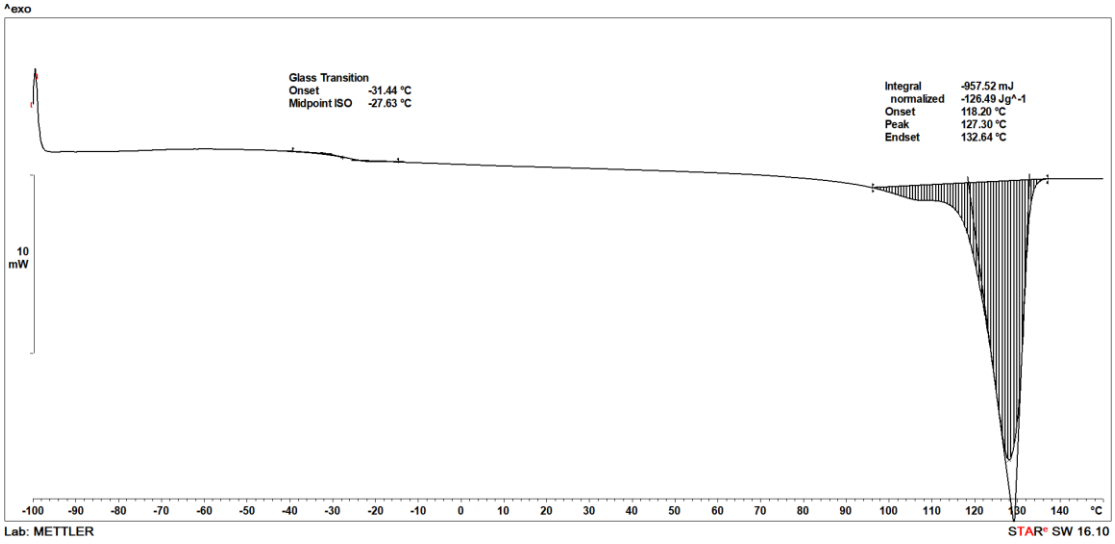


Figure S96. DSC curve of **2m′** (Table 2, entry 33).

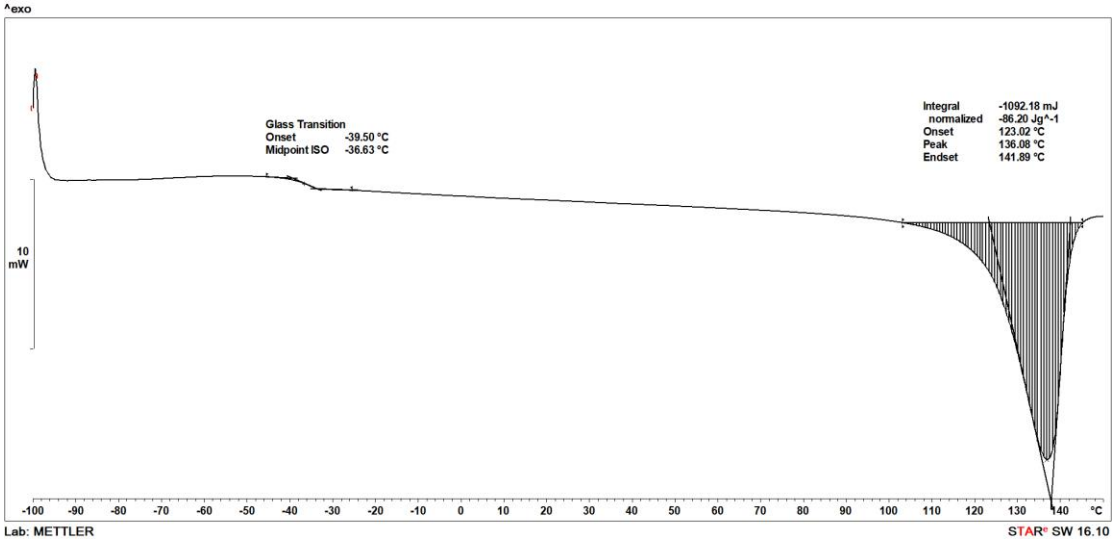


Figure S97. DSC curve of **2n′** (Table 2, entry 34).

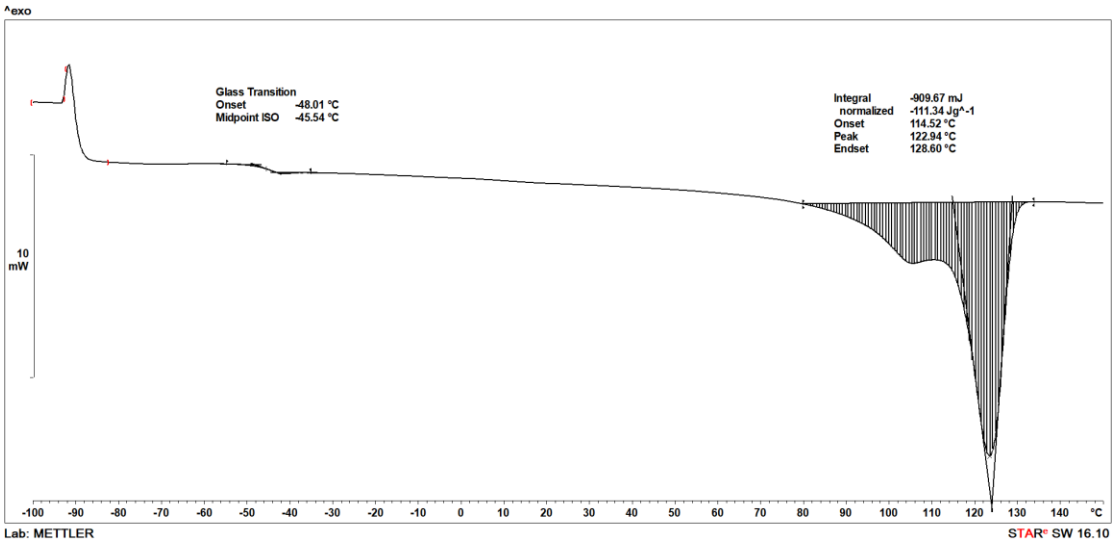


Figure S98. DSC curve of **2o′** (Table 2, entry 35).

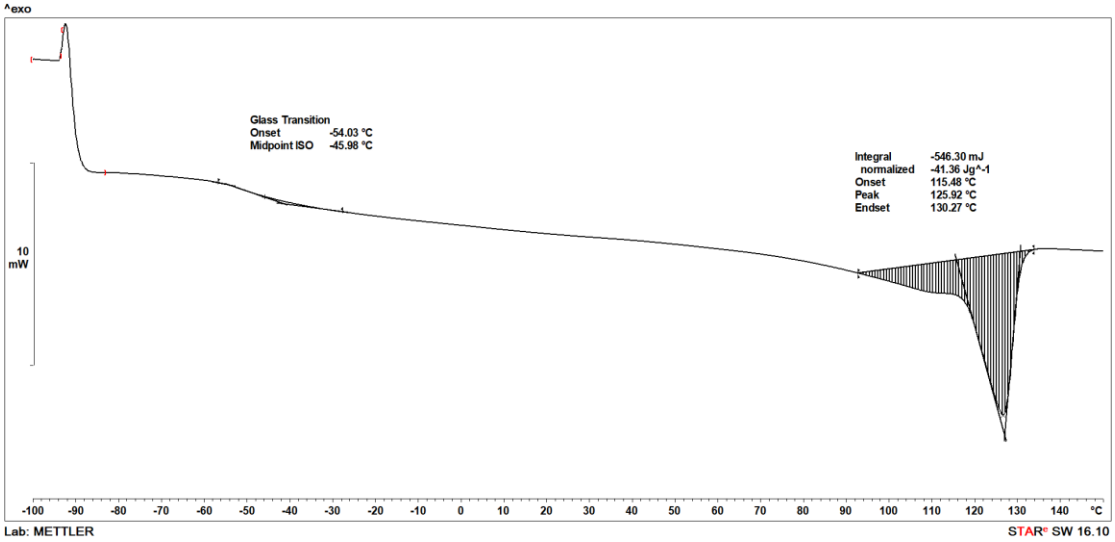


Figure S99. DSC curve of **2p′** (Table 2, entry 36).

GPC curves of copolymers

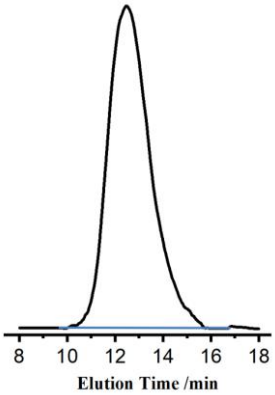


Figure S100. GPC curve of **2a** (Table 1, entry 1).

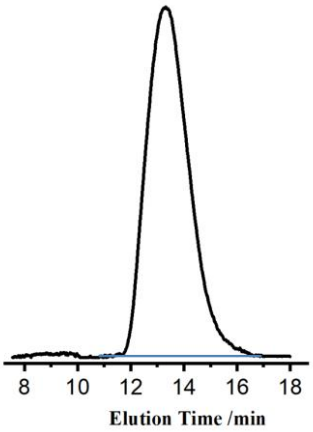


Figure S101. GPC curve of **2b** (Table 1, entry 2).

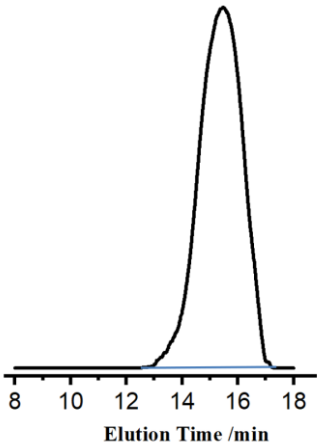


Figure S102. GPC curve of **2g** (Table 1, entry 7).

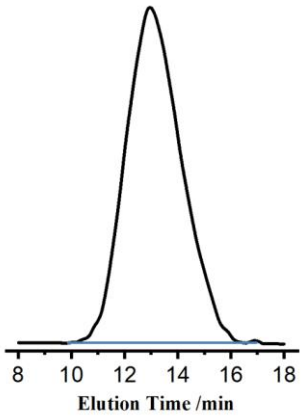


Figure S103. GPC curve of **2h** (Table 1, entry 8).

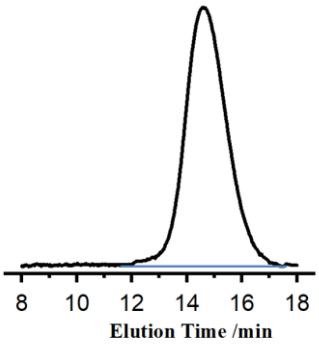


Figure S104. GPC curve of **2i** (Table 1, entry 9).

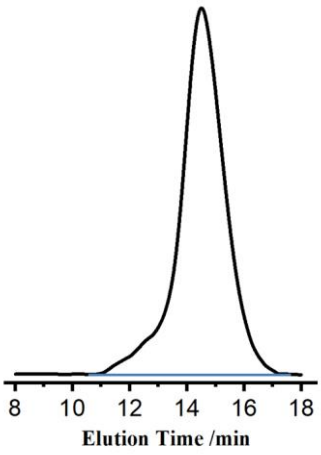


Figure S105. GPC curve of **2j** (Table 1, entry 10).

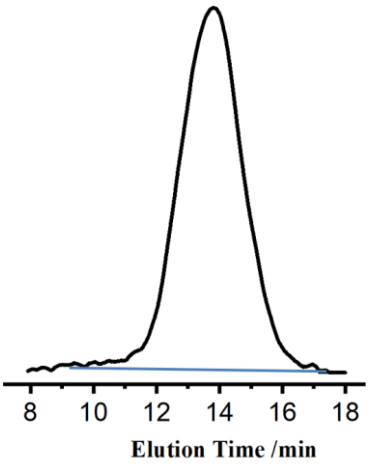


Figure S106. GPC curve of **2l** (Table 1, entry 12).

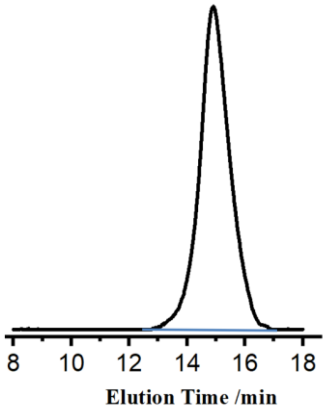


Figure S107. GPC curve of **2m** (Table 1, entry 13).

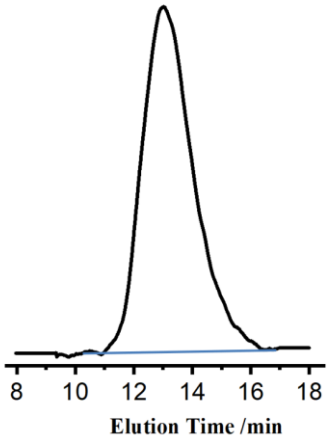


Figure S108. GPC curve of **2n** (Table 1, entry 14).

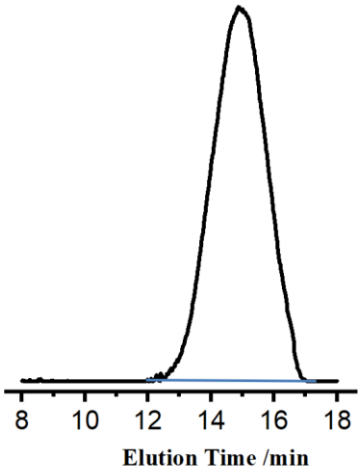


Figure S109. GPC curve of **2o** (Table 1, entry 15).

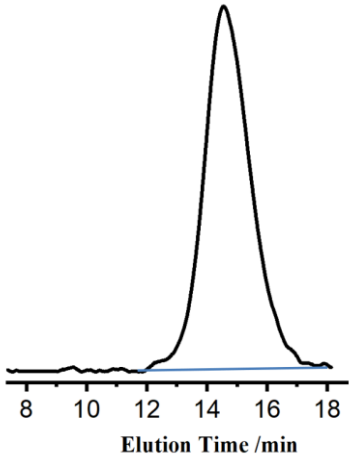


Figure S110. GPC curve of **2p** (Table 1, entry 16).

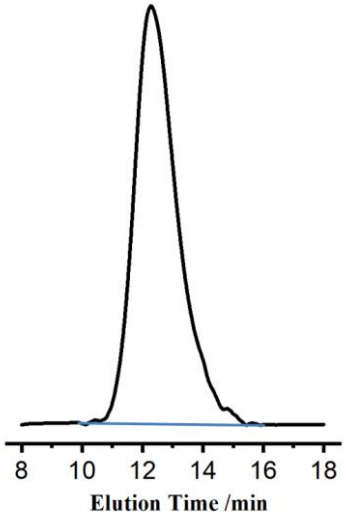


Figure S111. GPC curve of **2a′** (Table 2, entry 17).

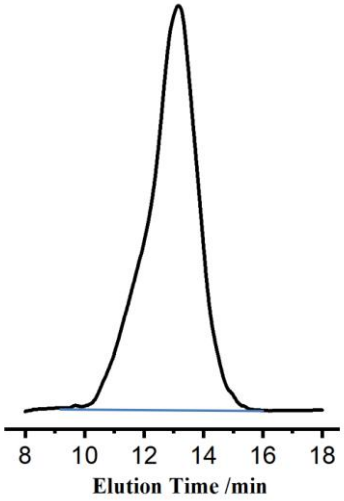


Figure S112. GPC curve of **2b′** (Table 2, entry 18).

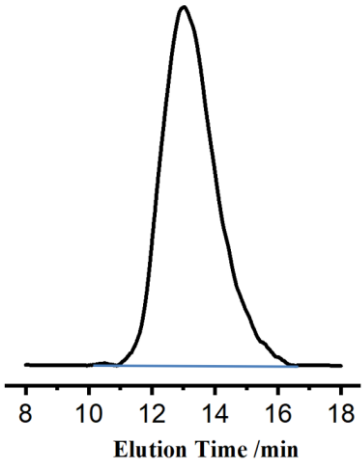


Figure S113. GPC curve of **2e′** (Table 2, entry 21).

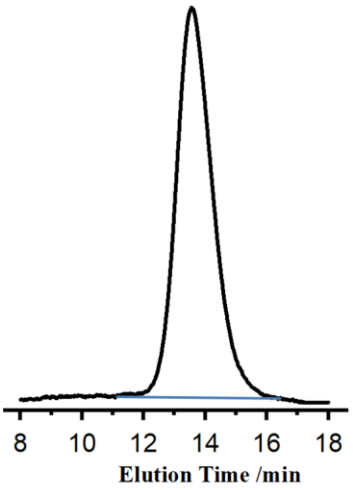


Figure S114. GPC curve of **2g′** (Table 2, entry 23).

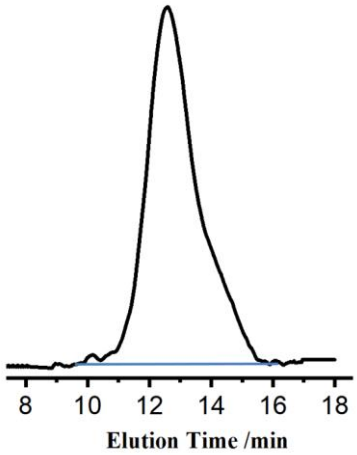


Figure S115. GPC curve of **2g′** (Table 2, entry 24).

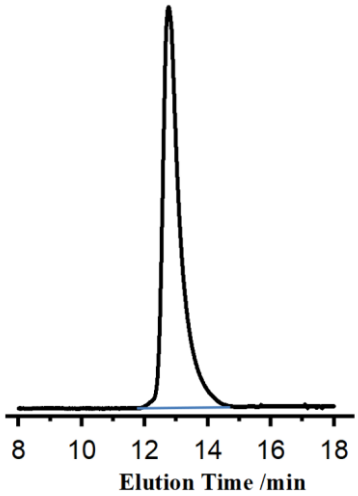


Figure S116. GPC curve of **2g′** (Table 2, entry 25).

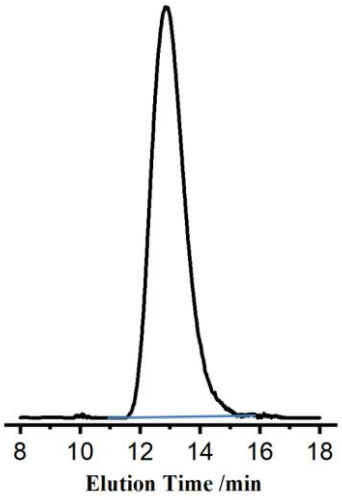


Figure S117. GPC curve of **2g′** (Table 2, entry 26).

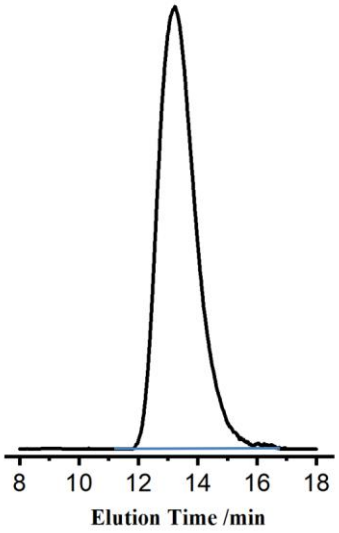


Figure S118. GPC curve of **2g′** (Table 2, entry 27).

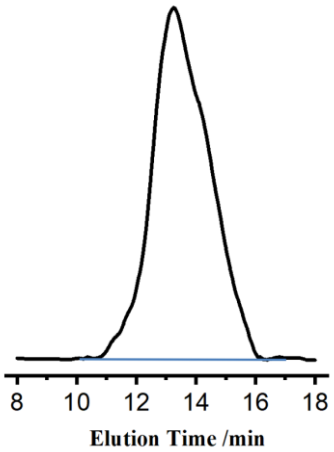


Figure S119. GPC curve of **2h′** (Table 2, entry 28).

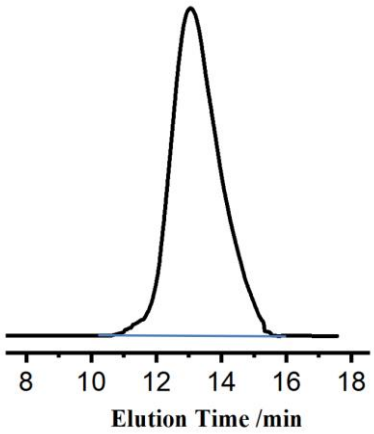


Figure S120. GPC curve of **2i′** (Table 2, entry 29).

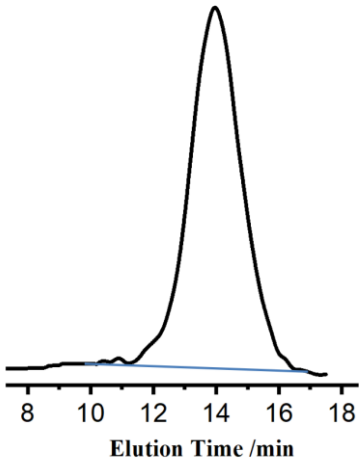


Figure S121. GPC curve of **2j′** (Table 2, entry 30).

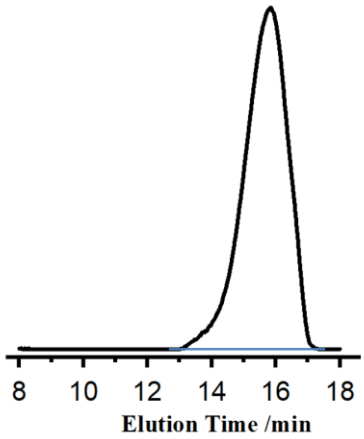


Figure S122. GPC curve of **2m′** (Table 2, entry 33).

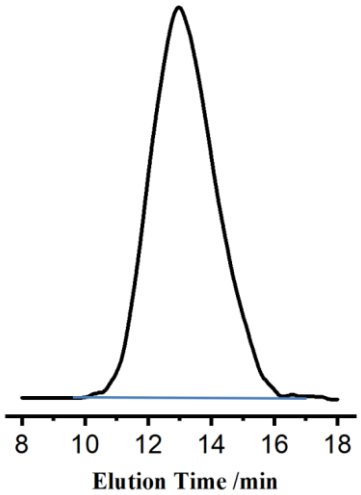


Figure S123. GPC curve of **2n′** (Table 2, entry 34).

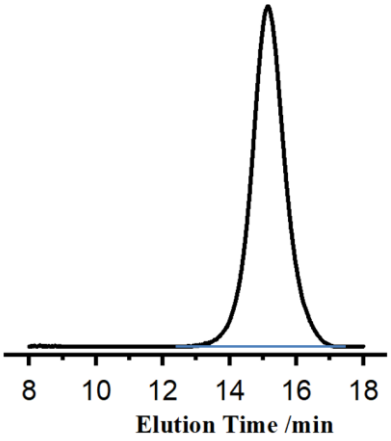


Figure S124. GPC curve of **2o′** (Table 2, entry 35).

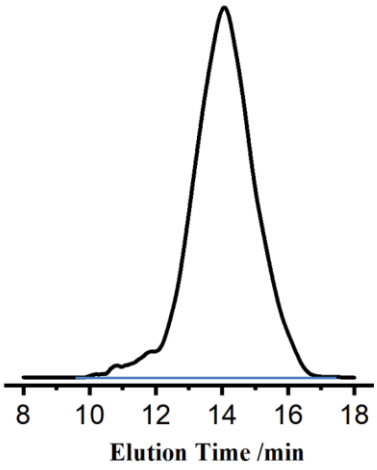
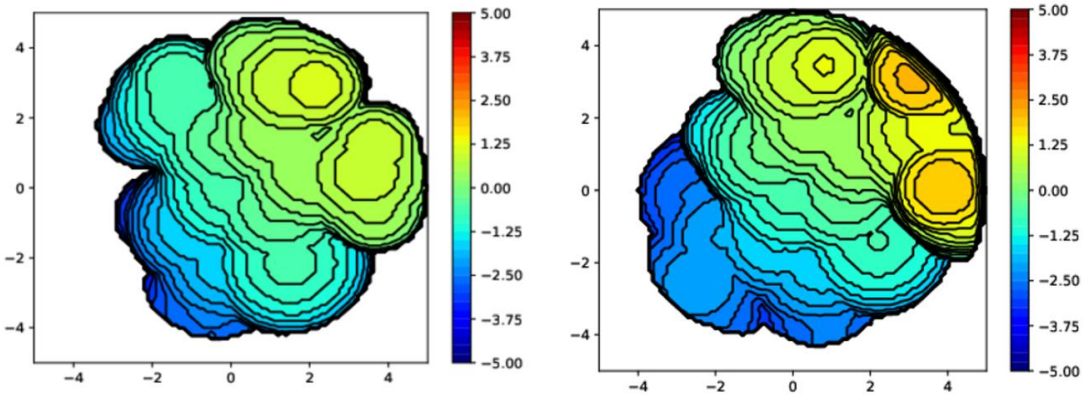


Figure S125. GPC curve of **2p′** (Table 2, entry 36).



Complex **1**: V_{buried} = 33.2% Complex **2**: V_{buried} = 36.5%

Figure S126. Topographical steric maps of **Sc-1** and **Sc-2.**

Table S2. The Buried Volume of **Sc-1** and **Sc-2** In the Different Sphere Radii.

Complex	Sphere radius	Buried volume (%)
Sc -1	3.5	38.9
	4	39.0
	4.5	37.3
	5	33.2
Sc -2	3.5	39.2
	4	39.8
	4.5	38.9
	5	36.5

Computational Procedures

All calculations were performed with Gaussian 16 program.[10] The B3PW91 hybrid exchange-correlation functional was utilized for geometry optimization.[11-13] The 6-31G* basis set was considered for C, H, and O, S, and F atoms, and the Si and Sc atoms were treated by the Stuttgart/Dresden effective core potential (ECP) and the associated basis sets.[14-15] The basis sets of Si were augmented with one d-polarization function (exponent of 0.284).[16] This basis set is denoted as "BSI". Meanwhile, harmonic vibration frequencies were carried out to characterize a minimum (N_{imag} = 0) or a transition state (N_{imag} = 1) and to provide thermodynamic data. The transition state structures are shown to connect the reactant and product on either side via intrinsic reaction coordinate (IRC) following. To obtain more reliable energy, the single-point calculations of optimized structures were carried out at the level of B3PW91-D3 (B3PW91 with Grimme's DFT-D3 correction)[17-18]/BSII, taking into account solvation effect of toluene with the SMD[19] solvation model. In the BSII, the 6-311+G(d,p) basis set was used for nonmetal atoms, while the basis sets together with associated pseudopotentials for Sc atom are the same as that in geometry optimization. Therefore, unless otherwise mentioned, the free energy (ΔG, 298.15 K, 1 atm) in solution, which was used for description of energy profiles, was obtained from the solvation single-point calculation and the gas-phase Gibbs free energy correction.[20]

Table S3. Relative energies for four possible insertion manners of polar monomer **1g**.

Insertion manners	**C1$_{1g}$**	**C1'$_{1g}$**	**TS1$_{1g}$**	**P1$_{1g}$**	**$\Delta G^{‡}$**
1,2-*si*[a]	******	**	**	**	**
1,2-*re*	******	-19.5	-6.8	-27.9	12.7
2,1-*si*	-17.1	-20.3	-9.2	-31.9	11.1
2,1-*re*	******	-20.3	2.4	-26.9	22.7

[a] 1,2-*si* pathway was not located.

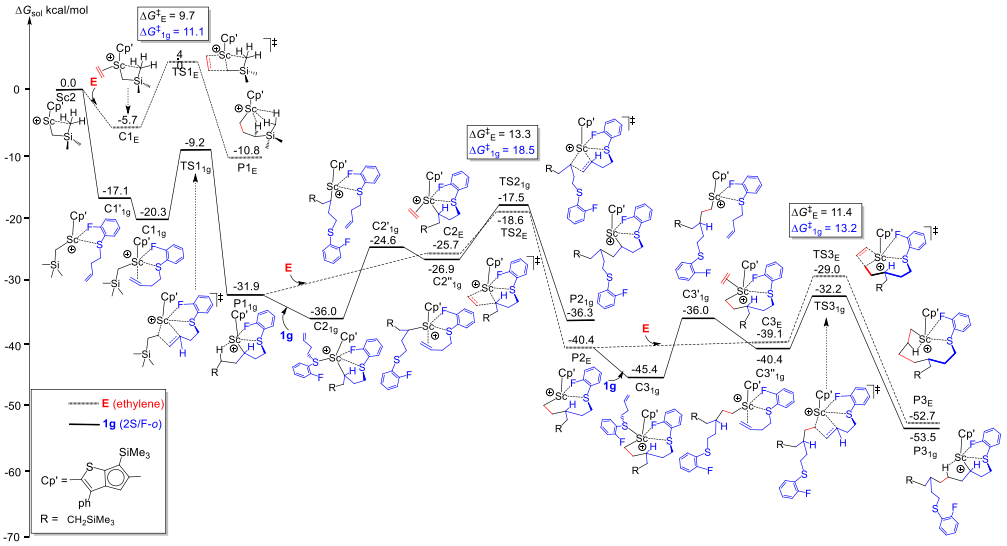


Figure S127. DFT-optimized energy profiles for copolymerization of ethylene (**E**, dashed line) and polar monomer **1g** (plain line).

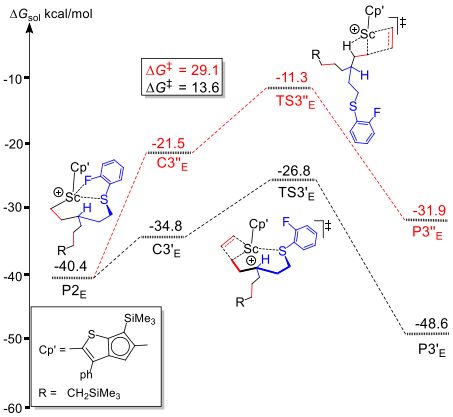


Figure S128. Energy profiles for other two insertion styles of ethylene, viz., stationary (just S-atom coordination, black line) and migratory (red line) insertions.

Table S4. The distances (D, Å) and Wiberg Bond Index (WBI) of Sc···S and Sc···F interactions in key intermediates and transition states.

Complexes	D_{Sc-F}	D_{Sc-S1}	D_{Sc-S2}	WBI_{Sc-F}	WBI_{Sc-S1}	WBI_{Sc-S2}
$C1_{1g}$	2.368	2.842		0.182	0.448	
$TS1_{1g}$	2.353	2.790		0.226	0.496	
$P1_{1g}$	2.298	2.737		0.222	0.490	
$C2_E$	2.339	2.752		0.197	0.466	
$TS2_E$	2.371	2.825		0.239	0.488	
$P2_E$	2.288	2.762		0.203	0.476	
$C3_{1g}$	2.377	2.913	2.850	0.169	0.416	0.430
$TS3_{1g}$	2.341	2.765		0.232	0.508	
$P3_{1g}$	2.263	2.718		0.234	0.494	

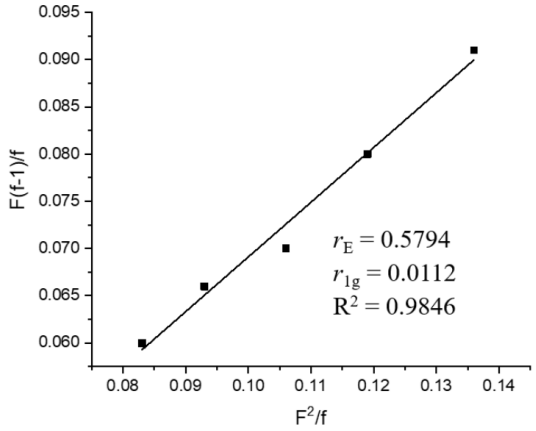
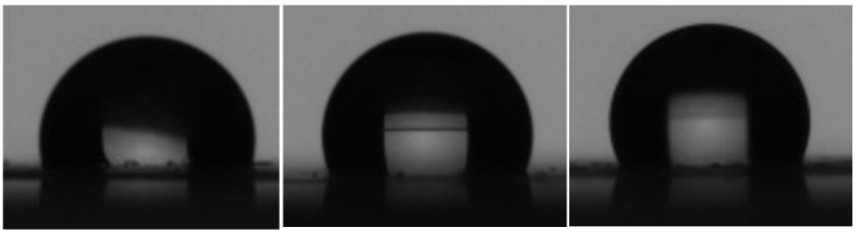


Figure S129. Fineman-Ross plot for copolymerization of ethylene and **1g** (2S/F-*o*).



(a) 101.0° (b) 102.3° (c) 107.9°

Figure S130. WCA of copolymers. (a) **2b′** (f_M = 8.8 mol%, table 2, entry 18); (b) **2g′** (f_M = 17.2 mol%, table 2, entry 23); (c) **2g′** (f_M = 44.9 mol%, table 2, entry 27).

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Cartesian coordinates for all of the calculated structures

58

Sc2, Esol(SCF Done) = -1310.408741 a.u.

Sc	-0.23064900	0.64251600	-0.13151300
S	-0.25962900	-1.27935300	-2.06195200
Si	-0.71134100	3.50911300	-0.02936900
C	-1.78200500	2.07380700	-0.60776000
H	-2.00057600	2.14946800	-1.68247500
H	-2.73183500	2.03584400	-0.06450200
C	-1.32989800	4.33925900	1.54718400
H	-2.25687200	4.88496500	1.33831200
H	-0.59938600	5.05463900	1.94069100
H	-1.54738700	3.60568600	2.33190100
C	-0.22097000	4.72741500	-1.38443700
H	0.18254700	4.21258700	-2.26398900
H	0.52865900	5.44496100	-1.03292700
H	-1.10285000	5.29134000	-1.70825500
C	1.01288400	2.65835400	0.49146800
H	1.03097100	1.94649400	1.34438600
H	1.61330100	3.49286500	0.87078800
H	1.63220900	2.24557100	-0.32794900
C	-1.66515800	-1.24344100	0.46970200
C	-1.09289100	-0.90033000	1.74161200
C	0.32538300	-0.95203200	1.67666500
C	0.69161700	-1.39677900	0.37452600
C	-0.53077300	-1.57365900	-0.34691100
C	1.84284900	-1.12347800	-0.46571400
C	1.48584300	-1.01679300	-1.79777400
C	-1.84847900	-0.56495300	2.99272700

H	-2.68071400	0.11753000	2.80199000
H	-1.19108100	-0.11003800	3.74020200
H	-2.26814400	-1.47506900	3.43942200
C	2.35469500	-0.88523100	-3.00899700
H	3.40737800	-0.97439600	-2.73071100
H	2.21379600	0.07194000	-3.52533000
H	2.12631500	-1.67868100	-3.72999500
Si	-3.49733900	-1.57550800	0.00584300
C	-4.69104800	-0.42376300	0.91359800
H	-5.69585600	-0.57602300	0.50123200
H	-4.74696500	-0.63929200	1.98515700
H	-4.44079000	0.63377100	0.78120200
C	-3.84380900	-3.37344500	0.48248900
H	-4.87082400	-3.64555900	0.21195400
H	-3.16627400	-4.06096800	-0.03563500
H	-3.72919200	-3.53431400	1.56012300
C	-3.69113900	-1.35192500	-1.86341800
H	-3.10235500	-2.07620200	-2.43793700
H	-4.74192400	-1.51594100	-2.13113000
H	-3.42319300	-0.34099200	-2.18931900
C	3.20200800	-0.95923800	0.08803500
C	3.63020700	-1.82622600	1.10661400
C	4.07770800	0.04198800	-0.36207600
C	4.90700900	-1.70396600	1.64676000
H	2.96655000	-2.61315100	1.45553200
C	5.35212000	0.16508700	0.18560100
H	3.75850800	0.73900300	-1.13313500
C	5.77069600	-0.70906300	1.18831100
H	5.22955000	-2.39027300	2.42456200
H	6.01769100	0.94669600	-0.16980400

H	6.76615800	-0.61388400	1.61243500
H	1.00070800	-0.73176200	2.49633000

6

E, ethylene, Esol(SCF Done) = -78.585701 a.u.

C	0.00000000	0.00000000	0.66524000
C	0.00000000	0.00000000	-0.66524000
H	0.00000000	-0.92428600	1.23866200
H	0.00000000	-0.92428600	-1.23866200
H	0.00000000	0.92428600	1.23866200
H	0.00000000	0.92428600	-1.23866200

23

1g, Esol(SCF Done) = -885.665283 a.u.

C	-1.65832200	0.89397400	-0.18395300
C	-2.89860600	1.20676600	0.35429500
C	-3.72198600	0.17595200	0.80316100
C	-3.29299100	-1.14783700	0.71635600
C	-2.03523500	-1.43885900	0.19192400
C	-1.19013600	-0.42177000	-0.27052100
H	-3.20425200	2.24743800	0.40203300
H	-4.69713900	0.41162000	1.22043100
H	-3.93128400	-1.95421800	1.06639000
H	-1.68633700	-2.46602200	0.13453100
S	0.36513800	-0.82858800	-1.02303600
C	1.55436300	0.05428500	0.06033200
H	1.42492000	-0.29391900	1.08987500
H	1.33922300	1.12577000	0.02230400
C	2.97947200	-0.22964900	-0.42472000
H	3.06195900	0.07322600	-1.47886800
H	3.18026500	-1.30714000	-0.38301900
C	3.99298900	0.51494000	0.39573800

H	3.92011700	1.60379200	0.36937800
C	4.94177500	-0.05493800	1.13879500
H	5.05079900	-1.13667000	1.19487900
H	5.64906100	0.53662000	1.71450500
F	-0.88638600	1.89997100	-0.63025600

64

C1$_E$, Esol(SCF Done) = -1389.021399 a.u.

Sc	0.47680800	0.84026800	0.46921800
S	0.52860300	-2.60954700	1.16343300
Si	-0.43054400	3.60693900	0.19189700
C	1.26110500	2.79361100	0.05182500
H	1.90596600	3.10574600	0.89038100
H	1.77115100	3.03828600	-0.88359500
C	-1.13749500	4.17182700	-1.46230600
H	-0.55408400	5.01503900	-1.84882500
H	-2.17758000	4.50105400	-1.36128900
H	-1.10442500	3.37230900	-2.21046100
C	-0.57179500	4.92336000	1.53893800
H	-0.20261300	4.56024400	2.50501600
H	-1.60800800	5.25399600	1.67191900
H	0.02904600	5.79750000	1.26422000
C	-1.61724100	2.14988500	0.81515700
H	-1.80187200	1.27383100	0.16171900
H	-2.60882700	2.61662900	0.84962600
H	-1.44867300	1.80315300	1.85016500
C	1.83893600	-0.74953500	-0.75438700
C	1.19852400	0.09190800	-1.73518400
C	-0.21235300	-0.05453500	-1.64465700
C	-0.49306600	-1.05754100	-0.66668100
C	0.76023600	-1.47015000	-0.14059200

C	-1.63295800	-1.64212700	0.01072100
C	-1.22911800	-2.50811700	1.00264300
C	1.88682800	0.92791300	-2.77185800
H	2.83305800	1.34123800	-2.41288900
H	1.25431000	1.76023000	-3.09611800
H	2.10465200	0.32058300	-3.65933800
C	-2.06054400	-3.40948200	1.85974500
H	-3.07597700	-3.47650200	1.46069400
H	-2.12683100	-3.05494900	2.89633500
H	-1.63980200	-4.42074200	1.88910500
Si	3.71787800	-1.09708400	-0.59790700
C	4.65439800	0.45507500	-0.04351500
H	5.73071200	0.24558600	-0.03021400
H	4.49246100	1.30355800	-0.71628000
H	4.37221100	0.77017000	0.96753500
C	4.35155000	-1.68168100	-2.28010800
H	5.40136700	-1.98572800	-2.19300500
H	3.78087400	-2.54577800	-2.63735500
H	4.29640800	-0.89751100	-3.04159800
C	3.96897400	-2.48070800	0.67033900
H	3.44689500	-3.39821400	0.37748400
H	5.03820400	-2.71836500	0.72436900
H	3.65027100	-2.21638300	1.68519500
C	-3.03177400	-1.35989300	-0.37568400
C	-3.39484600	-1.35384700	-1.73257700
C	-4.01678300	-1.07987000	0.58474300
C	-4.70653400	-1.08485300	-2.11441800
H	-2.65003600	-1.59183700	-2.48783200
C	-5.32882000	-0.81122800	0.19997600
H	-3.75099300	-1.06169400	1.63889400

C	-5.67727200	-0.81278400	-1.15004700
H	-4.97351200	-1.09769800	-3.16762000
H	-6.07916900	-0.59850600	0.95666400
H	-6.70076900	-0.60554300	-1.44951100
H	-0.93604400	0.46305200	-2.26525900
C	1.88251900	0.47777500	2.89072400
C	0.60951100	0.57107100	3.30670300
H	2.30672500	-0.47781700	2.58753700
H	-0.03491700	-0.30634300	3.35528300
H	0.20368400	1.50766600	3.68584000
H	2.55095600	1.33643900	2.90185000

64

TS1$_E$, Esol(SCF Done) = -1389.010936 a.u. i200

Sc	-0.49359900	0.92437000	-0.30878300
S	-0.51653500	-2.54727200	-1.41868100
Si	0.61935500	3.61597000	-0.12222800
C	-1.18014100	2.95828600	-0.11105400
H	-1.86222300	3.79768500	-0.26083000
H	-1.50928300	2.49169900	0.84951400
C	1.22707500	4.25478600	1.54308300
H	0.60885000	5.09524800	1.87756300
H	2.26237200	4.60782000	1.47023000
H	1.18601500	3.47873800	2.31519400
C	0.78020100	4.89567800	-1.49539200
H	0.51244400	4.49530400	-2.47895700
H	1.81221000	5.25961600	-1.55252200
H	0.13526300	5.75791200	-1.29281100
C	1.72272200	2.10002400	-0.63656900
H	1.82894200	1.24295900	0.05410100
H	2.74580400	2.49388400	-0.66965100

H	1.53881300	1.73243000	-1.66096300
C	-1.83639700	-0.87144000	0.66070200
C	-1.20019700	-0.16330900	1.74401100
C	0.21224600	-0.29286300	1.64424400
C	0.49763500	-1.15145300	0.53809100
C	-0.75368300	-1.49190300	-0.04863700
C	1.63853900	-1.69312800	-0.16893300
C	1.23335700	-2.47776100	-1.22670500
C	-1.89511200	0.54351500	2.87486000
H	-2.85087700	0.98310400	2.57450800
H	-1.27117200	1.33821300	3.29860800
H	-2.10520100	-0.16402500	3.68651800
C	2.06929800	-3.30209600	-2.15401900
H	3.07682400	-3.42389500	-1.74782200
H	2.15595600	-2.84393300	-3.14744500
H	1.63568600	-4.29857700	-2.29274900
Si	-3.70749200	-1.24052200	0.46944300
C	-4.70049000	0.34748200	0.16464800
H	-5.77087000	0.10903500	0.16798100
H	-4.53699500	1.11183700	0.93211900
H	-4.47230900	0.78546400	-0.81361400
C	-4.29858300	-2.08296300	2.05581800
H	-5.34188000	-2.39952300	1.93989200
H	-3.70049200	-2.97445300	2.27390600
H	-4.24947300	-1.41870600	2.92462500
C	-3.94728000	-2.41280200	-0.99511500
H	-3.42282700	-3.36272800	-0.84534700
H	-5.01519100	-2.64238300	-1.09278900
H	-3.62039700	-1.98803700	-1.95100500
C	3.03713100	-1.45311800	0.24646300

C	3.39839300	-1.56712100	1.59919200
C	4.02591300	-1.09363800	-0.68336900
C	4.70979500	-1.33505200	2.00613200
H	2.65247500	-1.87182700	2.32903600
C	5.33804300	-0.86366500	-0.27412300
H	3.76226400	-0.98523700	-1.73261900
C	5.68362500	-0.98251100	1.07146300
H	4.97455300	-1.44166100	3.05466300
H	6.09113000	-0.59039900	-1.00845000
H	6.70719500	-0.80584600	1.38984500
H	0.93054100	0.13047600	2.33887600
C	-1.90836600	2.09728700	-2.11931600
C	-1.49518400	0.79735300	-2.38524600
H	-2.92644100	2.29114000	-1.79675700
H	-2.19658700	-0.02701100	-2.28714400
H	-0.64400900	0.62189900	-3.04683200
H	-1.40827900	2.94457000	-2.57790500

64

P1$_E$, Esol(SCF Done) = -1389.037343 a.u.

Sc	-0.28019400	0.61760900	-0.27242000
S	-0.59974000	-1.64923400	-1.96211100
Si	1.01082100	3.51332400	-0.01602300
C	-0.63004500	2.95916500	0.82782400
H	-0.79672900	3.74519000	1.57798200
H	-0.49096100	2.07810200	1.49675900
C	2.26854400	3.94847100	1.31752100
H	1.91209600	4.78978900	1.92245800
H	3.22493500	4.24308800	0.87116700
H	2.45815400	3.10617100	1.99264200
C	0.66664500	4.92645000	-1.20957800

H	-0.02313100	4.63082000	-2.00725000
H	1.59631700	5.27157300	-1.67562000
H	0.22474500	5.77812900	-0.68033100
C	1.75553200	2.04200100	-1.02888800
H	2.10167200	1.17315400	-0.44036800
H	2.68457700	2.43417400	-1.46160800
H	1.17828000	1.71107600	-1.91015600
C	-1.95750200	-0.98091900	0.53371500
C	-1.32148000	-0.57146700	1.75492800
C	0.07462700	-0.83188100	1.70224300
C	0.35208400	-1.48054500	0.46617200
C	-0.89024400	-1.55598600	-0.23302500
C	1.51902700	-1.62547600	-0.38630300
C	1.15945000	-1.73634800	-1.71488700
C	-2.01202900	-0.00428600	2.96036000
H	-2.76099800	0.74711700	2.69433800
H	-1.29519000	0.45225400	3.65062000
H	-2.53012300	-0.79863200	3.51209200
C	2.01143000	-2.02588800	-2.91004300
H	2.99186900	-2.39295800	-2.59582800
H	2.16405100	-1.14005400	-3.53955700
H	1.54689600	-2.79301800	-3.53925500
Si	-3.82250600	-1.21924300	0.17165900
C	-4.87960400	0.27066600	0.66579500
H	-5.92097900	0.05690700	0.39556600
H	-4.86166400	0.46108300	1.74367700
H	-4.58888700	1.18769300	0.14395800
C	-4.36183200	-2.73416400	1.17137700
H	-5.41466400	-2.96533800	0.97096000
H	-3.76786900	-3.61571900	0.90623100

H	-4.25836800	-2.56914400	2.24954100
C	-4.03409300	-1.57434500	-1.67528500
H	-3.52358800	-2.49607800	-1.97668700
H	-5.10021700	-1.71504500	-1.89006600
H	-3.67820400	-0.75505200	-2.30917000
C	2.89321500	-1.66437800	0.15318700
C	3.13458000	-2.33977100	1.36160200
C	3.97224700	-1.04284100	-0.49702900
C	4.41848300	-2.40160900	1.89461700
H	2.31392100	-2.84130500	1.86776200
C	5.25560300	-1.10335000	0.04161800
H	3.80818400	-0.49962900	-1.42393100
C	5.48258300	-1.78360800	1.23715400
H	4.58982300	-2.93993400	2.82258400
H	6.07915600	-0.61733100	-0.47422200
H	6.48429600	-1.83309700	1.65441600
H	0.78443600	-0.61435900	2.49327600
C	-1.91312400	2.84579600	-0.05357200
C	-1.83682400	1.78500100	-1.16662200
H	-2.75465200	2.61748700	0.61060600
H	-2.82351300	1.42342700	-1.45883700
H	-1.36727600	2.20873300	-2.07401500
H	-2.10652800	3.84741200	-0.46132900

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C1'$_{1g}$, Esol(SCF Done) = -2196.119404 a.u.

Sc	-0.65556000	0.18975300	-0.02531200
S	-1.38411400	-3.07607200	-1.28000000
Si	-1.27362800	2.03659400	-3.13115200
C	-1.18963900	0.44208600	-2.09684400
H	-0.61973700	-0.29444600	-2.69104100

H	-2.22113700	0.03794300	-2.08342800
C	-1.51390100	3.58597500	-2.04724000
H	-2.41113900	3.50869200	-1.42073000
H	-1.63625500	4.47375300	-2.67906400
H	-0.65519600	3.77247600	-1.38972000
C	-2.72850800	1.94883200	-4.34603700
H	-2.63356800	1.08105800	-5.00873700
H	-2.77608400	2.84759200	-4.97229900
H	-3.68507400	1.86162800	-3.81692600
C	0.33950300	2.23569600	-4.11405100
H	1.21530500	2.29679400	-3.45780200
H	0.31566000	3.14913400	-4.71947000
H	0.49056900	1.38961700	-4.79441100
C	-2.32732800	-1.27121600	0.89169600
C	-1.56958300	-0.81151800	2.03322700
C	-0.22659100	-1.24684500	1.93053000
C	-0.11216500	-2.05129000	0.75443500
C	-1.40045800	-2.08058400	0.15043800
C	0.89388100	-2.77634700	0.00620100
C	0.33563700	-3.39017500	-1.09575500
C	-2.11316600	-0.02875500	3.19464500
H	-2.87769800	0.69472500	2.89482400
H	-1.31874400	0.50949600	3.72230800
H	-2.57919700	-0.70634500	3.92068700
C	0.98288000	-4.30993500	-2.08271400
H	1.92241700	-4.69834600	-1.68072700
H	1.20209700	-3.80394100	-3.03156400
H	0.33241600	-5.16117500	-2.31142000
Si	-4.20751500	-1.08457100	0.58791000
C	-4.65106600	0.74852900	0.36311200

H	-5.72690900	0.84368000	0.17273500
H	-4.42647600	1.35124500	1.25029500
H	-4.13039500	1.18908500	-0.49562700
C	-5.13737900	-1.80357200	2.06980000
H	-6.21680800	-1.77738000	1.87927800
H	-4.85287800	-2.84746300	2.24137500
H	-4.95035500	-1.24378400	2.99196900
C	-4.66315800	-2.03465600	-0.98044200
H	-4.45447900	-3.10556400	-0.88208500
H	-5.73872700	-1.92711900	-1.16509300
H	-4.13966400	-1.66172200	-1.86768100
C	2.30460300	-2.89407900	0.43254200
C	2.61262700	-3.17571200	1.77336200
C	3.36172300	-2.73102900	-0.47649200
C	3.93619000	-3.29589700	2.18908800
H	1.80685800	-3.33321500	2.48587900
C	4.68585100	-2.85444800	-0.05926400
H	3.14416200	-2.49829300	-1.51581200
C	4.97751100	-3.13596400	1.27483800
H	4.15453900	-3.52854200	3.22799400
H	5.49066900	-2.73304900	-0.77969100
H	6.00959900	-3.23668900	1.59911800
H	0.55929100	-1.04154400	2.64900300
C	-0.10442500	2.77286800	1.88109200
C	-0.61469200	3.74046200	2.72113500
C	0.26817500	4.33481300	3.62353800
C	1.60701600	3.94313800	3.66437700
C	2.08079300	2.95735900	2.80170700
C	1.22135000	2.35618700	1.87327600
H	-1.66174600	4.01941900	2.66702000

H	-0.09863500	5.10187800	4.29847700
H	2.28558600	4.40308000	4.37593400
H	3.11948400	2.64201200	2.84162100
C	2.64667200	2.12355000	-0.54858400
H	3.32924400	2.78843500	-0.01145600
H	1.90032300	2.72905600	-1.07055200
C	3.42099600	1.21073600	-1.50265800
H	2.71540000	0.56061400	-2.03965300
H	4.09260300	0.56089700	-0.92984400
C	4.21085000	2.03301400	-2.48412100
H	3.63386200	2.62145600	-3.19778000
C	5.54240900	2.07815300	-2.52011000
H	6.15645000	1.50118600	-1.83097800
H	6.06992200	2.68667400	-3.24924800
F	-0.98489200	2.17121400	0.98318900
S	1.80733800	1.10148900	0.74963900

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C1$_{1g}$, Esol(SCF Done) = -2196.132614 a.u.

Sc	0.57372100	-0.16565100	0.02355400
S	-1.44489900	-3.03704500	1.28736400
Si	4.02533500	0.72341100	1.09640300
C	2.67661700	-0.46809400	0.47464600
H	2.71668600	-1.36035300	1.12286100
H	3.05456400	-0.82340000	-0.50160800
C	5.08886700	1.26997800	-0.38006900
H	5.59431000	0.40881300	-0.83236500
H	5.86077100	1.98277900	-0.06780800
H	4.48829200	1.74951300	-1.16151400
C	5.12993400	-0.16074500	2.36297200
H	4.55702800	-0.49333200	3.23746400

H	5.92683900	0.50078400	2.72278800
H	5.60242700	-1.04498900	1.92013500
C	3.35586400	2.29846200	1.94388300
H	2.65486500	2.85256500	1.30747500
H	4.18833800	2.97492500	2.17283100
H	2.86017800	2.07846500	2.89742600
C	0.40915800	-2.39481500	-0.93729800
C	0.20064800	-1.44013300	-1.99698100
C	-1.00455700	-0.72062000	-1.77392400
C	-1.62871700	-1.25078100	-0.60700900
C	-0.74779800	-2.24494800	-0.10332200
C	-2.85364900	-1.12130300	0.15946400
C	-2.89537500	-2.03974400	1.18537300
C	1.08593700	-1.23090800	-3.19432500
H	2.14627200	-1.16698900	-2.93122500
H	0.80992000	-0.31750400	-3.73053200
H	0.97728500	-2.06504600	-3.89866200
C	-4.00590100	-2.33741300	2.14506600
H	-4.95034100	-1.93617400	1.76777300
H	-3.82803200	-1.90738600	3.13937700
H	-4.12739200	-3.41791200	2.27829800
Si	1.57062700	-3.91439600	-0.88796400
C	3.21045000	-3.63550400	-1.78926700
H	3.81205600	-4.54753200	-1.69154900
H	3.07344900	-3.45125500	-2.85931100
H	3.79274800	-2.81243600	-1.36319100
C	0.61296700	-5.30782900	-1.74242100
H	1.19514600	-6.23675700	-1.72705400
H	-0.34205200	-5.50127000	-1.24163000
H	0.40043400	-5.06273700	-2.78898900

C	1.91415000	-4.40131200	0.91062400
H	0.99876200	-4.63299600	1.46608400
H	2.53186100	-5.30751300	0.91934000
H	2.46372400	-3.62584400	1.45461300
C	-3.93845200	-0.17652200	-0.18148000
C	-4.32196300	0.00475300	-1.52042500
C	-4.61238600	0.55808000	0.80831100
C	-5.34330700	0.88935200	-1.85553400
H	-3.83623900	-0.57681500	-2.29926400
C	-5.63556100	1.44285200	0.47169600
H	-4.33465700	0.43362500	1.85249500
C	-6.00278400	1.61342300	-0.86209100
H	-5.63357600	1.00505700	-2.89635700
H	-6.14883100	1.99625400	1.25385200
H	-6.80255600	2.29990900	-1.12542700
H	-1.39349700	0.05802000	-2.42082900
C	1.18881100	2.92188900	-1.27013300
C	2.10419000	3.76580500	-1.86696600
C	1.89662900	5.13838000	-1.73613100
C	0.79014900	5.61927200	-1.03451200
C	-0.12537500	4.73767500	-0.46506800
C	0.07514600	3.35604600	-0.56217200
H	2.95121000	3.35920800	-2.40881400
H	2.59935600	5.82950600	-2.19079500
H	0.62667300	6.68878700	-0.94564600
H	-1.00508700	5.12261300	0.04235400
C	-1.45638000	2.61301900	1.74846000
H	-2.49842100	2.30296200	1.87779500
H	-1.42562000	3.70281400	1.82283400
C	-0.54487900	1.94519000	2.77055000

H	-0.92901500	2.19811200	3.77111400
H	0.46952400	2.35467200	2.71364400
C	-0.51978300	0.44737500	2.63867900
H	-1.47790600	-0.04652600	2.45782600
C	0.57454700	-0.31603400	2.81240200
H	1.54280000	0.11925900	3.04383900
H	0.50682700	-1.40173100	2.80932800
F	1.38211800	1.55618100	-1.38668700
S	-1.09028700	2.13802200	0.01141400

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TS1$_{1g}$, Esol(SCF Done) = -2196.118175 a.u.

Sc	0.41558300	0.02436300	-0.09212500
S	-1.12773600	-3.03975600	1.30912700
Si	4.04712500	0.45320300	1.47392300
C	2.46790500	-0.37209700	0.77035000
H	2.57906600	-1.45628700	0.88026800
H	2.52666700	-0.20206300	-0.33933600
C	5.43682000	0.26254700	0.19829100
H	5.65357000	-0.79227600	-0.00381800
H	6.35981900	0.72438300	0.56862200
H	5.18516000	0.74364700	-0.75441000
C	4.53923700	-0.42136500	3.08032600
H	3.78549600	-0.32720300	3.86984200
H	5.47163900	0.00692600	3.46627000
H	4.71447500	-1.48955600	2.90805800
C	3.77659300	2.30490900	1.80282500
H	3.46081600	2.83980600	0.89974300
H	4.71882000	2.75662500	2.13531200
H	3.03570000	2.49565600	2.58761000
C	0.42060200	-2.21887900	-1.08433700

C	0.01924500	-1.28070100	-2.10659800
C	-1.22769100	-0.69956900	-1.76580900
C	-1.67672800	-1.29002900	-0.54554300
C	-0.65958300	-2.19794000	-0.14546800
C	-2.83178400	-1.28925600	0.33204700
C	-2.67797600	-2.19690900	1.35422300
C	0.76305000	-0.97821100	-3.37941300
H	1.82855800	-0.78504600	-3.21580100
H	0.33403900	-0.10719000	-3.88542000
H	0.69412700	-1.82271300	-4.07650100
C	-3.64742600	-2.59328100	2.42444300
H	-4.65971800	-2.28251100	2.15230800
H	-3.40394400	-2.14342600	3.39551900
H	-3.65410900	-3.68001400	2.56306500
Si	1.72694300	-3.60260500	-1.23945900
C	3.36542100	-2.98370400	-1.96403800
H	4.09211000	-3.80482600	-1.93910400
H	3.26358800	-2.67501700	-3.00940200
H	3.79287500	-2.14973200	-1.39769100
C	0.98705600	-4.91033600	-2.39179100
H	1.67388900	-5.75800600	-2.50047600
H	0.03980000	-5.29240900	-1.99580600
H	0.79504400	-4.50567000	-3.39159800
C	2.03840900	-4.38716500	0.45772600
H	1.13695300	-4.86620600	0.85481600
H	2.79826500	-5.17059300	0.34913200
H	2.40624800	-3.67905300	1.20826200
C	-4.02956700	-0.45338500	0.10444000
C	-4.56393200	-0.32232700	-1.18809900
C	-4.66332400	0.22651600	1.15807900

C	-5.69363700	0.45868700	-1.41665800
H	-4.10774000	-0.86389300	-2.01245800
C	-5.79510000	1.00719200	0.92788000
H	-4.26527900	0.14295300	2.16657600
C	-6.31311800	1.12736600	-0.36063900
H	-6.09877100	0.53606300	-2.42211100
H	-6.27345700	1.52011200	1.75825100
H	-7.19713800	1.73282700	-0.54026700
H	-1.75866800	0.03197600	-2.36406200
C	1.18067200	3.11590000	-1.23028900
C	2.14703600	3.99752700	-1.67157700
C	1.85457400	5.35924200	-1.59506600
C	0.62311300	5.78908100	-1.09765100
C	-0.33331100	4.86589100	-0.68220000
C	-0.05851600	3.49362400	-0.73104100
H	3.09200400	3.63031000	-2.05811400
H	2.59100100	6.08184700	-1.93257500
H	0.39817000	6.85004200	-1.05015200
H	-1.30371900	5.20383300	-0.33007100
C	-1.59229400	2.52685100	1.46392700
H	-2.55226900	2.02151700	1.61539800
H	-1.74906700	3.59709700	1.62768400
C	-0.50037100	1.94275400	2.34486100
H	-0.79508000	2.10822900	3.39356800
H	0.42681600	2.51534700	2.20165900
C	-0.24586800	0.46638500	2.09778800
H	-1.10950100	-0.20115700	2.14546000
C	1.00568900	-0.07955700	2.40440800
H	1.74658700	0.54669000	2.88962500
H	1.08048700	-1.13709100	2.64040600

F	1.46461800	1.75567500	-1.29128100
S	-1.25915600	2.24390700	-0.32019100

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P1$_{1g}$, Esol(SCF Done) = -2196.154788 a.u.

Sc	0.20605600	0.17519600	-0.29022200
S	-0.79686200	-3.10096800	1.06323100
Si	4.16095900	0.08216000	1.95727400
C	2.36757400	0.14886200	1.21719500
H	2.37030900	-0.58880000	0.38595800
H	2.31240300	1.16709600	0.78964900
C	5.39680800	0.21897700	0.53117300
H	5.33849700	-0.64146300	-0.14439500
H	6.41986800	0.25853400	0.92302200
H	5.23779400	1.12922500	-0.05906200
C	4.38935800	-1.53605300	2.90425000
H	3.65394700	-1.64308000	3.70894300
H	5.38513300	-1.55943500	3.36228500
H	4.30817700	-2.40996600	2.24888100
C	4.33505100	1.57052500	3.11318100
H	4.19387100	2.51671900	2.57770300
H	5.34102300	1.58612300	3.54855200
H	3.62088900	1.53801000	3.94309300
C	0.37832800	-1.95810000	-1.41921500
C	-0.25358600	-1.03698000	-2.33614000
C	-1.50693600	-0.62835300	-1.81899600
C	-1.74157000	-1.33815700	-0.59958000
C	-0.59287200	-2.13827700	-0.37316500
C	-2.77174700	-1.49858900	0.40395000
C	-2.40435100	-2.43232000	1.34296100
C	0.29526000	-0.57584000	-3.65858500

H	1.34154000	-0.25782600	-3.60188300
H	-0.29170400	0.25926300	-4.05456700
H	0.24526400	-1.38429700	-4.39858100
C	-3.18682200	-2.96562700	2.50214200
H	-4.24502300	-2.71467400	2.39027600
H	-2.84028200	-2.55579200	3.45944400
H	-3.10315300	-4.05629700	2.56549400
Si	1.87293500	-3.08850200	-1.77450000
C	3.33493400	-2.11038100	-2.48759000
H	4.21414600	-2.76428400	-2.53475400
H	3.13902700	-1.76133800	-3.50659600
H	3.60585200	-1.24226800	-1.87541300
C	1.32063100	-4.40027200	-3.02073300
H	2.13868400	-5.10038000	-3.22736000
H	0.47365700	-4.97592000	-2.63194300
H	1.01555800	-3.95257700	-3.97277300
C	2.40070600	-3.92844400	-0.16175100
H	1.63169200	-4.61631500	0.20606200
H	3.30683000	-4.51993900	-0.33936400
H	2.62372700	-3.21284100	0.63722000
C	-4.05226700	-0.76090700	0.37961700
C	-4.78288800	-0.64904500	-0.81453700
C	-4.56390500	-0.14770600	1.53486300
C	-5.98684700	0.04973000	-0.84975800
H	-4.41765900	-1.14016300	-1.71288900
C	-5.77034300	0.54977300	1.49840400
H	-4.00830300	-0.21592100	2.46698400
C	-6.48484800	0.65214900	0.30573400
H	-6.54398700	0.11438200	-1.78064300
H	-6.15247700	1.01290700	2.40448300

H	-7.42655600	1.19328500	0.27746700
H	-2.18784000	0.06208400	-2.30371600
C	0.99332700	3.22766700	-1.31084300
C	1.95880800	4.11051300	-1.74969700
C	1.68716200	5.47231400	-1.61660900
C	0.47696500	5.89875200	-1.06715500
C	-0.47685600	4.97272900	-0.65175200
C	-0.22552900	3.59879800	-0.75771100
H	2.88546000	3.74485000	-2.17987600
H	2.42244800	6.19717200	-1.95181100
H	0.26733100	6.95996700	-0.97574200
H	-1.42947600	5.30829800	-0.25205200
C	-1.52447700	2.52298000	1.52808500
H	-2.44791300	1.98470700	1.76954500
H	-1.67220900	3.57944800	1.77342200
C	-0.31450000	1.89616700	2.20117100
H	-0.42082300	2.04445200	3.29010900
H	0.57878100	2.47892400	1.92099200
C	-0.13877800	0.41663900	1.84491000
H	-0.93727000	-0.18176400	2.29809900
C	1.24770200	-0.10429900	2.26919400
H	1.56115000	0.36377400	3.21665100
H	1.20137300	-1.18107300	2.46407900
F	1.26291300	1.86242900	-1.43841600
S	-1.43430100	2.36607200	-0.30957500

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$C2_{1g}$, Esol(SCF Done) = -3081.847975 a.u.

Sc	-0.16637500	-0.66867400	-0.08275400
S	-3.50234300	-1.74572500	-1.03565600
C	-0.77311500	-1.71213000	-2.22118300

C	0.03665100	-0.55820800	-2.51469900
C	-0.63877500	0.62403100	-2.10486900
C	-1.92877800	0.25038600	-1.61961200
C	-1.98244100	-1.16612400	-1.67268800
C	-3.12850300	0.85520300	-1.08103000
C	-4.05560900	-0.09907500	-0.73516400
C	1.36273200	-0.56172900	-3.21896600
H	1.97956800	-1.42130000	-2.94213000
H	1.93198000	0.34702700	-2.99945900
H	1.21635300	-0.59503800	-4.30607100
C	-5.44950000	0.08749200	-0.22379000
H	-5.75370400	1.13234800	-0.32757100
H	-5.53900500	-0.18804800	0.83480500
H	-6.16170200	-0.53061800	-0.78207600
Si	-0.57078500	-3.46657100	-2.95829800
C	1.02233400	-4.34619900	-2.42812700
H	1.09857400	-5.29151900	-2.97938800
H	1.92511500	-3.76679900	-2.64614400
H	1.02262700	-4.59046900	-1.36065400
C	-0.57326800	-3.27106000	-4.84289700
H	0.30918000	-2.73357700	-5.20536200
H	-0.57877500	-4.25832300	-5.32006100
H	-1.46393000	-2.72981800	-5.18048000
C	-2.05253100	-4.52909600	-2.45177600
H	-2.99609500	-4.11605100	-2.82420700
H	-1.93711200	-5.52743600	-2.89109900
H	-2.13362800	-4.65363700	-1.36672900
C	-3.36560700	2.31500500	-1.02718200
C	-3.19627300	3.09086200	-2.18485300
C	-3.79026900	2.95067800	0.14918700

C	-3.46163400	4.45811700	-2.16949600
H	-2.88175800	2.60998400	-3.10759800
C	-4.05070700	4.32063400	0.16559000
H	-3.91192300	2.36551400	1.05707300
C	-3.89085000	5.07801600	-0.99490500
H	-3.34595700	5.03838800	-3.08121700
H	-4.38368000	4.79569800	1.08475500
H	-4.10657800	6.14305400	-0.98553600
H	-0.26122300	1.63261200	-2.22849100
C	4.36859800	-1.55565100	0.05812900
C	-2.05095900	-1.25576100	2.68909700
C	-2.79824200	-0.77904700	3.74747800
C	-3.32147700	-1.71735300	4.63755400
C	-3.09207900	-3.08007000	4.44233500
C	-2.34147300	-3.52038000	3.35451700
C	-1.79329300	-2.59868100	2.45464200
H	-2.96057000	0.28654300	3.86995300
H	-3.91375100	-1.37792000	5.48179300
H	-3.50926600	-3.80515900	5.13424000
H	-2.18147900	-4.58174600	3.18797800
C	0.79051000	-3.50690300	1.74370100
H	1.16979200	-4.30884700	1.10167300
H	0.62310100	-3.92213700	2.74198100
C	1.71979400	-2.30573000	1.71670600
H	2.70858700	-2.66213900	2.05138100
H	1.40001900	-1.58651000	2.49057200
C	1.78380900	-1.65476500	0.32370700
H	1.85227700	-2.47352800	-0.41433800
C	3.03975900	-0.78075300	0.14597200
H	2.93886700	-0.16815500	-0.75899200

H	3.09995000	-0.06123300	0.97570700
F	-1.52064000	-0.32915400	1.80189300
S	-0.86677900	-3.10517000	1.02289200
H	4.51401300	-2.17089700	0.95826800
H	4.31829900	-2.26656900	-0.78068500
C	2.10279200	3.30816500	-0.74115800
C	2.50638100	4.32188800	-1.59661900
C	1.58711000	5.30691400	-1.95317500
C	0.28636500	5.27026800	-1.45205400
C	-0.10140300	4.25182100	-0.58415700
C	0.80676300	3.24994100	-0.22152400
H	3.52683100	4.32727100	-1.96639600
H	1.89398400	6.10559200	-2.62213900
H	-0.42939300	6.03860200	-1.72619300
H	-1.10981100	4.22507700	-0.18290300
S	0.27849400	1.97161300	0.90038500
C	1.43243400	2.20291500	2.31992500
H	1.51166300	3.28456000	2.46116000
H	2.41523600	1.81324700	2.04555100
C	0.89439300	1.54061500	3.58907800
H	0.74803200	0.46552000	3.41042000
H	-0.08349200	1.96614500	3.84318900
C	1.85483600	1.73172100	4.73016700
H	2.83408300	1.26499200	4.61616900
C	1.58518100	2.42953100	5.83298400
H	0.62202700	2.91330000	5.98562200
H	2.31662500	2.54079600	6.62851700
F	2.98966500	2.35661400	-0.40231300
Si	5.95289400	-0.50660200	-0.16761600
C	5.88222500	0.43270700	-1.81654000

H	5.05069000	1.14588200	-1.83343800
H	6.80778500	0.99715200	-1.97963400
H	5.76062600	-0.25406200	-2.66240900
C	7.44407400	-1.67792100	-0.16217300
H	8.37950800	-1.12247300	-0.29639500
H	7.51658800	-2.22754900	0.78350800
H	7.37522500	-2.41320300	-0.97227700
C	6.11232000	0.74062900	1.25703000
H	5.30239800	1.47892100	1.23510000
H	6.09393800	0.24012900	2.23244400
H	7.05887100	1.28895300	1.18572600

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C2'$_{1g}$, Esol(SCF Done) = -3081.827045 a.u.

Sc	0.70007400	0.10526800	-0.65476700
S	2.79370500	3.02517900	-0.24687800
C	1.65514800	1.40869600	-2.47113800
C	1.91922800	0.02165700	-2.76893700
C	2.73531400	-0.53784200	-1.74692800
C	3.10442400	0.50844400	-0.84663500
C	2.43322500	1.67523700	-1.29271400
C	3.87755300	0.70926100	0.36076800
C	3.82348400	2.02255000	0.77096800
C	1.51899200	-0.72498200	-4.00611300
H	0.50410000	-0.49067500	-4.33388200
H	1.58250900	-1.80526900	-3.84751000
H	2.19809000	-0.47314500	-4.83126000
C	4.53725800	2.68284300	1.90751200
H	5.36865500	2.05785200	2.24456700
H	3.87271900	2.85398200	2.76421500
H	4.94347500	3.65525200	1.60806500

Si	0.87457700	2.77337700	-3.55608100
C	-0.31801900	2.08513000	-4.85444000
H	-0.81062800	2.92709300	-5.35570900
H	0.19777800	1.50331600	-5.62453400
H	-1.10295200	1.45816800	-4.41705400
C	2.30089200	3.68170200	-4.40455900
H	2.86441300	3.00683600	-5.05816900
H	1.92047600	4.50647100	-5.01844200
H	2.99912000	4.10081700	-3.67180800
C	-0.07602400	3.97880000	-2.44068800
H	0.54969300	4.40506900	-1.64876600
H	-0.44685500	4.81612100	-3.04399300
H	-0.94881200	3.50650000	-1.97392200
C	4.66553500	-0.36253300	1.00623000
C	5.46818200	-1.21088300	0.22637700
C	4.62661500	-0.56673200	2.39422500
C	6.21366100	-2.22658300	0.81893400
H	5.52816000	-1.05228000	-0.84732800
C	5.37426600	-1.58344400	2.98565600
H	3.99726700	0.06912300	3.01180300
C	6.16960500	-2.41653700	2.20034600
H	6.83911400	-2.86531900	0.20098200
H	5.33392100	-1.72483300	4.06256700
H	6.75480100	-3.20722100	2.66175300
H	3.07416800	-1.56801800	-1.71438400
C	-0.70364700	-3.28964300	-2.11330800
C	-4.97144100	0.14714400	1.38309200
C	-5.92448900	-0.54949400	2.10947200
C	-7.26791400	-0.40689800	1.76678700
C	-7.63557600	0.42090300	0.70693600

C	-6.65857000	1.10084400	-0.01667000
C	-5.30070200	0.97508700	0.30670500
H	-5.60788500	-1.18336100	2.93189000
H	-8.02415300	-0.94480800	2.33104600
H	-8.68157500	0.53407600	0.43843100
H	-6.93550100	1.74381700	-0.84696200
C	-3.14779200	0.67125400	-1.51541900
H	-2.98050200	1.09036400	-2.51332600
H	-3.78147300	-0.21203800	-1.63255600
C	-1.80836300	0.27977600	-0.88263300
H	-1.99643200	-0.03060500	0.15486400
H	-1.24107400	1.25237800	-0.80052000
C	-1.00978600	-0.78866800	-1.62809500
H	-1.04093600	-0.59606300	-2.70853900
C	-1.46927600	-2.21867200	-1.32737400
H	-1.38288800	-2.41850600	-0.24690600
H	-2.54535400	-2.32617000	-1.54688400
F	-3.67256700	0.00001200	1.74134000
S	-4.09898300	1.93971300	-0.58346600
H	-0.81616100	-3.09856700	-3.19071900
H	0.37513400	-3.20460500	-1.90867200
C	0.66058800	-1.57512500	2.21306700
C	0.61429500	-2.80526200	2.83517300
C	0.29052900	-2.82665200	4.19107000
C	0.03977100	-1.63404500	4.87050700
C	0.11049200	-0.41114700	4.20790600
C	0.41345200	-0.36113300	2.84155600
H	0.81826200	-3.71008700	2.27297800
H	0.24187000	-3.77710700	4.71306100
H	-0.20252300	-1.65258000	5.92862000

H	-0.06391000	0.51015800	4.75474700
C	-0.93778300	2.10319400	2.37517700
H	-0.97359100	2.15002300	3.46660600
H	-1.81576200	1.56345900	2.01254300
C	-0.85151100	3.51779300	1.79744800
H	-0.78401000	3.46574900	0.70191800
H	0.05786900	4.01427800	2.15569100
C	-2.06734500	4.30889700	2.19419300
H	-3.01479400	3.96287200	1.78154000
C	-2.03884700	5.37131800	2.99838800
H	-1.10944400	5.74886900	3.42118400
H	-2.94486300	5.91349000	3.25460700
F	0.98639200	-1.55386300	0.85776300
S	0.59150100	1.16331700	1.93299600
Si	-1.21684500	-5.10528000	-1.79361800
C	-0.82419100	-5.56169700	0.01052900
H	-1.10461200	-6.60048000	0.21923200
H	0.25009900	-5.46431800	0.21173600
H	-1.36941100	-4.92499900	0.71751900
C	-0.21396800	-6.21694300	-2.95572800
H	-0.42118700	-5.98223300	-4.00618400
H	0.86385600	-6.10022200	-2.79224700
H	-0.46115700	-7.27297200	-2.79739400
C	-3.07147700	-5.33029300	-2.11895600
H	-3.68229600	-4.72699100	-1.43759500
H	-3.33166300	-5.04680500	-3.14542300
H	-3.36168200	-6.37845600	-1.98205500

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C2''$_{1g}$, Esol(SCF Done) = -3081.837532 a.u.

Sc	0.63054400	-0.60544400	0.02965500

S	3.32171600	-2.47316300	-1.65207000
C	1.13872100	-3.00525300	0.30384200
C	1.00087400	-2.44477400	1.62600200
C	2.00360800	-1.46208300	1.83591200
C	2.87274200	-1.46363300	0.70475400
C	2.31950800	-2.38021800	-0.22478200
C	4.10778400	-0.85155500	0.25952000
C	4.47809800	-1.32884000	-0.97670300
C	0.07895500	-2.91974200	2.70855600
H	-0.80632900	-3.42141400	2.31478900
H	-0.25055400	-2.09657500	3.35115300
H	0.60536400	-3.63928900	3.34955900
C	5.71248800	-1.03770700	-1.76997000
H	6.49268000	-0.63381900	-1.11881900
H	5.52571100	-0.30591000	-2.56675300
H	6.10227100	-1.94541500	-2.24332700
Si	0.39813200	-4.65106700	-0.32864400
C	-1.46762400	-4.81149000	-0.02656500
H	-1.84621900	-5.65318000	-0.61930800
H	-1.69064500	-5.03482300	1.02180800
H	-2.04574800	-3.92497700	-0.30615100
C	1.30073700	-6.03636200	0.59279900
H	1.12638800	-5.97824800	1.67269000
H	0.94882200	-7.01626100	0.24928100
H	2.38147600	-5.98579500	0.42130500
C	0.74926800	-4.83116100	-2.18517400
H	1.82371300	-4.85326500	-2.39693400
H	0.33573100	-5.78878600	-2.52429100
H	0.29473200	-4.04901500	-2.80331600
C	4.89732300	0.08476300	1.08807800

C	5.09972500	-0.18521500	2.45176700
C	5.46356800	1.24969200	0.54753200
C	5.84896200	0.67913300	3.24523100
H	4.69180100	-1.09573900	2.88267100
C	6.21463200	2.11332600	1.34289700
H	5.30447200	1.48599600	-0.50125100
C	6.40961500	1.83165200	2.69400900
H	6.00552900	0.44568300	4.29504500
H	6.64806600	3.00852100	0.90454800
H	6.99857400	2.50272700	3.31319700
H	2.12446500	-0.87986400	2.74307600
C	-1.69474100	2.43369600	1.03943100
C	-6.02009900	-0.28529700	-0.47102400
C	-6.98486100	0.24453700	-1.31332500
C	-8.30502100	0.31346700	-0.87228900
C	-8.63299600	-0.13855000	0.40485300
C	-7.64290100	-0.64707000	1.24199600
C	-6.30835700	-0.73551600	0.82046600
H	-6.69492000	0.58166600	-2.30382900
H	-9.07008400	0.72090200	-1.52662900
H	-9.65867900	-0.08454500	0.75772400
H	-7.89248600	-0.98369600	2.24417600
C	-3.67360400	-0.39529900	1.85957300
H	-3.44215700	-0.15065400	2.90284500
H	-3.98070500	0.52892100	1.36500700
C	-2.46627700	-1.04373500	1.17212200
H	-2.79976200	-1.37616900	0.18299800
H	-2.21295500	-1.95417900	1.72327700
C	-1.23454700	-0.14692400	1.05070000
H	-0.87540300	0.13215300	2.05905700

C	-1.48388200	1.13524100	0.23540000
H	-0.64692800	1.34829500	-0.48735900
H	-2.34205100	0.95954400	-0.42856600
F	-4.74554100	-0.35368900	-0.93320100
S	-5.13172900	-1.51729600	1.89386400
H	-2.36971000	2.21643800	1.87839500
H	-0.74939800	2.74218800	1.50494400
C	1.94854400	2.55672700	0.33634300
C	2.09900200	3.69985600	1.09675300
C	2.51644600	4.86092700	0.44772600
C	2.78082700	4.84402000	-0.92280600
C	2.64066100	3.66770200	-1.65542900
C	2.19904300	2.49609600	-1.02928300
H	1.89682800	3.67433700	2.16234300
H	2.64356600	5.77541400	1.01861500
H	3.11628400	5.74739400	-1.42285000
H	2.88514800	3.65454600	-2.71371400
C	1.14706700	1.23988200	-3.39532100
H	1.78308800	0.85120400	-4.19611100
H	1.05565000	2.32075100	-3.52727700
C	-0.21918100	0.55623000	-3.40131000
H	-0.57504300	0.53879100	-4.44270500
H	-0.94763800	1.14069400	-2.83050700
C	-0.17227900	-0.85363100	-2.88597300
H	0.65279200	-1.47754600	-3.23701000
C	-1.10522700	-1.39533100	-2.08479800
H	-1.97678100	-0.82898100	-1.76687700
H	-1.07899200	-2.44650700	-1.81412900
F	1.53531300	1.40380000	0.97313900
S	2.09866300	0.91924100	-1.84592100

Si	-2.44984700	3.92467200	0.10035900
C	-1.47783200	4.27209400	-1.49684900
H	-1.87358000	5.16510500	-1.99458500
H	-0.41490000	4.44760900	-1.29553700
H	-1.56343600	3.44159700	-2.20817900
C	-2.37304100	5.44176200	1.23268600
H	-2.90390800	5.26027200	2.17423000
H	-1.33859400	5.70993600	1.47670900
H	-2.83806800	6.31058900	0.75283600
C	-4.25054800	3.52977200	-0.33989700
H	-4.34034800	2.60572600	-0.92237900
H	-4.86012300	3.41323000	0.56359900
H	-4.69184800	4.33962200	-0.93234200

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TS2$_{1g}$, Esol(SCF Done) = -3081.847975 a.u.

Sc	0.86226300	-0.52766400	-0.30334800
S	4.10545800	-2.24866000	-1.00392800
C	1.47089000	-2.89942200	0.20746700
C	0.89750800	-2.32471100	1.39883200
C	1.71065800	-1.25320900	1.86012900
C	2.86849400	-1.19126100	1.03221000
C	2.69279600	-2.17347600	0.02113200
C	4.13849100	-0.49862600	0.95842300
C	4.91173500	-0.99235200	-0.06527200
C	-0.27506600	-2.84778400	2.17706300
H	-1.02418800	-3.32961200	1.54752300
H	-0.76507200	-2.05332700	2.75089700
H	0.06747300	-3.59711600	2.90280100
C	6.30822500	-0.62321600	-0.45289200
H	6.79856300	-0.09035600	0.36629800

H	6.32949400	0.02412300	-1.33912500
H	6.90309900	-1.51390800	-0.68320000
Si	1.14354600	-4.62165100	-0.55865800
C	-0.65428400	-5.20001000	-0.39972000
H	-0.76405100	-6.12641200	-0.97686600
H	-0.92732500	-5.43148200	0.63452100
H	-1.38395600	-4.48589700	-0.79706100
C	2.26885600	-5.81575500	0.38645200
H	2.02150100	-5.83368300	1.45360600
H	2.15913000	-6.83513500	-0.00187500
H	3.32183000	-5.52928000	0.28984100
C	1.61454700	-4.64416900	-2.39590000
H	2.61157500	-4.23367200	-2.59009500
H	1.62600800	-5.68704000	-2.73561000
H	0.89047700	-4.10977000	-3.02071200
C	4.55068000	0.54988700	1.91672100
C	4.36722500	0.35570600	3.29549400
C	5.12393900	1.75495700	1.48209000
C	4.75049700	1.33410400	4.20897200
H	3.94914100	-0.58200800	3.65235700
C	5.50845400	2.73286700	2.39789200
H	5.26012600	1.92950400	0.41776600
C	5.32243400	2.52622900	3.76382300
H	4.61281400	1.16018500	5.27291100
H	5.95453300	3.65804200	2.04218100
H	5.62552400	3.28682100	4.47813900
H	1.51337600	-0.65376100	2.74286600
C	-2.02057600	2.17655500	0.51091200
C	-6.58268100	-0.47851700	-0.23321800
C	-7.77718700	0.11714000	-0.60683700

C	-8.87314600	0.02906300	0.24981800
C	-8.75400700	-0.64039600	1.46678800
C	-7.53790100	-1.21296700	1.83266800
C	-6.42403800	-1.14511200	0.98522100
H	-7.83775100	0.62626500	-1.56366800
H	-9.81600600	0.48564100	-0.03678100
H	-9.60417800	-0.70897500	2.13899000
H	-7.43547200	-1.72293000	2.78624900
C	-3.61705100	-0.74947100	1.23030400
H	-3.11226500	-0.65105200	2.19830200
H	-4.10210400	0.20130700	1.00601000
C	-2.63644200	-1.17061900	0.13009200
H	-3.20198500	-1.20773800	-0.80759300
H	-2.32318300	-2.19983800	0.33593900
C	-1.39474500	-0.30708000	-0.06740200
H	-0.85293100	-0.27430800	0.92148000
C	-1.66261400	1.12578800	-0.55792800
H	-0.80219800	1.52049100	-1.13121100
H	-2.46442200	1.05357700	-1.30687200
F	-5.53325700	-0.39215300	-1.08222400
S	-4.94230700	-2.00922800	1.44053400
H	-2.66687200	1.73940100	1.28080200
H	-1.11363800	2.49518300	1.03988000
C	1.69740000	2.73243200	-0.19675800
C	1.47100800	3.99315000	0.31841200
C	1.88006600	5.08471900	-0.44754800
C	2.50077500	4.88573700	-1.68215700
C	2.74052600	3.59751300	-2.15389500
C	2.32830600	2.48524300	-1.41004200
H	0.99332800	4.11253900	1.28488300

H	1.71768800	6.09033700	-0.07232000
H	2.82185600	5.73897100	-2.27168500
H	3.26526000	3.45005800	-3.09344200
C	2.08466200	0.54773700	-3.52487800
H	2.74733700	-0.22728000	-3.92568500
H	2.23957600	1.45500700	-4.11569300
C	0.63855900	0.07626800	-3.50793100
H	0.37787800	-0.22965000	-4.53404100
H	-0.02119500	0.91933300	-3.26745500
C	0.41561900	-1.06985500	-2.53968100
H	1.10215300	-1.91340900	-2.62287000
C	-0.84128000	-1.31192000	-1.98137800
H	-1.69838700	-0.74517100	-2.33397200
H	-1.08232000	-2.30831200	-1.62130000
F	1.27968500	1.63782200	0.54747400
S	2.74041000	0.80436200	-1.82729100
Si	-2.94218500	3.72123300	-0.16905600
C	-2.11683000	4.31759600	-1.77157200
H	-2.62197500	5.21626600	-2.14438200
H	-1.06145000	4.57060100	-1.61882800
H	-2.17591900	3.56070300	-2.56271400
C	-2.88212600	5.08587000	1.14433300
H	-3.31583400	4.74503200	2.09148100
H	-1.85518600	5.41362100	1.34357400
H	-3.45161600	5.96334800	0.81706600
C	-4.74040600	3.23679000	-0.51902000
H	-4.81513200	2.34148400	-1.14655200
H	-5.27945700	3.03425800	0.41383400
H	-5.26688900	4.04868100	-1.03390000

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$P2_{1g}$, Esol(SCF Done) = -3081.847975 a.u.

Sc	-1.60350900	0.57347900	-0.39040800
S	-4.97984900	1.34050800	-1.20306700
C	-2.54025100	2.77193500	-0.27323300
C	-1.83733800	2.57127600	0.97118300
C	-2.44134600	1.51582900	1.70860000
C	-3.59443400	1.07764800	0.99082800
C	-3.63026000	1.83350600	-0.21182200
C	-4.64358900	0.08565500	1.08350100
C	-5.47471800	0.13940200	-0.01469800
C	-0.65977500	3.36265800	1.46785600
H	0.07956000	3.56083600	0.68676200
H	-0.15827500	2.84860600	2.29418300
H	-0.99288200	4.33614000	1.84953800
C	-6.72312200	-0.63903000	-0.28661000
H	-7.08509600	-1.10363500	0.63442900
H	-6.55980700	-1.43279800	-1.02657800
H	-7.51625000	0.01001900	-0.67370800
Si	-2.44677700	4.22840500	-1.51290200
C	-0.70485800	4.94669800	-1.67148000
H	-0.72231000	5.72097300	-2.44820500
H	-0.36070900	5.42323900	-0.74839400
H	0.03439600	4.19782400	-1.97478100
C	-3.63578200	5.55015100	-0.86477800
H	-3.32353900	5.91912400	0.11838800
H	-3.66640000	6.40520300	-1.55026400
H	-4.65408900	5.15756700	-0.76991800
C	-3.02422700	3.62304400	-3.21331400
H	-4.05878900	3.26329500	-3.20525600
H	-2.98033900	4.45890100	-3.92191400

H	-2.38418100	2.82612300	-3.60869200
C	-4.80830500	-0.81146400	2.24720900
C	-4.72199000	-0.29349700	3.54965000
C	-5.04165100	-2.18598500	2.08624600
C	-4.87286400	-1.12517900	4.65600400
H	-4.56525300	0.77271900	3.69246600
C	-5.19304700	-3.01660400	3.19502900
H	-5.09481700	-2.60750900	1.08554800
C	-5.10915600	-2.48913800	4.48272900
H	-4.81626900	-0.70491500	5.65654400
H	-5.37676300	-4.07816600	3.05160700
H	-5.23077000	-3.13613500	5.34704600
H	-2.10424100	1.15567600	2.67499200
C	3.07648600	-2.04062800	-0.69190000
C	6.83852700	1.66892700	0.63059400
C	8.19627600	1.52474900	0.38889200
C	9.07086300	1.43624800	1.47043300
C	8.57514200	1.48256100	2.77261200
C	7.20514100	1.60496400	2.99395200
C	6.30661300	1.70261300	1.92344600
H	8.54926500	1.49861200	-0.63738100
H	10.13688300	1.33056900	1.29108000
H	9.25239700	1.41162300	3.61869600
H	6.81185400	1.62536600	4.00633400
C	3.73258300	0.71254000	1.23749900
H	3.12862900	0.10873400	1.92608100
H	4.49972400	0.06063500	0.81560800
C	2.86208600	1.34581700	0.15693000
H	3.50376100	1.94888000	-0.49669700
H	2.17046700	2.05069900	0.63948200

C	2.05137800	0.36213800	-0.70925700
H	1.36374800	-0.18995600	-0.03853200
C	2.96291000	-0.68600100	-1.40371500
H	2.60171300	-0.85754700	-2.42485000
H	3.96032300	-0.23952400	-1.52493800
F	6.00841500	1.76852800	-0.42842600
S	4.58666600	1.98387800	2.25833800
H	3.38931200	-1.90561700	0.35278900
H	2.08300200	-2.51506900	-0.64178700
C	-1.21535300	-2.58393900	0.35536000
C	-0.65226300	-3.56703000	1.14148100
C	-0.78578200	-4.88657600	0.70875100
C	-1.47233400	-5.17625100	-0.47120500
C	-2.03729200	-4.15289000	-1.22858600
C	-1.90768200	-2.81775000	-0.82571600
H	-0.12974700	-3.30734200	2.05598800
H	-0.35474800	-5.68663400	1.30250800
H	-1.57920900	-6.20580300	-0.79837800
H	-2.59093400	-4.38077000	-2.13501900
C	-1.49964800	-1.30176800	-3.18521600
H	-2.03031800	-0.59475100	-3.83481600
H	-1.46335400	-2.26738000	-3.69907500
C	-0.12768300	-0.77949600	-2.78300500
H	0.47218100	-0.73615200	-3.70952100
H	0.36374600	-1.53523200	-2.15433600
C	-0.18233900	0.58175900	-2.07351900
H	-0.65768500	1.28971000	-2.78310400
C	1.20066000	1.16606400	-1.72573900
H	1.80708700	1.31223100	-2.63653200
H	1.04670700	2.18079800	-1.32864000

F	-1.08026100	-1.26309900	0.79171000
S	-2.66363700	-1.49226100	-1.75261100
Si	4.27598900	-3.30085100	-1.49384100
C	3.74378700	-3.64217000	-3.28440000
H	4.39961900	-4.39058700	-3.74409700
H	2.71834500	-4.02809800	-3.33289000
H	3.79532000	-2.73788600	-3.90161100
C	4.19167000	-4.90912300	-0.48912900
H	4.48471400	-4.74289300	0.55410000
H	3.17972600	-5.33150300	-0.49266000
H	4.86723700	-5.66503600	-0.90573800
C	6.04415200	-2.61846800	-1.46737100
H	6.12939700	-1.68791000	-2.03989800
H	6.37885300	-2.41527300	-0.44344800
H	6.74216100	-3.34085300	-1.90621500

87

C2$_E$, Esol(SCF Done) = -2274.748459 a.u.

Sc	0.01506300	0.03621500	-0.18273000
S	-2.95565900	1.02708000	1.54135100
C	5.65283900	-3.11492400	-0.02226000
H	5.60182300	-2.98533500	1.06528900
H	4.70661200	-3.55716700	-0.35615400
C	-0.16842900	0.27400800	2.24303500
C	0.48753300	-0.98573200	1.99468200
C	-0.39215200	-1.85593900	1.29839900
C	-1.65775500	-1.20273100	1.16814700
C	-1.49586200	0.08992100	1.72997800
C	-2.97840300	-1.43517500	0.61550600
C	-3.77906700	-0.32511000	0.76494900
C	1.85117100	-1.38696200	2.47512400

H	2.57949100	-0.57484300	2.39831600
H	2.23702200	-2.23994800	1.90851900
H	1.80689100	-1.69328600	3.52779500
C	-5.23022300	-0.15659400	0.43843900
H	-5.70831200	-1.13309000	0.32255200
H	-5.38375500	0.40755900	-0.49066500
H	-5.75266900	0.38319400	1.23576300
Si	0.37310800	1.61979000	3.49309000
C	2.03559900	2.42324800	3.06301000
H	2.32350200	3.09108600	3.88415700
H	2.84435700	1.69693800	2.93486400
H	1.97376100	3.03478900	2.15649200
C	0.50237100	0.77767400	5.18419300
H	1.31505100	0.04495000	5.22259300
H	0.69668000	1.52820200	5.95961600
H	-0.43105500	0.26452500	5.44010700
C	-0.95628000	2.96365300	3.57234300
H	-1.91884900	2.56613700	3.91150400
H	-0.64483000	3.72488100	4.29794100
H	-1.10744200	3.46819600	2.61207700
C	-3.40903600	-2.73175900	0.05198200
C	-3.04890300	-3.92845000	0.69432200
C	-4.16977100	-2.81042700	-1.12569300
C	-3.44049800	-5.16057200	0.17660700
H	-2.48417000	-3.88794500	1.62219100
C	-4.56221300	-4.04407600	-1.64159900
H	-4.44496000	-1.89790700	-1.64877700
C	-4.19774300	-5.22335000	-0.99339000
H	-3.16244200	-6.07439200	0.69488900
H	-5.15151600	-4.08359800	-2.55391500

H	-4.50443500	-6.18500300	-1.39507400
H	-0.15113800	-2.87171500	1.00546200
C	4.65757500	-0.18907200	-0.46007200
C	-1.71298500	2.04830600	-2.29572700
C	-2.59344900	2.20531000	-3.34663900
C	-2.85095400	3.50734600	-3.77716900
C	-2.23689300	4.59272100	-3.15073100
C	-1.36083700	4.39054000	-2.08664300
C	-1.07355100	3.09340400	-1.64492200
H	-3.05776100	1.34197000	-3.81172300
H	-3.53850700	3.66872700	-4.60168400
H	-2.44901900	5.60340500	-3.48526400
H	-0.89875300	5.23551700	-1.58430300
C	1.68891500	2.96534000	-1.02481100
H	2.31140900	3.32154500	-0.19747700
H	1.62100200	3.76505100	-1.76832400
C	2.21996900	1.65226000	-1.57525000
H	3.25681000	1.84644800	-1.89769500
H	1.67751600	1.40375200	-2.50361400
C	2.15567400	0.50749000	-0.54372200
H	2.41233600	0.94844400	0.43974500
C	3.21579900	-0.57551800	-0.83311900
H	2.96246100	-1.50603900	-0.30386200
H	3.18204700	-0.82458400	-1.90462800
F	-1.44540600	0.75409800	-1.86210000
S	0.00749400	2.78668700	-0.26411100
H	4.93506800	0.75841900	-0.94576000
H	4.71373000	0.00459600	0.62165900
C	-0.72116900	-2.19744500	-2.00228800
H	-1.65593600	-1.79503500	-2.38349400

H	-0.80765900	-3.08048900	-1.37638300
C	0.47008200	-1.67834200	-2.33531000
H	1.39856700	-2.12975200	-1.99772000
H	0.56026500	-0.84559500	-3.03175600
H	6.44524000	-3.84319000	-0.23032600
Si	6.01423700	-1.46879300	-0.89794600
C	6.05314700	-1.74252300	-2.77640200
H	6.24138100	-0.80470600	-3.31218900
H	6.85262500	-2.44229900	-3.04606100
H	5.11160200	-2.16171700	-3.15035800
C	7.68311500	-0.78587500	-0.31425500
H	7.91747900	0.16644400	-0.80387900
H	7.68870300	-0.61655900	0.76874400
H	8.49420700	-1.48608200	-0.54507200

87

TS2$_E$, Esol(SCF Done) = -2274.741465 a.u.

Sc	-0.17369900	-0.15145500	-0.34792200
S	-2.68984900	0.82818500	1.98459800
C	6.17109400	-2.62186200	-0.10204000
H	6.02381900	-2.43326200	0.96786400
H	5.38558900	-3.30880900	-0.43779100
C	-0.05694300	-0.55476200	2.07515600
C	0.29879900	-1.79581900	1.42901800
C	-0.79688800	-2.27546400	0.66834300
C	-1.89671800	-1.39101600	0.86807800
C	-1.43070700	-0.35223400	1.71795700
C	-3.26821500	-1.21878600	0.43320100
C	-3.81927500	-0.08224000	0.97491200
C	1.58171600	-2.55415600	1.61124700
H	2.45172900	-1.89806900	1.70690600

H	1.76206800	-3.23903400	0.77609800
H	1.53411300	-3.16600900	2.52094600
C	-5.22413400	0.42193500	0.87380700
H	-5.87544700	-0.35640500	0.46751500
H	-5.30241300	1.30330500	0.22421200
H	-5.61148400	0.70891100	1.85797200
Si	0.87727400	0.30964500	3.50043200
C	2.61580300	0.88331900	2.99816500
H	3.11184400	1.31717800	3.87501800
H	3.24775800	0.06296600	2.64231400
H	2.58774300	1.66070000	2.22631800
C	1.01826400	-0.93203700	4.92244700
H	1.64475300	-1.79125300	4.66094100
H	1.46572600	-0.44985600	5.79965000
H	0.03110400	-1.30795600	5.21282800
C	-0.12027600	1.80966100	4.07830200
H	-1.10666900	1.52049500	4.45657900
H	0.41505200	2.29629200	4.90254700
H	-0.25748700	2.55728100	3.28969200
C	-3.96626000	-2.19026400	-0.43542600
C	-3.87207700	-3.56555400	-0.16593800
C	-4.71953000	-1.77568800	-1.54475500
C	-4.51872400	-4.49455400	-0.97688600
H	-3.31074100	-3.90326600	0.70163400
C	-5.36645000	-2.70672400	-2.35488400
H	-4.78562500	-0.71666400	-1.78093600
C	-5.26795500	-4.06865100	-2.07378600
H	-4.44443100	-5.55393700	-0.74632200
H	-5.94492000	-2.36737200	-3.21006900
H	-5.77281800	-4.79441100	-2.70522700

H	-0.80074400	-3.19142100	0.08822300
C	4.51571400	-0.08050000	-0.83026800
C	-1.77952200	2.69091500	-1.39675900
C	-2.80044500	3.28930900	-2.10895300
C	-2.81764100	4.68297800	-2.16613300
C	-1.83409000	5.43000200	-1.51625600
C	-0.82266000	4.79164200	-0.80255700
C	-0.77483800	3.39347700	-0.74357100
H	-3.55295500	2.68244900	-2.60152900
H	-3.60805000	5.18281300	-2.71766800
H	-1.85945900	6.51445100	-1.55729100
H	-0.06698500	5.37000500	-0.27884400
C	1.88399000	2.47538900	-0.99318100
H	2.78608100	2.48707200	-0.37409800
H	1.85908900	3.39652800	-1.58336900
C	1.81100100	1.21523800	-1.85119600
H	2.60417000	1.25575300	-2.61072700
H	0.87338900	1.26261500	-2.43865000
C	1.93969800	-0.10263900	-1.05839300
H	1.88681500	0.11222100	0.04671200
C	3.25539800	-0.84418100	-1.26986400
H	3.20665400	-1.80068200	-0.73490600
H	3.34679200	-1.09851700	-2.33529000
F	-1.75453700	1.31123700	-1.34036600
S	0.47346200	2.54301800	0.20000100
H	4.59251000	0.87530000	-1.37017700
H	4.44526500	0.17674900	0.23693700
C	-0.70069500	-1.28957200	-2.34700200
H	-1.11420100	-0.58071300	-3.06244000
H	-1.39921700	-2.01881100	-1.94577400

C	0.66527000	-1.52429100	-2.33282500
H	1.07065900	-2.41997200	-1.86809200
H	1.29701700	-1.08822900	-3.10033100
H	7.12920000	-3.14223100	-0.21503200
Si	6.17767500	-1.00750800	-1.09758200
C	6.39878700	-1.38468300	-2.94295100
H	6.38031300	-0.46892400	-3.54544100
H	7.36410000	-1.87358700	-3.11805700
H	5.61987300	-2.05635300	-3.32219900
C	7.56982100	0.12484600	-0.49145900
H	7.59266400	1.06728200	-1.05077900
H	7.45621100	0.36626400	0.57171400
H	8.54509400	-0.35884100	-0.61870600

87

P2$_E$, Esol(SCF Done) = -2274.775092 a.u.

Sc	-0.63838900	0.03031800	-0.18055100
S	-3.05935700	0.15079200	2.25701700
C	6.20989500	-2.83463500	-0.63038500
H	5.82616100	-3.00537000	0.38239800
H	5.53206700	-3.32569200	-1.33806500
C	-0.43742000	-1.21044800	1.92562800
C	-0.05968300	-2.12609700	0.87383600
C	-1.13969000	-2.31785400	-0.02315800
C	-2.25414200	-1.57803700	0.47497500
C	-1.81655400	-0.92337000	1.65924300
C	-3.58516700	-1.18998100	0.05017400
C	-4.14052400	-0.28680200	0.92904100
C	1.24999000	-2.85255900	0.75933000
H	2.10691400	-2.22763800	1.02513800
H	1.40362000	-3.22893100	-0.25670700

H	1.25999000	-3.72073700	1.43077900
C	-5.52290900	0.28404500	0.93793300
H	-6.16149800	-0.26632000	0.24211900
H	-5.53566600	1.34216200	0.64669400
H	-5.96937300	0.21669900	1.93644500
Si	0.48678200	-0.83286800	3.55418000
C	2.30184700	-0.36105100	3.26660800
H	2.74999600	-0.09054800	4.23048100
H	2.89472000	-1.18382800	2.85497100
H	2.40489600	0.50836600	2.60739400
C	0.40009200	-2.38735300	4.62911600
H	0.91024500	-3.23465400	4.15813200
H	0.87682500	-2.20791000	5.59993600
H	-0.63961800	-2.67943700	4.81269800
C	-0.38201700	0.60492300	4.42676200
H	-1.40919800	0.35384900	4.71273900
H	0.16043200	0.84389600	5.34938100
H	-0.40592700	1.51449700	3.81586500
C	-4.24957800	-1.75889500	-1.14172300
C	-4.21686000	-3.14471400	-1.36395900
C	-4.90907700	-0.94377100	-2.07397800
C	-4.83504900	-3.69796600	-2.48196500
H	-3.72462500	-3.79141000	-0.64192600
C	-5.52645300	-1.49947500	-3.19260400
H	-4.92363100	0.13367400	-1.92943700
C	-5.49178500	-2.87766800	-3.39945100
H	-4.80977100	-4.77370400	-2.63351700
H	-6.03095500	-0.85363800	-3.90627700
H	-5.97361500	-3.31080800	-4.27154500
H	-1.12037100	-2.93930600	-0.90959500

C	4.69940400	-0.11219200	-0.80206500
C	-1.48301500	3.22422100	-0.56775800
C	-2.35142000	4.16892200	-1.07636800
C	-1.94195300	5.50137300	-1.05005900
C	-0.70049300	5.84572700	-0.51319000
C	0.14277500	4.86460700	0.00121600
C	-0.23362800	3.51595500	-0.03537200
H	-3.31177300	3.86674000	-1.48063100
H	-2.60085100	6.26923100	-1.44321100
H	-0.39189200	6.88595900	-0.48161500
H	1.09559300	5.14085300	0.44380900
C	2.31487300	2.30809300	-0.40919400
H	3.09909500	1.90221200	0.23623500
H	2.52076800	3.37262200	-0.55501000
C	2.21553700	1.54916400	-1.72578200
H	3.08176500	1.84477100	-2.33415200
H	1.33617100	1.90564300	-2.27655900
C	2.19830500	0.01123600	-1.58305200
H	1.87649100	-0.23414100	-0.54140800
C	3.60049300	-0.61273400	-1.74368300
H	3.49121300	-1.69963700	-1.63177100
H	3.90677400	-0.45130800	-2.78782100
F	-1.89637300	1.89805200	-0.58673100
S	0.79918900	2.23524200	0.65693500
H	4.88024900	0.96309500	-0.94798900
H	4.38974200	-0.23625300	0.24756000
C	-0.26401100	-0.27684300	-2.29380300
H	-0.48747400	0.72411800	-2.71531400
H	-0.94119000	-0.96689800	-2.81272600
C	1.20046100	-0.65097800	-2.55568600

H	1.31292100	-1.73902000	-2.45977200
H	1.51345500	-0.40985700	-3.58474900
H	7.18016400	-3.33930800	-0.70384300
Si	6.40035200	-0.98375800	-0.99849700
C	7.03712500	-0.73413500	-2.76649200
H	7.13520000	0.33001000	-3.01120600
H	8.02612000	-1.19176700	-2.88454700
H	6.37333800	-1.19235600	-3.50857600
C	7.59661700	-0.19668600	0.24286600
H	7.72250500	0.87576700	0.05384700
H	7.24383800	-0.31856900	1.27363300
H	8.58658300	-0.66216300	0.17507400

110

$C3_{1g}$, Esol(SCF Done) = -3160.472183 a.u.

Sc	-0.28900900	-0.37500700	-0.26420700
S	-2.73401200	1.70217300	-2.17143800
C	-0.66786600	-0.37215400	-2.70175300
C	0.75345500	-0.25282800	-2.48283400
C	1.04061800	0.96000000	-1.80128800
C	-0.17937300	1.67657200	-1.65438000
C	-1.20575300	0.85772000	-2.19942300
C	-0.64917100	2.95821800	-1.17364200
C	-1.99124600	3.11364100	-1.41532400
C	1.80925800	-1.16831300	-3.03506400
H	1.48291800	-2.20991600	-3.09805600
H	2.72743500	-1.13263400	-2.43828800
H	2.07867400	-0.84715400	-4.04943200
C	-2.86630700	4.29592500	-1.14748300
H	-2.25669600	5.16767700	-0.89624400
H	-3.55513500	4.10591900	-0.31581100

H	-3.47138800	4.54593300	-2.02669300
Si	-1.57274400	-1.69053000	-3.73798900
C	-1.42987700	-3.40038700	-2.92012100
H	-1.92316900	-4.15479600	-3.54486400
H	-0.38910800	-3.71561100	-2.78655400
H	-1.92165800	-3.41836000	-1.93972500
C	-0.82102500	-1.74639700	-5.47398200
H	0.22130500	-2.08090100	-5.46717100
H	-1.38894300	-2.43992100	-6.10547500
H	-0.85716200	-0.75790200	-5.94497800
C	-3.40243600	-1.22602300	-3.86261600
H	-3.54175500	-0.26960100	-4.37799100
H	-3.92947100	-1.99185600	-4.44448000
H	-3.89045700	-1.16020300	-2.88376900
C	0.23346000	3.96873400	-0.55260500
C	1.44095400	4.32895300	-1.17157700
C	-0.10484700	4.57992500	0.66402400
C	2.28028500	5.27776900	-0.59297600
H	1.70716400	3.88101400	-2.12577200
C	0.73597400	5.52976100	1.24140900
H	-1.02794300	4.29691500	1.16365500
C	1.93080100	5.88136700	0.61529300
H	3.20519900	5.55437600	-1.09240200
H	0.45762100	5.99370700	2.18410500
H	2.58521300	6.62345100	1.06444600
H	2.02584200	1.30735300	-1.51792700
C	5.79258500	-0.54274500	0.26445900
C	-0.90498100	-3.46677000	1.22079000
C	-1.76873000	-4.23229700	1.97883000
C	-1.31718500	-5.48103300	2.40342300

C	-0.04124000	-5.92115100	2.04850400
C	0.79305800	-5.12307300	1.27019700
C	0.37528000	-3.85243400	0.85372800
H	-2.75782500	-3.86246500	2.22817500
H	-1.96812600	-6.11006400	3.00245300
H	0.30254000	-6.90062000	2.36635500
H	1.77000400	-5.49175500	0.97184500
C	2.96792400	-2.71419600	0.68320700
H	3.70275700	-2.68718300	-0.12693200
H	3.06866500	-3.67924900	1.18787600
C	3.15223600	-1.54141700	1.63348200
H	4.05607400	-1.75874200	2.22025700
H	2.32858100	-1.52729200	2.35705900
C	3.30339800	-0.17871900	0.92013900
H	3.04756600	-0.32754500	-0.14260200
C	4.75384100	0.33846400	0.96816500
H	4.76780400	1.34191800	0.52074000
H	5.03574600	0.47833900	2.02238900
F	-1.35137800	-2.22489400	0.78484800
S	1.33772100	-2.79103500	-0.19742200
H	5.82776000	-1.54421300	0.71979000
H	5.50224800	-0.69597900	-0.78700300
C	0.85014700	0.50344500	1.35349200
H	0.58730400	-0.24233200	2.13679100
H	0.25062600	1.40028800	1.59715200
C	2.32854900	0.87663200	1.45940500
H	2.49056400	1.80806000	0.90150800
H	2.60414500	1.10727000	2.50238700
C	-5.22664300	1.09575800	0.71866000
C	-6.52743400	0.75591100	0.37119300

C	-6.80081300	-0.54853300	-0.03000100
C	-5.77941500	-1.49830300	-0.07935600
C	-4.48019100	-1.14065600	0.27160600
C	-4.18302200	0.16547400	0.67845100
H	-7.30135800	1.51515900	0.42086200
H	-7.81525700	-0.82191000	-0.30497500
H	-5.99340400	-2.51498100	-0.39533800
H	-3.68382000	-1.87557000	0.22724000
S	-2.53810400	0.69877000	1.11902700
C	-2.44080800	0.19289600	2.88785800
H	-1.38499200	0.31143200	3.15042100
H	-2.69262700	-0.87036100	2.95754600
C	-3.31628300	1.03918700	3.81483800
H	-4.36343500	0.96896400	3.49267100
H	-3.02233900	2.09158800	3.73543300
C	-3.18637200	0.56490400	5.23547500
H	-3.58040300	-0.43030000	5.44817700
C	-2.62971100	1.27010400	6.22025400
H	-2.23280200	2.27013000	6.05532000
H	-2.56309200	0.88108500	7.23259600
F	-4.97693300	2.35259000	1.11057400
Si	7.58581300	0.13428700	0.26898600
C	7.63365900	1.82046000	-0.59949600
H	7.02660800	2.56608900	-0.07333800
H	8.66047700	2.20200800	-0.64030300
H	7.26585600	1.75024200	-1.62998700
C	8.67967200	-1.10119100	-0.66586300
H	9.72035200	-0.75804200	-0.69169900
H	8.66844400	-2.08759100	-0.18753600
H	8.34635700	-1.22604000	-1.70277600

C	8.19686900	0.31153600	2.05622800
H	8.16747800	-0.64778600	2.58620800
H	9.23362800	0.66707200	2.07438100
H	7.59298400	1.02923000	2.62325500

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C3'$_{1g}$, Esol(SCF Done) = -3160.451146 a.u.

Sc	-1.79914600	-0.53390000	0.34639000
S	-4.94476600	-0.66633200	2.00961100
Si	5.76358200	-2.59026500	-2.93336300
C	4.86937800	-2.10410400	-1.31474500
H	5.46849400	-1.31132000	-0.84734300
H	4.92621100	-2.96569100	-0.63229200
C	7.53275400	-3.11262300	-2.49563900
H	8.07122200	-2.30445500	-1.98735300
H	8.09923000	-3.37803700	-3.39575100
H	7.53611500	-3.98451900	-1.83125200
C	5.80772200	-1.10162600	-4.11263400
H	4.79970200	-0.78950200	-4.40982500
H	6.35945300	-1.34857400	-5.02715900
H	6.30322000	-0.24123800	-3.64765900
C	4.85793300	-4.03408200	-3.77143600
H	4.80086700	-4.90573200	-3.10888900
H	5.38468200	-4.34405100	-4.68150400
H	3.83581700	-3.76143800	-4.05926500
C	-2.76649000	-2.54763800	1.26761600
C	-2.30585300	-2.87915100	-0.05357500
C	-3.00880500	-2.09615400	-1.01635600
C	-4.00473300	-1.33629900	-0.33047200
C	-3.83148000	-1.60988300	1.05089600
C	-5.02730900	-0.34724800	-0.60057900

C	-5.62815700	0.07638500	0.56551400
C	-1.28221200	-3.91260100	-0.42113400
H	-0.40845900	-3.89372800	0.23426500
H	-0.93998300	-3.77363600	-1.45160200
H	-1.72043500	-4.91660100	-0.35865500
C	-6.78600000	1.00698300	0.74293200
H	-7.31921400	1.13066000	-0.20348100
H	-6.46644500	1.99941200	1.08571700
H	-7.49427500	0.61847500	1.48286800
Si	-2.31580200	-3.23149700	2.99460200
C	-0.88108400	-4.45958000	2.95424600
H	-0.71509500	-4.82856400	3.97368200
H	-1.09837000	-5.32726800	2.32332900
H	0.05610000	-4.00756600	2.61349300
C	-3.86493600	-4.07482800	3.67711300
H	-3.68198500	-4.43868200	4.69493200
H	-4.72187700	-3.39352700	3.71402800
H	-4.14591000	-4.93381400	3.05781100
C	-1.84970300	-1.74485500	4.08374400
H	-2.65310200	-0.99974000	4.13288000
H	-1.65608800	-2.07715600	5.11054300
H	-0.93549900	-1.25567000	3.72446200
C	-5.40558400	0.07197600	-1.96693700
C	-5.56343100	-0.89295400	-2.97541500
C	-5.61033500	1.42146700	-2.29387100
C	-5.92318800	-0.51881400	-4.26715700
H	-5.43223100	-1.94474500	-2.73453300
C	-5.97177900	1.79374000	-3.58738500
H	-5.47506200	2.18469000	-1.53186500
C	-6.12930800	0.82557400	-4.57783500

H	-6.05396300	-1.28069100	-5.03093100
H	-6.13058700	2.84326900	-3.82097400
H	-6.41489400	1.11560700	-5.58520600
H	-2.85668400	-2.14481000	-2.08958300
C	6.88967300	1.23214700	0.75254300
C	7.66149800	1.99121000	-0.11510600
C	7.41991900	3.35979600	-0.21661300
C	6.40454500	3.94534000	0.53847600
C	5.62559600	3.16085900	1.38633500
C	5.85421700	1.78404000	1.51419200
H	8.44982600	1.50469200	-0.68117200
H	8.02749200	3.96380300	-0.88442400
H	6.21323500	5.01202400	0.46362400
H	4.82435200	3.60909600	1.96717200
C	4.24542600	-0.54613200	1.73855600
H	3.67851700	-1.11359700	2.48704700
H	5.06473900	-1.18332300	1.40032700
C	3.33549700	-0.12626700	0.58839300
H	3.90585200	0.48536200	-0.12330200
H	2.56227600	0.53485600	1.00080100
C	2.68060700	-1.31225000	-0.15651800
H	2.71885600	-2.20099800	0.49438800
C	3.40974700	-1.66302100	-1.46803500
H	2.84369500	-2.46207000	-1.96895100
H	3.35437500	-0.78975500	-2.13645700
F	7.14974100	-0.08532800	0.84943400
S	4.93016700	0.84897100	2.70890800
C	1.18434200	-1.03560200	-0.43858500
C	0.27109600	-0.98037400	0.79691800
H	0.82414900	-1.82492400	-1.11662600

H	0.57885900	-0.14675700	1.46123900
H	1.11838000	-0.09612600	-1.01281600
H	0.40194300	-1.89347000	1.39502400
C	-1.79561600	2.16665600	-1.60456100
C	-1.56741100	2.72678300	-2.84427000
C	-1.83448200	4.08725400	-2.99285200
C	-2.32625700	4.83011800	-1.91832300
C	-2.55939500	4.22317100	-0.68674900
C	-2.27967900	2.86277100	-0.50415400
H	-1.19328600	2.11696000	-3.65981200
H	-1.66288700	4.56156800	-3.95402700
H	-2.54050300	5.88716100	-2.04194900
H	-2.96244900	4.80101200	0.13992500
C	-1.50937500	2.90876900	2.24519700
H	-1.60238600	2.30746200	3.15634600
H	-2.00113000	3.86704700	2.44050300
C	-0.04854100	3.10230100	1.84591200
H	-0.00313100	3.61651500	0.87583900
H	0.44725000	2.13252900	1.72708900
C	0.65840500	3.92138100	2.89204700
H	0.28323100	4.93562700	3.03688600
C	1.68262000	3.48864000	3.62741800
H	2.10674600	2.49355500	3.50800500
H	2.15453200	4.13007800	4.36677900
F	-1.52655800	0.80826200	-1.45701300
S	-2.59714900	2.02441200	1.03521000

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C3''$_{1g}$, Esol(SCF Done) = -3160.463076 a.u.

Sc	1.69448900	-0.54775100	-0.00221800
S	4.85012100	-1.88206300	-1.19952100

Si	-5.73471100	3.69055600	0.52203900
C	-4.82201400	2.10169700	1.06526700
H	-5.50252900	1.26371300	0.86592700
H	-4.70611400	2.14082400	2.15898100
C	-7.36533100	3.79675000	1.48230800
H	-7.98903400	2.91376700	1.30159900
H	-7.94177500	4.68048700	1.18525200
H	-7.18683300	3.86279900	2.56182500
C	-6.09051600	3.62015300	-1.34261900
H	-5.16664600	3.58291800	-1.93176200
H	-6.65214000	4.50490300	-1.66441900
H	-6.68735100	2.73681600	-1.59823600
C	-4.66838800	5.21772700	0.90129200
H	-4.42721200	5.27831000	1.96911600
H	-5.19952100	6.13722200	0.62890600
H	-3.72567200	5.20290800	0.34149600
C	2.70139600	-2.65696600	0.71230400
C	2.30049600	-1.94944000	1.90682900
C	3.02770600	-0.73594400	2.00959700
C	3.97665100	-0.69088700	0.94460600
C	3.75492500	-1.85169300	0.16059800
C	5.03560200	0.16075900	0.44331200
C	5.61172100	-0.37634700	-0.68395300
C	1.33810600	-2.43275300	2.95121400
H	0.42186500	-2.84826700	2.52444300
H	1.05612300	-1.61909800	3.62628900
H	1.80453000	-3.21519300	3.56351100
C	6.78188600	0.11958300	-1.47261500
H	7.35543800	0.83868200	-0.88142400
H	6.47218200	0.61706200	-2.40090000

H	7.45089200	-0.70291900	-1.74843900
Si	2.42782900	-4.50941200	0.33034800
C	0.68410200	-5.10266600	0.77826800
H	0.54657100	-6.11662400	0.38358500
H	0.54532600	-5.15660900	1.86262800
H	-0.11952800	-4.48057200	0.36922900
C	3.69795900	-5.45627100	1.36544300
H	3.61238000	-6.53428800	1.18515200
H	4.71947400	-5.15123400	1.11359100
H	3.54882100	-5.28262700	2.43672100
C	2.75996600	-4.85193000	-1.50628400
H	3.76532100	-4.54067300	-1.81056000
H	2.69629200	-5.93398800	-1.67396600
H	2.03427100	-4.38155200	-2.17893100
C	5.46146500	1.40643000	1.11633700
C	5.63710600	1.42748300	2.50951200
C	5.69124400	2.58796500	0.39453600
C	6.03700100	2.59286800	3.15776200
H	5.48647900	0.51562000	3.08163500
C	6.09167600	3.75360600	1.04523800
H	5.54483100	2.59496500	-0.68265500
C	6.26564500	3.75993400	2.42832900
H	6.18035000	2.58698600	4.23498300
H	6.26764000	4.65854600	0.46951200
H	6.58120300	4.66766600	2.93522300
H	2.90742400	-0.00222200	2.79939600
C	-7.17358400	-1.49477000	0.14617100
C	-8.09278500	-1.28938700	-0.87241800
C	-8.08083900	-2.13736500	-1.97810100
C	-7.14413900	-3.16730900	-2.05422200

C	-6.21390200	-3.34024000	-1.03171700
C	-6.20892000	-2.50639800	0.09521500
H	-8.81570400	-0.48530500	-0.77470700
H	-8.80531400	-1.99184400	-2.77427500
H	-7.13203500	-3.83346100	-2.91217200
H	-5.47533700	-4.13495400	-1.09016400
C	-4.26398900	-1.25816900	1.75328900
H	-3.58300800	-1.49563800	2.57988000
H	-4.99645100	-0.54276900	2.13115900
C	-3.48129100	-0.70376900	0.56649000
H	-4.16673700	-0.53232700	-0.27456400
H	-2.78754000	-1.48823100	0.23643800
C	-2.70596600	0.59809000	0.87517000
H	-2.56460900	0.67400000	1.96546500
C	-3.45800600	1.86042800	0.41007200
H	-2.81066300	2.72984000	0.59865600
H	-3.57727900	1.80586800	-0.68347400
F	-7.21697100	-0.67638400	1.21586700
S	-5.09296900	-2.85950600	1.43089700
C	-1.29112800	0.56344900	0.24678400
C	-0.30908400	-0.43529200	0.87807300
H	-0.87428100	1.57911000	0.32005900
H	-0.75210700	-1.44391200	0.92053200
H	-1.41876200	0.38083600	-0.83537200
H	-0.15389300	-0.15042500	1.93329600
C	1.67500900	2.78831000	-0.34253500
C	1.18736200	3.98189600	0.15012500
C	1.07265400	5.04800800	-0.74085100
C	1.45592900	4.89479000	-2.07416700
C	1.96177600	3.68020700	-2.53135400

C	2.06246800	2.58844300	-1.66170600
H	0.90649100	4.06623700	1.19462600
H	0.69014300	6.00027200	-0.38715200
H	1.37633600	5.73135700	-2.76145000
H	2.29114900	3.58561300	-3.56197200
C	1.96181900	0.56479500	-3.68280600
H	2.72923400	-0.00007300	-4.22285300
H	1.76846900	1.47877500	-4.24931900
C	0.70257000	-0.27071100	-3.49377100
H	0.35636700	-0.57932200	-4.49232700
H	-0.10397500	0.32910400	-3.05600300
C	0.95695200	-1.50517500	-2.67391600
H	1.89170100	-2.03452500	-2.87519800
C	0.08748200	-2.03595100	-1.79716000
H	-0.88129100	-1.58223800	-1.60603600
H	0.28851000	-2.98497300	-1.30866100
F	1.79664400	1.72245500	0.53096500
S	2.78971000	1.02089100	-2.10475900

110

TS3$_{1g}$, Esol(SCF Done) = -3160.453959 a.u.

Sc	-1.85662600	0.56934100	-0.48383400
S	-5.55125400	0.66114200	-0.21213800
Si	5.52669800	-3.25079800	-0.60096200
C	4.52296700	-1.79195800	0.12229500
H	5.24650600	-1.00853800	0.38165900
H	4.08873800	-2.12650000	1.07703600
C	6.81030300	-3.78311800	0.68659700
H	7.47972500	-2.95413700	0.94315800
H	7.42747400	-4.60693700	0.31002100
H	6.33038300	-4.12211900	1.61200000

C	6.39249600	-2.70777100	-2.19935300
H	5.67393300	-2.42028200	-2.97567400
H	7.00678500	-3.52099800	-2.60295200
H	7.05269100	-1.85133700	-2.01954600
C	4.36015800	-4.70617800	-0.97702600
H	3.84007400	-5.04070300	-0.07102100
H	4.92417100	-5.56100400	-1.36777200
H	3.60758600	-4.43749700	-1.72811100
C	-3.26267600	2.51561400	0.19631400
C	-2.18377800	2.37314100	1.14313200
C	-2.29415800	1.12662000	1.81955100
C	-3.48065100	0.48173300	1.36388800
C	-4.04765300	1.33124300	0.37434200
C	-4.24744300	-0.72432200	1.60453200
C	-5.39613800	-0.73831200	0.84841900
C	-1.15547600	3.41408200	1.48044100
H	-0.81605900	3.97358200	0.60385000
H	-0.27714500	2.96819800	1.95865400
H	-1.57036700	4.14138900	2.18973100
C	-6.50603400	-1.74109300	0.84354500
H	-6.44892900	-2.37172300	1.73480200
H	-6.46482600	-2.39397800	-0.03778700
H	-7.48396000	-1.24704900	0.83914700
Si	-3.88521900	4.12958900	-0.61975100
C	-2.57131300	5.05290200	-1.62989300
H	-3.00039700	6.01297900	-1.94235400
H	-1.66331700	5.28011400	-1.06192300
H	-2.29053100	4.51622400	-2.54249300
C	-4.49183300	5.24511100	0.78389800
H	-4.94696700	6.15512300	0.37550800

H	-5.24568300	4.73488600	1.39328700
H	-3.67320000	5.55043700	1.44444200
C	-5.33428200	3.72604300	-1.77234100
H	-6.19677000	3.33008700	-1.22602600
H	-5.65913200	4.64986500	-2.26610800
H	-5.07159100	3.01209500	-2.56151600
C	-3.85161800	-1.75454800	2.58882200
C	-3.42767400	-1.37567100	3.87281500
C	-3.87803800	-3.12082900	2.26886800
C	-3.04817800	-2.33493700	4.80801900
H	-3.42498300	-0.32369800	4.14661500
C	-3.49895800	-4.07977400	3.20649900
H	-4.18905500	-3.43201500	1.27460200
C	-3.08222300	-3.69007700	4.47846200
H	-2.73508600	-2.02368700	5.80107400
H	-3.52918400	-5.13350100	2.94166200
H	-2.78938100	-4.43763800	5.21051700
H	-1.61655700	0.76697100	2.58707500
C	7.07166000	1.66614000	1.02375300
C	8.24081700	1.67785800	0.27748900
C	8.55170900	2.80766200	-0.47679800
C	7.68534400	3.90001600	-0.48375200
C	6.50445400	3.85787700	0.25406600
C	6.17237100	2.73718400	1.02776900
H	8.89820800	0.81461200	0.31407400
H	9.47084600	2.83065000	-1.05515100
H	7.92328200	4.78327000	-1.06935500
H	5.82001600	4.70144200	0.24338600
C	3.82019000	1.26046600	1.62387000
H	2.92889100	1.31305500	2.26210800

H	4.39953200	0.39388400	1.94781800
C	3.41721600	1.16021700	0.15501700
H	4.31881300	1.16878700	-0.47126400
H	2.86702700	2.07336000	-0.10406200
C	2.57474500	-0.09465600	-0.17825800
H	2.12701800	-0.47491300	0.75566700
C	3.42084300	-1.23365700	-0.78310500
H	2.74002700	-2.04947600	-1.06952900
H	3.86187000	-0.86991400	-1.72328800
F	6.79731600	0.57043500	1.76060000
S	4.72595500	2.79103400	2.05730800
C	1.41230800	0.24907400	-1.14005600
C	0.33277300	1.15045400	-0.54888600
H	0.97366700	-0.69568500	-1.49663800
H	0.70840100	2.15227900	-0.32889000
H	1.84157100	0.72969700	-2.03091800
H	0.04537000	0.74597400	0.46242500
C	-1.07855100	-2.66208900	-0.77325900
C	-0.13739700	-3.65514300	-0.59047000
C	-0.19643500	-4.75935100	-1.44044000
C	-1.18475400	-4.84031700	-2.42313400
C	-2.12981600	-3.82664400	-2.56183800
C	-2.08122000	-2.69844300	-1.73387700
H	0.61345400	-3.56295400	0.18686900
H	0.53086600	-5.55715200	-1.32735300
H	-1.23098500	-5.70674000	-3.07565400
H	-2.91691300	-3.91257800	-3.30547700
C	-3.20648500	-0.75981700	-3.48115300
H	-4.14739000	-0.20938000	-3.59482600
H	-3.23018900	-1.60292400	-4.17760500

C	-2.00400000	0.14903500	-3.68376100
H	-2.03984300	0.52201700	-4.71991500
H	-1.08093400	-0.44246500	-3.60960900
C	-1.97029600	1.31016000	-2.70846900
H	-2.87507800	1.91604000	-2.64145300
C	-0.76399300	1.90648400	-2.33875200
H	0.15708200	1.61818000	-2.83565800
H	-0.77378800	2.92271200	-1.95729600
F	-1.02291400	-1.55015900	0.05697300
S	-3.30923900	-1.40496100	-1.76231400

110

$P3_{1g}$, Esol(SCF Done) = -3160.486816 a.u.

Sc	-2.52489700	0.33627600	-0.05630800
S	-5.15534400	1.87616600	-1.79587400
Si	7.25228500	-0.86313300	-3.05923100
C	6.08523500	-1.17111500	-1.57651700
H	6.66184900	-0.94361900	-0.67037500
H	5.87508500	-2.25082100	-1.53547100
C	8.77704700	-1.96984200	-2.84604700
H	9.28815500	-1.76185800	-1.89898800
H	9.49678900	-1.81005100	-3.65720400
H	8.50126600	-3.03081300	-2.84971700
C	7.78033200	0.96031900	-3.09073800
H	6.92409300	1.62855300	-3.23893000
H	8.48818500	1.14515700	-3.90715100
H	8.27149300	1.24683900	-2.15344400
C	6.37072000	-1.29562900	-4.68576300
H	6.03523700	-2.33948600	-4.69155100
H	7.04622500	-1.16023700	-5.53849400
H	5.49519000	-0.65791200	-4.85497100

C	-2.89680800	2.72331600	-0.05000700
C	-2.67995000	2.35507600	1.32914700
C	-3.69303200	1.45697200	1.76128700
C	-4.62752300	1.29955900	0.69307900
C	-4.12548600	2.06181400	-0.39666800
C	-5.82676500	0.55199300	0.37569900
C	-6.23410600	0.79617500	-0.91805600
C	-1.60374000	2.88397000	2.23462100
H	-0.62897700	2.95108900	1.74424900
H	-1.49475300	2.25797700	3.12631300
H	-1.86306900	3.89365900	2.57742200
C	-7.46136100	0.31164400	-1.62351800
H	-8.18653300	-0.07043700	-0.90007900
H	-7.23614500	-0.49182600	-2.33637600
H	-7.93786700	1.12209500	-2.18595300
Si	-2.09356600	4.12598600	-1.06959100
C	-0.21316700	4.22279300	-0.86169400
H	0.15720200	5.04076000	-1.49190800
H	0.09435900	4.44530600	0.16489400
H	0.29219800	3.30810300	-1.18965900
C	-2.87833500	5.74680000	-0.48659600
H	-2.49886100	6.59015000	-1.07543200
H	-3.96776700	5.72023900	-0.59859600
H	-2.65286600	5.94641100	0.56685300
C	-2.48258700	3.84038000	-2.90124600
H	-3.55184200	3.93124600	-3.12043200
H	-1.96559100	4.59951700	-3.50037900
H	-2.14152700	2.85821500	-3.24779800
C	-6.53094000	-0.30078900	1.35679500
C	-6.75062200	0.16767100	2.66242200

C	-6.98474500	-1.58580000	1.02086100
C	-7.41119200	-0.62271400	3.59907100
H	-6.42664400	1.16942600	2.93298800
C	-7.64667200	-2.37498800	1.95963800
H	-6.80899500	-1.97228000	0.02004600
C	-7.86181500	-1.89633200	3.25116000
H	-7.58401800	-0.23858100	4.60081800
H	-7.99450900	-3.36615300	1.68059000
H	-8.38078100	-2.51035100	3.98198100
H	-3.76261000	1.02195800	2.75280300
C	8.04511700	-0.12053200	2.19679700
C	9.08689100	0.77556900	2.00662500
C	9.08221700	1.97932300	2.70865300
C	8.03291900	2.27361200	3.57826300
C	6.98443400	1.37003300	3.73623300
C	6.96875600	0.14885400	3.04834600
H	9.89291900	0.51010900	1.32948200
H	9.89930900	2.68231700	2.57415900
H	8.02449800	3.21026300	4.12823400
H	6.15768700	1.59916000	4.40272000
C	5.02255600	-1.44869200	1.73197500
H	4.22990900	-2.17246200	1.96011000
H	5.79054200	-1.97791200	1.16449600
C	4.45541600	-0.26455300	0.95414900
H	5.25016700	0.47409700	0.78664500
H	3.71729300	0.23619400	1.59368400
C	3.82262300	-0.65592500	-0.40506400
H	3.60908600	-1.73813200	-0.39305400
C	4.76824600	-0.38901600	-1.59344200
H	4.22419700	-0.62113100	-2.52059200

H	4.97597700	0.69120600	-1.62924400
F	8.07789100	-1.28676600	1.52223700
S	5.67945300	-1.02440600	3.38822200
C	2.48406700	0.07204800	-0.62959400
C	1.35007500	-0.40563100	0.28043600
H	2.17668900	-0.05709300	-1.67655600
H	1.63566200	-0.28465100	1.33356500
H	2.63477900	1.15312400	-0.48803900
H	1.18612800	-1.48093900	0.13007600
C	-3.04566300	-2.88645200	0.42564700
C	-3.00741900	-3.99354100	1.24725600
C	-3.31884900	-5.22667800	0.67395900
C	-3.66006000	-5.31124200	-0.67658000
C	-3.69738500	-4.16562300	-1.46810900
C	-3.37687900	-2.91552500	-0.92346900
H	-2.74503300	-3.89167500	2.29508400
H	-3.29843800	-6.11976600	1.29079800
H	-3.90838200	-6.27302000	-1.11448700
H	-3.98231800	-4.22821700	-2.51452000
C	-1.84163900	-1.49101300	-2.81672800
H	-1.95210400	-0.71046800	-3.57826600
H	-1.78808000	-2.45877500	-3.32568700
C	-0.65857600	-1.21764700	-1.89760600
H	0.26022800	-1.37198200	-2.48682100
H	-0.63422800	-2.00426800	-1.12766200
C	-0.72371700	0.17705300	-1.26764300
H	-0.47823600	0.95466600	-1.99661200
C	0.03958700	0.36662200	0.03541900
H	0.22926700	1.43609600	0.18673600
H	-0.61090900	0.09674400	0.93680000

F	-2.72973200	-1.65422000	1.00165700
S	-3.45388900	-1.42629200	-1.90552900

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C3$_E$, Esol(SCF Done) = -2353.379042 a.u.

Sc	-0.63189300	0.75295300	0.74461200
S	-2.52192900	1.15404300	-2.36933400
Si	7.45574900	-0.15555600	-0.06125200
C	5.72312200	-0.15252200	-0.88160300
H	5.58539300	-1.14250300	-1.33855900
H	5.75446900	0.56620700	-1.71462200
C	8.72759000	-0.62235900	-1.38616400
H	8.52652000	-1.61664200	-1.80167700
H	9.74005000	-0.63679700	-0.96653400
H	8.72211400	0.09542400	-2.21458100
C	7.49058000	-1.42991400	1.34540300
H	6.77529500	-1.18114700	2.13805200
H	8.48604900	-1.47084400	1.80245200
H	7.25386300	-2.43586000	0.97911800
C	7.84204300	1.57026600	0.62566500
H	7.80653500	2.33045900	-0.16336600
H	8.84792600	1.59241900	1.06079100
H	7.13856100	1.86683700	1.41230400
C	-2.14671200	2.61743700	0.18974100
C	-2.51910400	2.16501000	1.50552600
C	-2.98346600	0.82203600	1.45253700
C	-3.01076900	0.42536000	0.08629300
C	-2.47287900	1.51058400	-0.66015300
C	-3.45352800	-0.68358500	-0.73362000
C	-3.28211600	-0.40681700	-2.06996300
C	-2.60800600	3.01604400	2.74084100

H	-1.88840600	3.83800200	2.74302900
H	-2.47749500	2.43108500	3.65834100
H	-3.60616100	3.46933600	2.79909000
C	-3.66695200	-1.23124200	-3.25685000
H	-4.39870000	-1.99066600	-2.96819600
H	-2.80123900	-1.74386700	-3.69583900
H	-4.11257900	-0.61034600	-4.04171200
Si	-1.78632800	4.39794900	-0.39670400
C	-0.65527400	5.35056400	0.79326500
H	-0.30883100	6.26215500	0.29146300
H	-1.17563100	5.66690700	1.70333600
H	0.23238700	4.77670400	1.07906200
C	-3.45545500	5.28632300	-0.51367800
H	-3.31953200	6.31136200	-0.87833500
H	-4.12977400	4.76978500	-1.20563700
H	-3.95198700	5.34216800	0.46149100
C	-0.97948700	4.34876000	-2.10829100
H	-1.62855100	3.88771000	-2.86052200
H	-0.78436000	5.37647700	-2.43777400
H	-0.02337100	3.81565500	-2.10055700
C	-4.08408400	-1.90166000	-0.18023300
C	-5.07933800	-1.79131500	0.80480900
C	-3.71313400	-3.18371400	-0.61393900
C	-5.68645500	-2.92710600	1.33372400
H	-5.39945800	-0.80581400	1.13307800
C	-4.32269700	-4.31976700	-0.08428800
H	-2.93381400	-3.29027600	-1.36392600
C	-5.31043000	-4.19566800	0.89135700
H	-6.46439100	-2.82081100	2.08517900
H	-4.02431600	-5.30411700	-0.43560800

H	-5.78827200	-5.08113300	1.30148000
H	-3.34106400	0.24595100	2.29938100
C	-0.15658100	-2.61739500	1.01549000
C	-0.04902000	-3.73784600	1.81452900
C	0.40837000	-4.91230800	1.21835400
C	0.72816100	-4.93133600	-0.14006200
C	0.58846800	-3.78376200	-0.91680900
C	0.14736500	-2.58637700	-0.33918700
H	-0.31725500	-3.69013500	2.86479100
H	0.50698500	-5.81193900	1.81772900
H	1.07759800	-5.84944700	-0.60231100
H	0.81840000	-3.81467700	-1.97766900
C	1.46675300	-0.85311200	-2.16576600
H	1.31559300	0.10066000	-2.68345700
H	1.46648000	-1.63039600	-2.93609100
C	2.76768800	-0.88314200	-1.37082800
H	3.55043800	-1.11895600	-2.10261000
H	2.75313700	-1.73366700	-0.67365800
C	3.18366900	0.38908900	-0.62495400
H	3.29616800	1.19664900	-1.36391700
C	4.55704500	0.18818300	0.05261600
H	4.78863800	1.11787800	0.59114800
H	4.45875700	-0.59027100	0.82541000
F	-0.60604900	-1.44384000	1.60595900
S	-0.12686400	-1.09155900	-1.26305500
C	2.14239700	0.86729600	0.41645900
C	1.05215400	1.83877500	-0.05999100
H	2.68600500	1.33244500	1.24745900
H	0.94498000	1.82766700	-1.15449400
H	1.71550800	-0.06094600	0.88248400

H	1.28023900	2.87070600	0.22033500
C	0.15784000	0.67258000	3.49911700
C	0.57997700	1.90725200	3.18970000
H	0.84491700	-0.17015400	3.52681100
H	1.61731500	2.10691700	2.94034300
H	-0.86579700	0.47979500	3.81646000
H	-0.08273400	2.76565800	3.22591000

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TS3$_E$, Esol(SCF Done) = -2353.367511 a.u.

Sc	0.75444400	0.63077900	-1.00876100
S	1.86881600	1.32672700	2.43838000
Si	-7.48065200	-0.41239300	0.30415700
C	-5.65766200	-0.45668700	0.89993400
H	-5.52982000	-1.39458500	1.45850100
H	-5.53041300	0.35458300	1.63277700
C	-8.59363500	-0.59801200	1.82613600
H	-8.40838300	-1.54588700	2.34463200
H	-9.65121400	-0.57860800	1.53892500
H	-8.42960400	0.21503800	2.54276600
C	-7.78907700	-1.84255500	-0.90405800
H	-7.16894100	-1.75770300	-1.80399600
H	-8.83645800	-1.85253800	-1.22720800
H	-7.57841000	-2.81231000	-0.43801000
C	-7.82965800	1.24325800	-0.55444600
H	-7.63358600	2.08949800	0.11436100
H	-8.88091800	1.30060900	-0.85968000
H	-7.22022900	1.37553800	-1.45597700
C	1.69470800	2.75000600	-0.17166300
C	2.41311300	2.43032400	-1.37976500
C	3.12738700	1.21466500	-1.21398100

C	2.96518600	0.78928100	0.13571100
C	2.07427300	1.71283000	0.74547000
C	3.46539600	-0.22511800	1.03914100
C	2.98502900	-0.03300500	2.31198700
C	2.53164600	3.29577300	-2.60242200
H	1.57164700	3.65628200	-2.98311900
H	3.04158000	2.76470100	-3.41260200
H	3.13722400	4.18188800	-2.37449900
C	3.29412900	-0.79902000	3.55833900
H	4.20786800	-1.38408900	3.42309400
H	2.48541800	-1.49241300	3.82365500
H	3.44341300	-0.12685100	4.41046300
Si	0.90647100	4.41471700	0.32818900
C	-0.10771700	5.20647000	-1.06378400
H	-0.53885200	6.14224200	-0.68755800
H	0.50063100	5.46208000	-1.93701000
H	-0.94138300	4.57583200	-1.39129800
C	2.32969100	5.56972000	0.80278700
H	1.94250000	6.53674700	1.14471700
H	2.93002800	5.14100800	1.61269400
H	2.99634000	5.75814400	-0.04602100
C	-0.22084100	4.15511800	1.82962400
H	0.33044600	3.79569100	2.70514900
H	-0.67163400	5.11614300	2.10530000
H	-1.03970400	3.45615600	1.62636500
C	4.41881300	-1.27917800	0.62968200
C	5.55187500	-0.94764100	-0.13063300
C	4.21609100	-2.62329800	0.97795700
C	6.45582900	-1.93054300	-0.52472300
H	5.73807100	0.09192300	-0.38796500

C	5.12230200	-3.60593200	0.58307300
H	3.33603200	-2.89966700	1.55305500
C	6.24428400	-3.26302800	-0.16968400
H	7.33388600	-1.65366400	-1.10216400
H	4.95023900	-4.64167400	0.86419100
H	6.95236300	-4.02849300	-0.47503000
H	3.74830300	0.74526600	-1.96949400
C	0.79480800	-2.78052100	-1.29194000
C	0.90874200	-3.86751800	-2.13430200
C	0.37341100	-5.07938900	-1.69834000
C	-0.24136400	-5.16486600	-0.44868000
C	-0.32405200	-4.04863000	0.38135800
C	0.19189400	-2.81739400	-0.03999800
H	1.40141900	-3.76450700	-3.09556000
H	0.44337900	-5.95479300	-2.33626000
H	-0.65216900	-6.11111000	-0.11012100
H	-0.78678900	-4.13522500	1.35957800
C	-1.38602500	-1.31900600	1.82496000
H	-1.33043400	-0.38036000	2.38931800
H	-1.31905500	-2.12619200	2.56121400
C	-2.68307000	-1.42223000	1.02983900
H	-3.44921600	-1.67110500	1.77526500
H	-2.64101500	-2.28315900	0.34796000
C	-3.14275400	-0.17588000	0.26491500
H	-3.11569300	0.67687800	0.96115000
C	-4.60721500	-0.32530900	-0.20674700
H	-4.83854000	0.55924100	-0.81685400
H	-4.67025300	-1.18519600	-0.89072500
F	1.31654400	-1.56844000	-1.71562800
S	0.23282800	-1.33961500	0.94532300

C	-2.22697200	0.15597200	-0.94544900
C	-1.31471000	1.37165600	-0.78568900
H	-2.86235700	0.33522300	-1.82195000
H	-0.83313300	1.38886900	0.23095400
H	-1.65247700	-0.75004100	-1.21561500
H	-1.86701600	2.31147300	-0.83520600
C	0.39149300	0.78963800	-3.32339800
C	-0.61147700	1.65789800	-2.91527900
H	0.12420000	-0.19552600	-3.70261100
H	-1.65376600	1.41778000	-3.09349500
H	1.36004300	1.17397300	-3.62862900
H	-0.40677700	2.71907600	-2.81047400

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P3$_E$, Esol(SCF Done) = -2353.406372 a.u.

Sc	0.82945200	0.47424100	-0.99577500
S	1.31487400	1.55716300	2.41075400
Si	-7.16581600	-0.71698000	0.67031900
C	-5.26644900	-0.75363100	0.93848900
H	-5.06123100	-1.55512300	1.66362000
H	-4.98370200	0.18443200	1.43975500
C	-7.98375900	-0.46310000	2.36049800
H	-7.73289400	-1.27522800	3.05272800
H	-9.07519200	-0.43578400	2.26386300
H	-7.66793800	0.48053200	2.82028400
C	-7.73287200	-2.36222700	-0.08488400
H	-7.28702800	-2.53510100	-1.07123900
H	-8.82160200	-2.36986000	-0.21184800
H	-7.47031400	-3.21002800	0.55876700
C	-7.61544800	0.71533500	-0.48974900
H	-7.27347400	1.67705900	-0.08952600

H	-8.70253400	0.77849000	-0.61534400
H	-7.17824000	0.58776600	-1.48685100
C	1.01065100	2.78978400	-0.28218000
C	1.88250600	2.62665300	-1.42257500
C	2.89875000	1.68383000	-1.11379600
C	2.76287900	1.31196700	0.25852600
C	1.60837700	1.97804100	0.74174200
C	3.39530800	0.45579100	1.23968600
C	2.73954700	0.51939500	2.44764400
C	1.81431000	3.38096300	-2.71699600
H	0.79632400	3.46242900	-3.10556600
H	2.43142600	2.89834400	-3.48071100
H	2.19973800	4.39986900	-2.58189600
C	3.09670800	-0.12954600	3.74685500
H	4.14115400	-0.45262000	3.73129100
H	2.47383600	-1.01028400	3.95026900
H	2.96810600	0.56424000	4.58486800
Si	-0.26484500	4.17074100	0.07494300
C	-1.20234900	4.73846100	-1.46702100
H	-1.94886300	5.48203600	-1.16222000
H	-0.54659700	5.21880100	-2.19957600
H	-1.73727200	3.92253500	-1.96392400
C	0.71455400	5.61911900	0.79825200
H	0.04091900	6.44086300	1.06816900
H	1.25951900	5.31876900	1.69978700
H	1.44320200	6.00516200	0.07696300
C	-1.51405600	3.54596200	1.35873200
H	-1.03984100	3.27885900	2.30928800
H	-2.23388800	4.34539700	1.57213800
H	-2.08510600	2.68035300	1.00368600

C	4.62086600	-0.32437800	0.96625100
C	5.69862800	0.27290500	0.29287900
C	4.73582500	-1.66738200	1.35699000
C	6.85791900	-0.45044400	0.02585200
H	5.63548500	1.31867600	0.00302600
C	5.89717700	-2.38966600	1.08908900
H	3.90398900	-2.15107500	1.86287900
C	6.96142800	-1.78381400	0.42288500
H	7.68689400	0.03155400	-0.48545700
H	5.96950100	-3.42835900	1.40085400
H	7.86798400	-2.34603200	0.21659700
H	3.67179700	1.35444100	-1.79977100
C	1.71686400	-2.70396500	-1.24698600
C	2.20222700	-3.65353700	-2.12061900
C	1.78618300	-4.97163800	-1.93244900
C	0.91763600	-5.28826100	-0.88811300
C	0.45545400	-4.30112100	-0.01885100
C	0.84855700	-2.96976200	-0.19372700
H	2.88069800	-3.36597500	-2.91695200
H	2.14578500	-5.74671100	-2.60171500
H	0.59886800	-6.31557800	-0.74074600
H	-0.20786000	-4.57150400	0.79615900
C	-1.24891800	-2.07024600	1.54004300
H	-1.43217400	-1.26231600	2.25828800
H	-1.08401900	-2.97728000	2.13022800
C	-2.43001300	-2.22818600	0.58844000
H	-3.24107300	-2.61635800	1.21905500
H	-2.22673100	-3.01175300	-0.15348200
C	-2.89705700	-0.94027800	-0.10912100
H	-2.66336100	-0.09513600	0.56092900

C	-4.42536800	-0.93347800	-0.32838400
H	-4.66494400	-0.12643900	-1.03426500
H	-4.70144400	-1.86700600	-0.84101200
F	2.12293500	-1.38660000	-1.41960100
S	0.40559400	-1.61344500	0.87271600
C	-2.15989600	-0.71319100	-1.44352600
C	-1.96400400	0.76047600	-1.80054100
H	-2.71168900	-1.20319800	-2.25874500
H	-1.43728000	1.28138800	-0.96156700
H	-1.18823900	-1.23509300	-1.43261700
H	-2.93722800	1.26854400	-1.81400300
C	0.21587500	0.42740100	-3.07933500
C	-1.21103400	0.99590900	-3.11951200
H	0.20518200	-0.64919800	-3.33194500
H	-1.80990300	0.57336300	-3.94074400
H	0.85771900	0.90638200	-3.82660900
H	-1.17163100	2.07612400	-3.30360500