Supporting Information for

On the diastereoselectivity of the addition of propargylic magnesium reagents to fluorinated aromatic sulfinyl imines

Alberto Llobat, Jorge Escorihuela, Santos Fustero and Mercedes Medio-Simón*

Departamento de Química Orgánica, Universitat de València, Av. Vicent Andrés Estellés s/n, 46100 Burjassot, València, Spain.

Email: Mercedes.Medio@uv.es
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I. General Methods.

Reactions were carried out under nitrogen atmosphere unless otherwise indicated. As a heat source oil baths were used. CH$_2$Cl$_2$ (DCM) was used without further purification. The reactions were monitored with the aid of TLC on 0.25 mm pre-coated silica-gel plates. Visualization was carried out with UV light and aqueous ceric ammonium molybdate solution or potassium permanganate stain. Flash column chromatography was performed with the indicated solvents on silica gel 60 (particle size: 0.040–0.063 mm). $^1$H, $^{13}$C and $^{19}$F NMR spectra were recorded on a 300 MHz Bruker Avance III 300 spectrometer. Chemical shifts are given in ppm (δ), referenced to the residual proton resonances of the solvents. Coupling constants (J) are given in Hertz (Hz). The letters m, s, d, t, and q stand for multiplet, singlet, doublet, triplet, and quartet, respectively. The letters br indicate that the signal is broad. DEPT experiments were performed to assign CH, CH$_2$ and CH$_3$. A QTOF mass analyzer system has been used for HRMS measurements. Melting points were measured on a Büchi B–540 apparatus and are uncorrected. Optical rotations were measured on a Jasco P–1020 polarimeter at 25 °C.

II. General procedure for the condensation of N-tert-butanesulfinyl aldimines 1.

![Reaction scheme]

The corresponding aldehyde (5 mmol) was dissolved in DCM (0.1 M) at room temperature in a round-bottomed flask. Titanium tetroxide (IV) (20 mmol) and (R)-tert-butylsulfinamide (6 mmol) were added and the mixture was stirred at room temperature overnight. Once the reaction was complete (TLC analysis), an aqueous saturated solution of NaHCO$_3$ was added and the mixture was filtered on Celyte® in order to remove the titanium salts. Finally, the filtered organic phase is dried over anhydrous Na$_2$SO$_4$, concentrated under reduced pressure and the crude mixture was purified by column chromatography using deactivated silica gel (n-hexane:EtOAc).
(R,E)-2-Methyl-N-((perfluorophenyl)methylene)propane-2-sulfinamide (1a). According to general procedure from 1.00 g (5.1 mmol) of 2,3,4,5,6-pentafluorobenzaldehyde, compound 1a was obtained as a yellow solid after column chromatography on silica gel using n-hexane:EtOAc (4:1) as eluent (1.28 g, 84% yield). Mp: 96–98 °C; [α]^{25}_D = -55.1 (c 1.0, CHCl₃); \(^1\)H NMR (300 MHz, CDCl₃): δ (ppm) 8.71 (s, 1H), 1.27 (s, 9H); \(^{19}\)F NMR (282 MHz, CDCl₃): δ (ppm) -139.90 – -140.05 (m, 2F), -147.20 – -147.38 (m, 1F), -160.75 – -160.96 (m, 2F); \(^{13}\)C \(^1\)H NMR (75 MHz, CDCl₃): δ (ppm) 151.2, 148.1 – 144.3 (m, 2C – F), 145.3 – 141.5 (m, 1C – F), 139.8 – 135.9 (m, 2C – F), 109.7 – 109.4 (m, 1C), 58.5, 22.5. HRMS (ESI) m/z: [M + H\(^+\)] Calcd for C₁₁H₁₁F₅NOS 300.0403; Found 300.0409.

(R,E)-2-Methyl-N-(2,3,5,6-tetrafluorobenzylidene)propane-2-sulfinamide (1b). According to general procedure from 500 mg (2.81 mmol) of 2,3,5,6-tetrafluorobenzaldehyde, compound 1b was obtained as a white solid after column chromatography on silica gel using n-hexane:EtOAc (4:1) as eluent (636 mg, 80% yield). Mp: 74–76 °C; [α]^{25}_D = -50.6 (c 1.0, CHCl₃); \(^1\)H NMR (300 MHz, CDCl₃): δ (ppm) 8.69 (s, 1H), 7.24 – 7.13 (m, 1H), 1.20 (s, 9H); \(^{19}\)F NMR (282 MHz, CDCl₃): δ (ppm) -138.03 – -138.17 (m, 2F), -141.02 – -141.16 (m, 2F); \(^{13}\)C \(^1\)H NMR (75 MHz, CDCl₃): δ (ppm) 151.9, 147.9 – 144.19 (m, 2C – F), 147.3 – 143.7 (m, 2C – F), 114.4 (t, \(J = 10.8 \) Hz), 109.1 (t, \(J = 22.6 \) Hz), 58.4, 22.4. HRMS (ESI) m/z: [M + H\(^+\)] Calcd for C₁₁H₁₂F₄NOS 282.0579; Found 282.0570.

(R,E)-2-Methyl-N-(2,4,6-trifluorobenzylidene)propane-2-sulfinamide (1c). According to general procedure, from 500 mg (3.12 mmol) of 2,4,6-trifluorobenzaldehyde, compound 1c was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (4:1) as eluent (612 mg, 72% yield); [α]^{25}_D = -64.2 (c 1.0, CHCl₃); \(^1\)H NMR (300 MHz, CDCl₃): δ (ppm) 8.68 (s, 1H), 6.76 – 6.68 (m, 2H), 1.22 (s, 9H); \(^{19}\)F NMR (282 MHz, CDCl₃): δ (ppm) -99.93 (t, \(J = 9.7 \) Hz, 1F), -106.89 (d, \(J = 9.7 \) Hz, 2F); \(^{13}\)C \(^1\)H NMR (75 MHz, CDCl₃): δ (ppm) 164.8 (dt, \(^3\)J\(_{CF} = 257.0 \) Hz, \(^3\)J\(_{CF} = 15.8 \) Hz), 162.7 (ddd, \(^3\)J\(_{CF} = 257.0 \) Hz, \(^3\)J\(_{CF} = 15.8 \) Hz, \(J = 8.5 \) Hz), 152.3, 101.3 (td, \(J = 25.7, 3.9 \) Hz), 58.0, 22.5. HRMS (ESI): m/z Calcd for C₁₁H₁₃F₃NOS [M+H\(^+\)]: 264.0661; Found 264.0664.
(R,E)-N-(2,6-Difluorobenzylidene)-2-methylpropane-2-sulfinamide (1d). According to general procedure, from 500 mg (3.52 mmol) of 2,6-difluorobenzaldehyde, compound 1d was obtained as a white solid after column chromatography on silica gel using n-hexane:EtOAc (4:1) as eluent (783 mg, 91% yield). Mp: 49–51 °C; [α]25o = −61.7 (c 1.0, CHCl3); 1H NMR (300 MHz, CDCl3): δ (ppm) 8.77 (s, 1H), 7.45–7.35 (m, 1H), 6.98–6.91 (m, 2H), 1.23 (s, 9H); 19F NMR (282 MHz, CDCl3): δ (ppm) -110.72 (s, 2F); 13C {1H} NMR (75 MHz, CDCl3): δ (ppm) 163.8 (d, JCF = 5.8 Hz), 160.3 (d, JCF = 5.8 Hz), 153.3, 133.7 (t, J = 11.0 Hz), 112.2 (d, J = 25.2 Hz), 58.0, 22.5. HRMS (ESI) m/z: [M + H]+ Calcd for C11H14F2NOS 246.0759; Found 246.0758.

(R,E)-N-(2-Fluorobenzylidene)-2-methylpropane-2-sulfinamide (1e). According to general procedure, from 500 mg (4.03 mmol) of 2-fluorobenzaldehyde, compound 1e was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (4:1) as eluent (611 mg, 67% yield); [α]25D = −78.3 (c 1.0, CHCl3); 1H NMR (300 MHz, CDCl3): δ (ppm) 8.76 (s, 1H), 7.86 (td, J = 7.6 Hz, 1H), 7.39–7.32 (m, 1H), 7.09 (t, J = 7.6 Hz, 1H), 7.03–6.97 (m, 1H), 1.13 (s, 9H); 19F NMR (282 MHz, CDCl3): δ (ppm) -118.18 (s, 1F); 13C {1H} NMR (75 MHz, CDCl3): δ (ppm) 160.4 (d, JCF = 256.9 Hz), 156.4 (d, J = 5.4 Hz), 134.2 (d, J = 8.8 Hz), 128.6 (d, J = 2.0 Hz), 124.5 (d, J = 3.7 Hz), 122.0 (d, J = 9.4 Hz), 116.2 (d, J = 20.8 Hz), 57.8, 22.6. HRMS (ESI) m/z: [M + H+] Calcd for C13H15FNOS 228.0853; Found 228.0853.

(R,E)-N-benzylidene-2-methylpropane-2-sulfinamide (1f). Spectroscopic data of compound 1f were in agreement with those previously reported.[1]

III. General procedure for the diastereoselective propargylation of sulfinyl imines.

III.a. General procedure for the propargylation reaction to sulfinamides 3 in THF.

First, a 1 M solution of Grignard reagent in diethyl ether was prepared by adding magnesium turnings (214 mg, 11 mmol), mercury chloride (II) (19 mg, 1.7 mol%), two iodine balls and Et₂O (5 mL, 1 M) to a sealed tube under a nitrogen atmosphere. This mixture was cooled to 0 °C and propargyl bromide was added slowly (0.56 mL, 5 mmol). The mixture was then heated an oil
bath and stirred at 35 °C for 1.5 h. After this time, the mixture was cooled to room temperature, the stirring stopped, and the solution was used as a reagent in the next step without purification.

Next, for the asymmetric propargylation, a solution of the corresponding fluorinated imine 1 (1 mmol) in THF (0.1 M) was cooled to −78 °C. The freshly prepared Grignard reagent (1.5 mmol) was slowly added, and the reaction mixture was stirred at this temperature until the reaction was complete (TLC analysis, typically 24 h). The reaction mixture was then quenched with a saturated aqueous solution of NH₄Cl and extracted with EtOAc. The combined organic phases were dried over anhydrous Na₂SO₄, concentrated and the crude mixture was purified by flash column chromatography using deactivated silica gel (n-hexane:EtOAc).

(RS,R)-2-Methyl-N-(1-(perfluorophenyl)but-3-yn-1-yl)propane-2-sulfinamide (3a). According to general procedure, from 506 mg (0.91 mmol) of 1a, compound 3a was obtained as a yellowish oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (383 mg, 67% yield); [α]25°D = +45.4 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 4.89–4.80 (m, 1H), 3.99 (d, J = 10.6 Hz), 2.81 (ddd, J = 16.7, 6.8, 2.6 Hz, 1H), 2.71 (ddd, J = 16.7, 8.2, 2.6 Hz, 1H) 1.98 (t, J = 2.6 Hz, 1H), 1.18 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -142.77 – -142.90 (m, 2F), -154.15 – -154.30 (m, 1F), -161.19 – -161.38 (m, 2F); ¹³C {¹H} NMR (75 MHz, CDCl₃): δ (ppm) 146.6–143.1 (m, 2C–F), 142.9–139.2 (m, 1C–F), 139.0–135.6 (m, 2C–F), 115.2–114.8 (m, 1C), 78.4, 71.6, 56.7, 51.0, 26.3, 22.3 HRMS (ESI) m/z: [M + H⁺] Calcd for C₁₄H₁₅F₅NOS 340.0790; Found 340.0791.

(RS,R)-2-Methyl-N-(1-(2,3,5,6-tetrafluorophenyl)but-3-yn-1-yl)propane-2-sulfinamide (3b). According to general procedure, from 103 mg (0.37 mmol) of 1b, compound 3b was obtained as a white solid after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (71 mg, 61% yield). Mp: 82–84 °C; [α]25°D = +51.2 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.07–6.96 (m, 1H), 4.97–4.88 (m, 1H), 4.04 (d, J = 10.5 Hz), 2.84 (ddd, J = 16.7, 7.0, 2.6 Hz, 1H), 2.74 (ddd, J = 16.7, 7.9, 2.6 Hz, 1H) 1.99 (t, J = 2.6 Hz, 1H), 1.22 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) 138.15 – -138.27 (m, 2F), -143.32 – -143.45 (m, 2F); ¹³C {¹H} NMR (75 MHz, CDCl₃): δ (ppm) 147.8–143.1 (m, 2C–F), 142.9–139.2 (m, 1C–F), 139.0–135.6 (m, 2C–F), 115.2–114.8 (m, 1C), 78.7, 71.4, 56.7, 51.4, 26.4, 22.4 HRMS (ESI) m/z: [M + H⁺] Calcd for C₁₄H₁₆F₄NOS 322.0879; Found 322.0883.
III.b. General procedure for the propargylation reaction to sulfinamides 3’ in DCM.

First, a 1 M solution of Grignard reagent in diethyl ether was prepared by adding magnesium turnings (214 mg, 11 mmol), mercury chloride (II) (19 mg, 1.7 mol%), two iodine balls and Et₂O (5 mL, 1 M) to a sealed tube under a nitrogen atmosphere. This mixture was cooled to 0 °C and propargyl bromide was added slowly (0.56 mL, 5 mmol). The mixture was then stirred at 35 °C for 1.5 h. After this time, the mixture was cooled to room temperature, the stirring stopped, and the solution was used as a reagent in the next step without purification.

Next, for the asymmetric propargylation, a solution of the corresponding fluorinated imine 1 (1 mmol) in DCM (0.1 M) was cooled to −48 °C. The freshly prepared Grignard reagent (1.5 mmol) was slowly added, and the reaction mixture was stirred at this temperature until the reaction was complete (TLC analysis, typically 18–24 h). The reaction mixture was then quenched with a saturated aqueous solution of NH₄Cl and extracted with EtOAc. The combined organic phases were dried over anhydrous Na₂SO₄, concentrated and the crude mixture was purified by flash column chromatography using deactivated silica gel (n-hexane:EtOAc).

(Rₛ,S)-2-Methyl-N-(1-(perfluorophenyl)but-3-yn-1-yl)propane-2-sulfinamide (3’a). According to general procedure, from 51 mg (0.17 mmol) of 1a, compound 3’a was obtained as a yellowish solid after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (46 mg, 80% yield). Mp: 83–85 ºC; [α]²⁵,D = −50.3 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.08–6.97 (m, 1H), 4.99 (q, J = 7.8 Hz, 1H), 4.00 (d, J = 7.4 Hz), 2.97 (ddd, J = 16.6, 6.4, 2.6 Hz, 1H), 2.84 (ddd, J = 16.6, 8.2, 2.6 Hz, 1H) 2.04 (t, J = 2.6 Hz, 1H), 1.18 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -141.91 -142.04 (m, 2F), -153.65 -153.81 (m, 1F), -161.10 -161.30 (m, 2F); ¹³C (¹H) NMR (75 MHz, CDCl₃): δ (ppm) 146.8–143.1 (m, 2C–F), 142.8–139.5 (m, 2C–F), 136.2–135.7 (m, 1C–F), 114.4–113.9 (m, 1C), 78.3, 72.1, 56.4, 50.9, 26.5, 22.3. HRMS (ESI) m/z: [M + H⁺] Calcd for C₁₄H₁₅F₅NOS 340.0790; Found 340.0788.
(R,S)-2-Methyl-N-(1-(2,3,5,6-tetrafluorophenyl)but-3-yn-1-yl)propane-2-sulfinamide (3’b).

According to general procedure, from 517 mg (0.91 mmol) of 1b, compound 3’b was obtained as a white solid after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (405 mg, 68% yield). Mp: 58–60 °C; [α]25D = −49.4 (c 1.0, CHCl3); 1H NMR (300 MHz, CDCl3): δ (ppm) 7.08–6.97 (m, 1H), 5.01 (q, J = 7.8 Hz, 1H), 4.04 (d, J = 7.8 Hz), 2.97 (dd, J = 16.6, 6.4, 2.6 Hz, 1H), 2.84 (ddd, J = 16.6, 8.1, 2.6 Hz, 1H) 2.02 (t, J = 2.6 Hz, 1H), 1.16 (s, 9H); 19F NMR (282 MHz, CDCl3): δ (ppm) -138.28 – -138.41 (m, 2F), -142.64 – -142.77 (m, 2F); 13C (1H) NMR (75 MHz, CDCl3): δ (ppm) 147.7–144.06 (m, 2C–F), 146.2–142.7 (m, 2C–F), 119.9 (t, J = 14.7 Hz, 1C), 105.8 (t, J = 22.6 Hz, 1C), 78.4, 71.9, 56.4, 51.3, 26.5, 22.3. HRMS (ESI) m/z: [M + H+] Calcd for C14H16F3NOS 322.0879; Found 322.0883.

(R,S)-2-Methyl-N-(1-(2,4,6-trifluorophenyl)but-3-yn-1-yl)propane-2-sulfinamide (3’c).

According to general procedure, from 282 mg (0.91 mmol) of 1c, compound 3’c was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (290 mg, 89% yield); [α]25D = −53.4 (c 1.0, CHCl3); 1H NMR (300 MHz, CDCl3): δ (ppm) 6.66–6.56 (m, 2H), 4.89 (q, J = 7.3 Hz, 1H), 3.97 (d, J = 7.3 Hz, 1H), 2.90 (dd, J = 16.6, 6.8, 2.6 Hz, 1H), 2.75 (dd, J = 16.6, 8.0, 2.6 Hz, 1H), 1.96 (t, J = 2.6 Hz, 1H), 1.10 (s, 9H); 19F NMR (282 MHz, CDCl3): δ (ppm) -107.66 (t, JFF = 6.7 Hz, 1F), -110.12 (d, JFF = 6.7 Hz, 2F); 13C (1H) NMR (75 MHz, CDCl3): δ (ppm) 162.2 (dt, JCF = 250 Hz, 3JCF = 15.9 Hz, C-F), 161.2 (dd, JCF = 250 Hz, 3JCF = 14.8, 11.0 Hz, C-F) 112.8 (td, J = 17.1, 4.9 Hz), 101.0–100.2 (m, 1C), 79.1, 71.5, 56.1, 50.3, 26.4, 22.3. HRMS (ESI) m/z: [M + H+] Calcd for C14H12F3NOS 304.0974; Found 304.0977.

(R,S)-N-(1-(2,6-Difluorophenyl)but-3-yn-1-yl)-2-methylpropane-2-sulfinamide (3’d).

According to general procedure, from 223 mg (0.91 mmol) of 1d, compound 3’d was obtained as a white solid after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (179 mg, 70% yield). Mp: 70–72 °C; [α]25D = −44.9 (c 1.0, CHCl3); 1H NMR (300 MHz, CDCl3): δ (ppm) 7.24–7.14 (m, 1H), 6.87–6.78 (m, 2H), 4.94 (dd, J = 14.8, 7.7 Hz, 1H), 4.00 (d, J = 7.7 Hz, 1H), 2.93 (ddd, J = 16.6, 6.7, 2.6 Hz, 1H), 2.77 (ddd, J = 16.6, 8.0, 2.6 Hz, 1H), 1.93 (t, J = 2.6 Hz, 1H), 1.09 (s, 9H); 19F NMR (282 MHz, CDCl3): δ (ppm) -113.52 (s, 2F); 13C (1H) NMR (75 MHz, CDCl3): δ (ppm) 161.0 (d, JCF = 248.7 Hz, 3JCF = 8.1 Hz), 129.8 (t, J = 10.7 Hz), 116.5 (t, J = 16.7 Hz), 111.8 (d, J = 26.2 Hz), 79.3, 71.3, 56.1, 50.8, 26.6, 22.3. HRMS (ESI) m/z: [M + H+] Calcd for C14H12F2NOS 286.1072; Found 286.1073.
(R,S)-N-(1-(2-Fluorophenyl)but-3-yn-1-yl)-2-methylpropane-2-sulfinamide (3′e). According to general procedure, from 74 mg (0.33 mmol) of 1e, compound 3′e was obtained as a white solid after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (76 mg, 86% yield). Mp: 100–102 °C; [α]D = −47.6 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.31 (td, J = 7.5, 1.2 Hz, 1H), 7.25–7.17 (m, 1H), 7.06 (td, J = 7.5, 1.2 Hz, 1H), 6.97 (ddd, J = 10.6, 8.2, 1.2 Hz, 1H), 4.81 (dd, J = 12.2, 5.1 Hz, 1H), 3.95 (d, J = 5.1 Hz, 1H), 2.82–2.64 (m, 2H), 2.02 (t, J = 2.6 Hz, 1H), 1.15 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -117.85 (s, 1F); ¹³C {¹H} NMR (75 MHz, CDCl₃): δ (ppm) 160.4 (d, JCF = 247.3 Hz), 129.5 (d, J = 8.4 Hz), 128.7 (d, J = 4.1 Hz), 127.6 (d, J = 12.5 Hz), 124.1 (d, J = 3.5 Hz), 115.7 (d, J = 21.8 Hz), 79.5, 72.2, 56.0, 51.9, 27.3, 22.5. HRMS (ESI) m/z: [M + H⁺] Calcd for C₁₄H₁₈FNOS 268.1166; Found 268.1163.

(R,S)-N-(1-Phenylbut-3-yn-1-yl)-2-methylpropane-2-sulfinamide (3′f). Spectroscopic data of compound 3′f were in agreement with those previously reported.[¹]

IV. General procedure for the propargylation reaction in DCM.

First, a 1 M solution of Grignard reagent in diethyl ether was prepared by adding magnesium turnings (214 mg, 11 mmol), mercury chloride (II) (19 mg, 1.7 mol%), two iodine balls and Et₂O (5 mL, 1 M) to a sealed tube under a nitrogen atmosphere. This mixture was cooled to 0 °C and the corresponding bromide was added slowly (0.56 mL, 5 mmol). The mixture was then heated an oil bath and stirred at 35 °C for 1.5 h. After this time, the mixture was cooled to room temperature, the stirring stopped, and the solution was used as a reagent in the next step without purification.

For the next asymmetric propargylation, a solution of the corresponding fluorinated imine 1 (1 mmol) in DCM (0.1 M) was cooled to −48 °C. The freshly prepared Grignard reagent (1.5 mmol) was slowly added, and the reaction mixture was stirred at this temperature until the reaction was complete (TLC analysis, typically 18–24 h). The reaction mixture was then quenched with a saturated aqueous solution of NH₄Cl and extracted with EtOAc. The combined
organic phases were dried over anhydrous Na₂SO₄, concentrated and the crude mixture was purified by flash column chromatography using deactivated silica gel (n-hexane:EtOAc).

(R,s)-2-Methyl-N-(1-(perfluorophenyl)-2-phenyl-3λ³-buta-2,3-dien-1-yl)propane-2-sulfinamide (4ab). According to general procedure from 51 mg (0.17 mmol) of 1a, compound 4ab was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (51 mg, 72% yield); [α]²⁰⁰ = −90.9 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.38–7.29 (m, 5H), 5.95–5.92 (m, 1H), 5.44–5.32 (m, 2H), 4.19 (d, J = 4.8 Hz, 1H), 1.17 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -141.48 – -141.58 (m, 2F), -147.20 – -153.90 (t, J = 21.0 Hz, 1F), -161.46 – -161.64 (m, 2F); ¹³C [¹H] NMR (75 MHz, CDCl₃): δ (ppm) 207.4, 147.6–144.0 (m, 2C–F), 146.5–143.0 (m, 2C–F), 132.9, 128.8, 127.8, 126.6, 120.5 (t, J = 13.8 Hz, C–F), 106.6, 105.7 (t, J = 22.6 Hz, C), 83.0, 56.5, 49.0, 22.4. HRMS (ESI) m/z: [M + H⁺]
Calcd for C₂₀H₁₂F₃NOS 416.1099; Found 416.1102.

(R,s)-2-Methyl-N-(2-methyl-1-(perfluorophenyl)-3λ³-buta-2,3-dien-1-yl)propane-2-sulfinamide (4ac). According to general procedure from 53 mg (0.18 mmol) of 1a, compound 4ac was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (54 mg, 85% yield); [α]²⁰⁰ = -93.1 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 5.20–5.15 (m, 1H), 4.99–4.86 (m, 2H), 4.09 (d, J = 6.4 Hz, 1H), 1.73 (t, J = 3.1 Hz, 3H), 1.16 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -142.44 – -142.56 (m, 2F), -147.20 – -154.45 – -154.60 (m, 1F), -161.58 – -161.76 (m, 2F); ¹³C [¹H] NMR (75 MHz, CDCl₃): δ (ppm) 205.0, 146.7–143.0 (m, 2C–F), 142.6–142.1 (m, 1C–F), 139.4–135.6 (m, 2C–F), 115.1–114.6 (m, 1C), 99.0, 79.9, 56.4, 52.4, 22.4, 16.2. HRMS (ESI) m/z: [M + H⁺] Calcd for C₁₅H₁₂F₃NOS 354.0943; Found 354.0946.

(R,s)-2-Methyl-N-(2-phenyl-1-(2,3,5,6-tetrafluorophenyl)-3λ³-buta-2,3-dien-1-yl)propane-2-sulfinamide (4bb). According to general procedure from 50 mg (0.18 mmol) of 1b, compound 4bb was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (48 mg, 68% yield); [α]²⁰⁰ = -61.6 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.39–7.28 (m, 5H), 7.01–6.90 (m, 1H), 5.98–5.94 (m, 1H), 5.44–5.32 (m, 2H), 4.22 (d, J = 5.3 Hz, 1H), 1.17 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) -138.64 – -138.76 (m, 2F), -142.19 – -142.32 (m, 2F); ¹³C [¹H] NMR (75 MHz, CDCl₃): δ (ppm) 207.3, 147.7–144.0 (m, 2C–F), 146.4–143.0 (m, 2C–F), 132.9, 128.8, 127.8, 126.6, 120.5.
(t, J = 13.8 Hz, C), 106.6, 105.7 (t, J = 22.6 Hz, CH), 83.0, 56.5, 49.0, 22.4. HRMS (ESI) m/z: [M + H'] Calcd for C_{20}H_{20}F_{2}NOS 398.1203; Found 398.1196.

**(R,s)-2-Methyl-N-(2-methyl-1-(2,3,5,6-tetrafluorophenyl)-3λ^5-buta-2,3-dien-1-yl)propane-2-sulfinamide (4bc).** According to general procedure from 50 mg (0.18 mmol) of 1b, compound 4bc was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (60 mg, 88% yield); [α]^{25}_{D} = −79.4 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.06–6.95 (m, 1H), 5.23–5.19 (m, 1H), 4.98–4.86 (m, 2H), 4.15 (d, J = 6.9 Hz, 1H), 1.73 (t, J = 3.1 Hz, 3H), 1.15 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) −138.70 (m, 2F), 145.8 (m, 2C); ¹³C {¹H} NMR (75 MHz, CDCl₃): δ (ppm) 205.1, 147.1–144.4 (m, 2C–F), 145.8–143.1 (m, 2C–F), 120.7 (t, J = 14.4 Hz, C), 105.3, 99.1, 79.8, 56.4, 52.8, 22.4, 16.2. HRMS (ESI) m/z: [M + H'] Calcd for C_{19}H_{19}F₄NOS 336.1040; Found 336.1040.

**(R,s)-2-Methyl-N-(2-phenyl-1-(2,4,6-trifluorophenyl)-3λ^5-buta-2,3-dien-1-yl)propane-2-sulfinamide (4cb).** According to general procedure, from 55 mg (0.19 mmol) of 1c, compound 4cb was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (53 mg, 72% yield); [α]^{25}_{D} = −96.4 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.38–7.26 (m, 5H), 6.61–6.55 (m, 2H), 5.91–5.86 (m, 2H), 4.16 (d, J = 5.1 Hz, 1H), 1.15 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) −107.78 (t, J_{CF} = 6.9 Hz, 1F), −109.61 (d, J_{CF} = 6.2 Hz, 2F); ¹³C {¹H} NMR (75 MHz, CDCl₃): δ (ppm) 207.5, 162.2 (dt, J_{CF} = 250 Hz, J_{CF} = 10.6 Hz, C–F), 161.4 (ddd, J_{CF} = 250 Hz, J_{CF} = 14.8, 10.6 Hz, C–F), 131.7, 128.6, 127.6, 126.6, 113.3 (td, J = 16.0, 4.9 Hz), 107.1, 101.0–100.2 (m, 1C), 82.5, 56.3, 48.1, 22.4. HRMS (ESI) m/z: [M + H'] Calcd for C_{20}H_{21}F₃NOS 380.1298; Found 380.1290.

**(R,s)-2-Methyl-N-(2-methyl-1-(2,4,6-trifluorophenyl)-3λ^5-buta-2,3-dien-1-yl)propane-2-sulfinamide (4cc).** According to general procedure, from 53 mg (0.20 mmol) of 1c, compound 4cc was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (43 mg, 68% yield); [α]^{25}_{D} = −153.1 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 6.68–6.62 (m, 2H), 5.18–5.13 (m, 1H), 4.96–4.85 (m, 2H), 4.12 (d, J = 6.5 Hz, 1H), 1.71 (t, J = 3.1 Hz, 3H), 1.15 (s, 9H); ¹⁹F NMR (282 MHz, CDCl₃): δ (ppm) −108.31 (t, J_{CF} = 6.6 Hz, 1F), −110.59 (d, J_{CF} = 6.6 Hz, 2F); ¹³C {¹H} NMR (75 MHz, CDCl₃): δ (ppm) 205.0,
162.0 (dt, $^{1}J_{CF} = 250$ Hz, $^{3}J_{CF} = 15.8$ Hz, C–F), 161.2 (ddd, $^{1}J_{CF} = 250$ Hz, $^{3}J_{CF} = 14.8$, 10.8 Hz, C–F), 113.4 (td, $J = 16.6$, 4.9 Hz), 100.9–100.2 (m, 1C), 99.7, 79.4, 56.2, 51.7, 22.4, 16.2. HRMS (ESI) m/z: [M + H$^+$] Calcd for C$_{15}$H$_{19}$F$_{3}$NOS 318.1135; Found 318.1134.

(R$_{S,S}$)-N-(1-(2,6-Difluorophenyl)-2-phenyl-3$\lambda^3$-buta-2,3-dien-1-yl)-2-methylpropane-2-sulfinamide (4db). According to general procedure, from 55 mg (0.22 mmol) of 1d, compound 4db was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (59 mg, 73% yield); [α]$^{25}_{D} = -96.5$ (c 1.0, CHCl$_3$); $^{1}$H NMR (300 MHz, CDCl$_3$): δ (ppm) 7.38–7.23 (m, 5H), 7.20–7.12 (m, 1H), 6.82–6.76 (m, 2H), 5.94–5.90 (m, 1H), 5.38–5.26 (m, 2H), 4.21 (d, $J = 5.8$ Hz, 1H), 1.13 (s, 9H); $^{19}$F NMR (282 MHz, CDCl$_3$): δ (ppm) -112.94 (s, 2F); $^{13}$C {^1H} NMR (75 MHz, CDCl$_3$): δ (ppm) 207.6, 161.2 (dd, $J = 250$, 7.8 Hz, 2C–F), 133.5, 131.7, 129.6 (t, $J = 10.7$ Hz, 1C), 128.5, 127.4, 126.7, 117.0 (t, $J = 15.8$ Hz, C–F), 111.7 (d, $J = 26.0$ Hz, CH), 82.5, 56.3, 48.6, 22.4. HRMS (ESI) m/z: [M + H$^+$] Calcd for C$_{20}$H$_{22}$F$_2$NOS 362.1380; Found 362.1385.

(R$_{S,S}$)-N-(1-(2,6-Difluorophenyl)-2-methyl-3$\lambda^3$-buta-2,3-dien-1-yl)-2-methylpropane-2-sulfinamide (4dc). According to general procedure, from 60 mg (0.24 mmol) of 1d, compound 4dc was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (6:1) as eluent (51 mg, 70% yield); [α]$^{25}_{D} = -128.7$ (c 1.0, CHCl$_3$); $^{1}$H NMR (300 MHz, CDCl$_3$): δ (ppm) 7.24–7.18 (m, 1H), 6.88–6.82 (m, 2H), 5.22–5.17 (m, 1H), 4.94–4.82 (m, 2H), 4.17 (d, $J = 7.1$ Hz, 1H), 1.69 (t, $J = 3.1$ Hz, 3H), 1.13 (s, 9H); $^{19}$F NMR (282 MHz, CDCl$_3$): δ (ppm) -113.89 (s, 2F); $^{13}$C {^1H} NMR (75 MHz, CDCl$_3$): δ (ppm) 205.0, 161.0 (dd, $J = 250$, 8.0 Hz, 2C–F), 129.3 (t, $J = 10.6$ Hz, 1C), 117.1 (t, $J = 16.3$ Hz, C–F), 111.6 (d, $J = 26.0$ Hz, CH), 99.9, 79.2, 56.2, 52.2, 22.4, 16.2. HRMS (ESI) m/z: [M + H$^+$] Calcd for C$_{20}$H$_{22}$F$_2$NOS 300.1228; Found 300.1228.

(R$_{S,S}$)-N-(1-(2-Fluorophenyl)-2-phenyl-3$\lambda^3$-buta-2,3-dien-1-yl)-2-methylpropane-2-sulfinamide (4eb). According to general procedure, from 51 mg (0.22 mmol) of 1e, compound 4eb was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (10:1) as eluent (46 mg, 61% yield); [α]$^{25}_{D} = -81.7$ (c 1.0, CHCl$_3$); $^{1}$H NMR (300 MHz, CDCl$_3$): δ (ppm) 7.33–7.29 (m, 2H), 7.23–7.08 (m, 5H), 7.02–6.92 (m, 2H), 5.79–5.75 (m, 1H), 5.31–5.18 (m, 2H), 3.83 (d, $J = 4.3$ Hz, 1H), 1.10 (s, 9H); $^{19}$F NMR (282 MHz, CDCl$_3$): δ (ppm) -117.63 (s, 1F); $^{13}$C {^1H} NMR (75 MHz, CDCl$_3$): δ (ppm) 208.4, 160.8 (d, $J = 250$ Hz, C–F), 133.5, 129.5 (d, $J = 8.4$
Hz), 129.4 (d, J = 3.6 Hz), 128.6, 127.7 (d, J = 12.8 Hz), 127.4, 126.6, 124.1 (d, J = 3.6 Hz), 115.5 (d, J = 21.9 Hz), 108.4, 82.5, 56.2, 51.0, 22.5. HRMS (ESI) m/z: [M + H⁺] Calcd for C₃₀H₂ₙNOS 344.1475; Found 344.1479.

(Rₛ,S)-N-(1-{2-Fluorophenyl}-2-methyl-3λ³-buta-2,3-dien-1-yl)-2-methylpropane-2-sulfinamide (4ec). According to general procedure, from 53 mg (0.22 mmol) of 1e, compound 4ec was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (10:1) as eluent (55 mg, 84% yield); [α]²⁵_D = −133.4 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.34–7.22 (m, 2H), 7.14–7.00 (m, 2H), 5.12–5.08 (m, 1H), 4.98–4.88 (m, 2H), 3.88 (d, J = 3.7 Hz, 1H), 1.63 (t, J = 3.1 Hz, 3H), 1.16 (s, 9H); ¹³C [¹H] NMR (75 MHz, CDCl₃): δ (ppm) 133.4 (c 1.0, CHCl₃): δ (ppm) 129.3 (d, J = 2.6 Hz), 127.6 (d, J = 12.7 Hz), 124.1 (d, J = 3.6 Hz), 115.5 (d, J = 22.0 Hz), 101.4, 79.2, 56.1, 53.4, 22.6, 16.3. HRMS (ESI) m/z: [M + H⁺] Calcd for C₁₅H₁₁FNOS 282.1324; Found 282.1322.

(Rₛ,R)-N-(1,2-Diphenyl-3λ³-buta-2,3-dien-1-yl)-2-methylpropane-2-sulfinamide (4fb). According to general procedure, from 55 mg (0.26 mmol) of 1f, compound 4fb was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (10:1) as eluent (44 mg, 52% yield); [α]²⁵_D = −124.4 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.36–7.28 (m, 5H), 4.91–4.87 (m, 2H), 4.87 (m, 1H), 3.88 (d, J = 3.5 Hz, 1H), 1.11 (s, 9H); ¹³C [¹H] NMR (75 MHz, CDCl₃): δ (ppm) 208.2, 140.2, 133.8, 128.5, 128.4, 127.9, 127.3, 126.8, 109.4, 81.9, 57.2, 56.1, 22.6. HRMS (ESI) m/z: [M + H⁺] Calcd for C₁₅H₁₂NOS 326.1572; Found 326.1573.

(Rₛ,R)-2-Methyl-N-(2-methyl-1-phenyl-3λ³-buta-2,3-dien-1-yl)propane-2-sulfinamide (4fc). According to general procedure, from 76 mg (0.36 mmol) of 1f, compound 4fc was obtained as a colorless oil after column chromatography on silica gel using n-hexane:EtOAc (10:1) as eluent (64 mg, 67% yield); [α]²⁵_D = −128.5 (c 1.0, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.28–7.23 (m, 5H), 4.91–4.87 (m, 2H), 4.68–4.65 (m, 1H), 3.83 (d, J = 2.0 Hz, 1H), 1.50 (t, J = 3.0 Hz, 3H), 1.11 (s, 9H); ¹³C [¹H] NMR (75 MHz, CDCl₃): δ (ppm) 204.5, 140.0, 128.4, 128.3, 128.0, 102.1, 78.7, 59.3, 55.9, 22.6, 16.2. HRMS (ESI) m/z: [M + H⁺] Calcd for C₁₅H₁₂NOS 264.1416; Found 264.1417.
V. X-ray structure of compound 3b (Deposition Number 2067822).

Experimental
Single crystals of C_{14}H_{15}F_{4}NOS [CCDC 2067822] were obtained by slow evaporation method at room temperature using chloroform as solvent. A suitable crystal was selected and mounted on a SuperNova, Single source at offset, Atlas diffractometer. The crystal was kept at 150.00(10) K during data collection. Using Olex2,[2] the structure was solved with the ShelXS[3] structure solution program using Direct Methods and refined with the ShelXL[4] refinement package using Least Squares minimization. Displacement ellipsoids are drawn at the 50% probability level.
Table S1. Crystal data and structure refinement for CCDC 2067822.

| Description                        | Value                        |
|------------------------------------|------------------------------|
| Identification code                | CCDC 2067822                 |
| Empirical formula                  | C_{14}H_{15}F_{4}NOS         |
| Formula weight                     | 321.33                       |
| Temperature/K                      | 150.4(5)                     |
| Crystal system                     | monoclinic                   |
| Space group                         | P2_1                         |
| a/Å                                | 7.8963(3)                    |
| b/Å                                | 10.1860(3)                   |
| c/Å                                | 10.2163(4)                   |
| α/°                                | 90.0                         |
| β/°                                | 107.419(4)                   |
| γ/°                                | 90.0                         |
| Volume/Å³                          | 784.04(5)                    |
| Z                                  | 2                            |
| ρ_{calc}/g/cm³                     | 1.361                        |
| μ/mm⁻¹                             | 2.221                        |
| F(000)                             | 332.0                        |
| Crystal size/mm³                   | 0.343 × 0.272 × 0.114        |
| Radiation                          | CuKα (λ = 1.54184)           |
| 2θ range for data collection/°     | 9.072 to 137.984             |
| Index ranges                       | -9 ≤ h ≤ 9, -12 ≤ k ≤ 12, -12 ≤ l ≤ 11 |
| Reflections collected              | 14341                        |
| Independent reflections            | 2909 [R_{int} = 0.0352, R_{sigma} = 0.0300] |
| Data/restraints/parameters         | 2909/2/196                   |
| Goodness-of-fit on F²              | 1.046                        |
| Final R indexes [I>2σ (I)]         | R₁ = 0.0378, wR₂ = 0.0932    |
| Final R indexes [all data]         | R₁ = 0.0431, wR₂ = 0.0977    |
| Largest diff. peak/hole / e Å⁻³    | 0.21/-0.40                   |
| Flack parameter                    | -0.007(10)                   |
| Friedel coverage                   | 99%                          |
| Flack x                            | -0.007(10)                   |
| Hooft y                            | -0.013(5)                    |
| P2(wrong)                          | <10⁻⁹⁹                      |
Table S2. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for CCDC 2067822. U(eq) is defined as 1/3 of the trace of the orthogonalised $U_{ij}$ tensor.

| Atom  | x     | y     | z     | U(eq)  |
|-------|-------|-------|-------|--------|
| S1    | 3522.0(11) | 6708.1(9) | 2607.7(8) | 33.6(2)  |
| F4    | 4687(3)  | 5356(2)  | 6429(2)  | 50.3(6)  |
| F1    | 2501(3)  | 2462(2)  | 2698(2)  | 48.8(6)  |
| F2    | 248(3)   | 1452(3)  | 3927(3)  | 66.0(8)  |
| F3    | 2387(4)  | 4366(3)  | 7621(3)  | 62.5(8)  |
| O1    | 1894(3)  | 6848(3)  | 3034(3)  | 45.9(7)  |
| N1    | 4058(4)  | 5140(3)  | 2522(3)  | 33.4(7)  |
| C5    | 3694(5)  | 3926(4)  | 4536(4)  | 33.8(8)  |
| C10   | 3599(6)  | 4386(4)  | 5788(4)  | 39.1(9)  |
| C1    | 4966(5)  | 4525(4)  | 3852(4)  | 34.1(8)  |
| C3    | 7718(5)  | 4199(4)  | 3220(5)  | 39.9(9)  |
| C6    | 2532(5)  | 2917(4)  | 3947(4)  | 39.5(9)  |
| C9    | 2411(6)  | 3876(4)  | 6411(4)  | 46.0(11) |
| C7    | 1363(5)  | 2402(4)  | 4579(5)  | 45.8(10) |
| C11   | 2858(6)  | 7089(4)  | 767(4)   | 48.6(11) |
| C8    | 1272(5)  | 2878(4)  | 5804(5)  | 47.7(11) |
| C2    | 6338(5)  | 3519(4)  | 3664(4)  | 39.2(9)  |
| C4    | 8790(6)  | 4789(4)  | 2885(5)  | 46.5(10) |
| C14   | 1323(7)  | 6221(6)  | -14(5)   | 66.2(15) |
| C12   | 4480(7)  | 6912(6)  | 264(5)   | 69.5(15) |
| C13   | 2295(10) | 8533(6)  | 710(6)   | 81.0(18) |
Table S3. Anisotropic Displacement Parameters ($\text{Å}^2\times10^3$) for CCDC 2067822. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+...].$

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|------|---------|---------|---------|---------|---------|---------|
| S1   | 34.7(4) | 36.1(4) | 34.8(4) | 1.8(4)  | 17.5(3) | -0.4(4) |
| F4   | 64.6(15)| 46.1(13)| 45.6(14)| -8.6(11)| 24.8(12)| -6.9(12)|
| F1   | 49.3(14)| 52.3(14)| 45.9(14)| -7.0(11)| 15.7(11)| -10.5(11)|
| F2   | 55.8(15)| 66.2(19)| 74.6(18)| 7.5(15) | 17.3(13)| -25.9(14)|
| F3   | 77(2)   | 72.7(19)| 53.9(16)| 5.8(14) | 43.4(15)| 13.5(14)|
| O1   | 44.4(14)| 52.7(16)| 50.1(16)| 1.9(15) | 28.4(12)| 5.7(13) |
| N1   | 36.3(16)| 35.7(16)| 30.7(16)| 0.9(13) | 13.9(13)| 1.2(13) |
| C5   | 32.9(18)| 35.1(18)| 36.3(19)| 6.8(16) | 14.8(16)| 4.6(15) |
| C10  | 43(2)   | 39(2)   | 41(2)   | 7.1(18) | 21.2(19)| 7.3(17) |
| C1   | 36(2)   | 35.6(18)| 34.4(19)| 2.2(15) | 16.4(17)| 0.1(15) |
| C3   | 37(2)   | 44(2)   | 41(2)   | -0.3(18)| 16.0(18)| 4.3(17) |
| C6   | 41(2)   | 40(2)   | 39(2)   | 5.2(17) | 14.1(17)| 2.1(16) |
| C9   | 49(3)   | 52(2)   | 45(3)   | 14(2)   | 27(2)   | 15(2)   |
| C7   | 36(2)   | 44(2)   | 57(3)   | 9(2)    | 15.3(19)| -4.5(18)|
| C11  | 57(3)   | 53(3)   | 40(2)   | 10.6(18)| 20(2)   | 6.8(19) |
| C8   | 36(2)   | 58(3)   | 56(3)   | 23(2)   | 25(2)   | 8.8(18) |
| C2   | 36(2)   | 43(2)   | 43(2)   | 5.2(18) | 17.7(18)| 3.1(17) |
| C4   | 41(2)   | 50(2)   | 57(3)   | -2(2)   | 27(2)   | 1.7(18) |
| C14  | 61(3)   | 89(4)   | 41(2)   | -1(2)   | 4(2)    | 8(3)    |
| C12  | 79(3)   | 95(4)   | 47(3)   | 14(3)   | 38(2)   | 1(3)    |
| C13  | 119(5)  | 61(3)   | 58(3)   | 30(3)   | 19(3)   | 27(3)   |

Table S4. Bond Lengths for CCDC 2067822.

| Atom | Atom | Length/Å |
|------|------|----------|
| S1   | O1   | 1.482(2) |
| S1   | N1   | 1.662(3) |
| S1   | C11  | 1.837(4) |
| F4   | C10  | 1.344(5) |
| F1   | C6   | 1.350(5) |
| F2   | C7   | 1.343(5) |
| F3   | C9   | 1.338(5) |
| N1   | C1   | 1.473(5) |
| C5   | C10  | 1.385(5) |
| C5   | C1   | 1.513(5) |
| C5   | C6   | 1.390(5) |

---S17---
Table S5. Bond Angles for CCDC 2067822.

| Atom | Atom | Atom | Angle/˚ | Atom | Atom | Atom | Angle/˚ |
|------|------|------|---------|------|------|------|---------|
| O1   | S1   | N1   | 111.37(16) | C7   | C6   | C5   | 121.8(4) |
| O1   | S1   | C11  | 105.90(18) | F3   | C9   | C10  | 119.0(4) |
| N1   | S1   | C11  | 98.53(17) | F3   | C9   | C8   | 120.3(4) |
| C1   | N1   | S1   | 114.9(2) | C8   | C9   | C10  | 120.8(4) |
| C10  | C5   | C1   | 121.2(4) | F2   | C7   | C6   | 118.3(4) |
| C10  | C5   | C6   | 116.0(3) | F2   | C7   | C8   | 120.3(4) |
| C6   | C5   | C1   | 122.8(3) | C8   | C7   | C6   | 121.4(4) |
| F4   | C10  | C5   | 119.6(3) | C14  | C11  | S1   | 110.7(3) |
| F4   | C10  | C9   | 118.4(3) | C14  | C11  | C12  | 111.9(4) |
| C9   | C10  | C5   | 122.0(4) | C14  | C11  | C13  | 111.2(4) |
| N1   | C1   | C5   | 112.9(3) | C12  | C11  | S1   | 108.0(3) |
| N1   | C1   | C2   | 109.5(3) | C12  | C11  | C13  | 111.3(4) |
| C5   | C1   | C2   | 112.2(3) | C13  | C11  | S1   | 103.4(3) |
| C4   | C3   | C2   | 177.1(5) | C7   | C8   | C9   | 118.0(4) |
| F1   | C6   | C5   | 119.1(3) | C3   | C2   | C1   | 109.7(3) |
| F1   | C6   | C7   | 119.1(4) | C3   | C2   | C1   | 109.7(3) |

Table S6. Torsion Angles for CCDC 2067822.

| A  | B  | C  | D  | Angle/˚ | A  | B  | C  | D  | Angle/˚ |
|----|----|----|----|---------|----|----|----|----|---------|
| S1 | N1 | C1 | C5 | 88.9(3) | C5 | C1 | C2 | C3 | -170.3(4) |
| S1 | N1 | C1 | C2 | -145.3(3) | C5 | C6 | C7 | F2 | 178.2(4) |
| F4 | C10| C9 | F3 | 0.1(5) | C5 | C6 | C7 | C8 | 1.2(6) |
| F4 | C10| C9 | C8 | -179.7(4) | C10| C5 | C1 | N1 | -117.2(4) |
| F1 | C6 | C7 | F2 | 0.7(6) | C10| C5 | C1 | C2 | 118.5(4) |
| F1 | C6 | C7 | C8 | -176.3(4) | C10| C5 | C6 | F1 | 177.2(3) |
| F2 | C7 | C8 | C9 | -178.2(4) | C10| C5 | C6 | C7 | -0.4(5) |
| F3 | C9 | C8 | C7 | -179.2(4) | C10| C9 | C8 | C7 | 0.5(6) |
| O1 | S1 | N1 | C1 | -79.2(3) | C1 | C5 | C10| F4 | -1.9(6) |
| O1 | S1 | C11| C14| -55.3(4) | C1 | C5 | C10| C9 | 178.2(3) |
| O1 | S1 | C11| C12| -178.0(3) | C1 | C5 | C6 | F1 | -1.4(5) |
| O1 | S1 | C11| C13| 63.9(4) | C1 | C5 | C6 | C7 | -178.9(4) |
| N1 | S1 | C11| C14| 59.9(3) | C6 | C5 | C10| F4 | 179.6(3) |
| N1 | S1 | C11| C12| -62.8(4) | C6 | C5 | C10| C9 | -0.4(6) |
| N1 | S1 | C11| C13| 179.1(4) | C6 | C5 | C1 | N1 | 61.2(4) |
| N1 | C1 | C2 | C3 | 63.5(4) | C6 | C5 | C1 | C2 | -63.1(5) |
| C5 | C10| C9 | F3 | -179.9(4) | C6 | C7 | C8 | C9 | -1.3(6) |
| C5 | C10| C9 | C8 | 0.3(6) | C11| S1 | N1 | C1 | 169.9(3) |
Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for CCDC 2067822.

| Atom  | x     | y     | z     | U(eq) |
|-------|-------|-------|-------|-------|
| H1A   | 5638.4| 5232.15| 4471.87| 41    |
| H8    | 448.01| 2530.47| 6225.37| 57    |
| H2A   | 6888.9| 3056.96| 4540.74| 47    |
| H2B   | 5738.85| 2859.15| 2968.33| 47    |
| H4    | 9660.65| 5267.34| 2612.2 | 56    |
| H14A  | 1730.49| 5309.89| 10.25 | 99    |
| H14B  | 880.82| 6517.29| -968.6 | 99    |
| H14C  | 366.81| 6275.22| 413.08 | 99    |
| H12A  | 5480.32| 7409.25| 857.29 | 104   |
| H12B  | 4209.18| 7234.84| -679.71| 104   |
| H12C  | 4792.5| 5979.41| 293.06 | 104   |
| H13A  | 1300.73| 8622.97| 1092.41| 121   |
| H13B  | 1926.56| 8833.03| -244.99| 121   |
| H13C  | 3295.96| 9065.04| 1246.76| 121   |
| H1    | 3250(60)| 4590(50)| 1970(50)| 97    |
VI. X-ray structure of compound 3’b (Deposition Number 2067817).

Experimental
Single crystals of $\text{C}_{14}\text{H}_{15}\text{F}_4\text{NOS}$ [CCDC 2067817] were obtained by vapour diffusion method using dichloromethane and $n$-hexane (1:1) and slow evaporation in glass vial. A suitable crystal was selected and mounted on a SuperNova, Single source at offset, Atlas diffractometer. The crystal was kept at 150.00(10) K during data collection. Using Olex2,[2] the structure was solved with the ShelXS[3] structure solution program using Direct Methods and refined with the ShelXL[4] refinement package using Least Squares minimization. Displacement ellipsoids are drawn at the 50% probability level.
Table S8. Crystal data and structure refinement for CCDC 2067817.

| Property                      | Value                                      |
|-------------------------------|--------------------------------------------|
| Identification code           | CCDC 2067817                               |
| Empirical formula             | C_{14}H_{15}F_{4}NOS                       |
| Formula weight                | 321.33                                     |
| Temperature/K                 | 150.00(10)                                 |
| Crystal system                | monoclinic                                 |
| Space group                   | P2_1                                       |
| a/Å                           | 8.87345(12)                                |
| b/Å                           | 5.57753(8)                                 |
| c/Å                           | 15.18268(19)                               |
| α/°                           | 90.0                                       |
| β/°                           | 101.7056(13)                               |
| γ/°                           | 90.0                                       |
| Volume/Å³                     | 735.793(18)                                |
| Z                             | 2                                          |
| \(\rho_{\text{calc}}\)/cm³  | 1.450                                      |
| \(\mu\)/mm⁻¹                 | 2.372                                      |
| F(000)                        | 332.0                                      |
| Crystal size/mm³              | 0.297 × 0.165 × 0.067                      |
| Radiation                     | CuKα (\(\lambda = 1.54184\))              |
| 2Θ range for data collection/°| 10.18 to 137.99                            |
| Index ranges                  | -10 ≤ h ≤ 10, -6 ≤ k ≤ 6, -18 ≤ l ≤ 18    |
| Reflections collected         | 13571                                      |
| Independent reflections       | 2686 [\(R_{\text{int}} = 0.0408, R_{\text{sigma}} = 0.0263\)] |
| Data/restraints/parameters    | 2686/2/196                                 |
| Goodness-of-fit on \(F^2\)    | 1.039                                      |
| Final R indexes [\(I \geq 2\sigma (I)\)] | \(R_1 = 0.0330, wR_2 = 0.0877\)            |
| Final R indexes [all data]    | \(R_1 = 0.0342, wR_2 = 0.0891\)            |
| Largest diff. peak/hole / e Å⁻³| 0.30/-0.16                                |
| Flack parameter               | 0.00(2)                                    |
| Friedel coverage              | 99%                                        |
| Flack x                       | -0.007(10)                                 |
| Hooft y                       | -0.013(5)                                  |
| P2(wrong)                     | <10⁻⁹⁹                                     |
Table S9. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for CCDC 2067817. $U_{eq}$ is defined as $1/3$ of the trace of the orthogonalised UIJ tensor.

| Atom | x      | y      | z      | U(eq)   |
|------|--------|--------|--------|---------|
| S1   | 1263.3(7) | 2075.0(13) | 7843.6(3) | 21.78(18) |
| F1   | 4575(2)  | 3228(4)  | 6268.6(11) | 34.6(4)   |
| F2   | 3720(2)  | 3291(4)  | 4482.7(12) | 41.0(5)   |
| F3   | 805(2)   | -3727(4) | 4576.9(12) | 38.8(5)   |
| F4   | 1643(2)  | -3832(4) | 6358.7(11) | 32.2(4)   |
| O1   | 2023(2)  | 3790(4)  | 8548.6(14) | 32.2(5)   |
| N1   | 2294(3)  | -413(5)  | 7835.4(15) | 25.9(5)   |
| C1   | 3632(3)  | -290(6)  | 7400.3(17) | 24.4(6)   |
| C5   | 3122(3)  | -275(5)  | 6386.3(17) | 22.4(6)   |
| C6   | 3617(3)  | 1498(5)  | 5867.7(18) | 24.7(6)   |
| C7   | 3181(3)  | 1532(6)  | 4941.6(18) | 28.5(7)   |
| C8   | 2227(3)  | -206(6)  | 4488.9(18) | 30.0(6)   |
| C9   | 1735(3)  | -1983(6) | 4989.3(18) | 27.4(6)   |
| C10  | 2172(3)  | -2034(6) | 5917.2(19) | 23.9(6)   |
| C11  | 4663(3)  | -2477(6) | 7726.4(18) | 28.9(7)   |
| C12  | 5386(3)  | -2250(6) | 8678(2)   | 32.1(7)   |
| C13  | 5926(4)  | -1967(7) | 9452(2)   | 39.6(8)   |
| C14  | -322(3)  | 646(5)   | 8275.5(17) | 23.2(6)   |
| C15  | 298(4)   | -538(6)  | 9182.5(18) | 29.5(6)   |
| C16  | -1418(3) | 2689(6)  | 8373(2)   | 32.4(7)   |
| C17  | -1090(4) | -1150(6) | 7569(2)   | 32.0(7)   |
Table S10. Anisotropic Displacement Parameters (Å²×10³) for CCDC 2067817. The Anisotropic displacement factor exponent takes the form: -2π²[h²a*²U11+2hka*b*U12+...].

| Atom | U11  | U22  | U33  | U23  | U13  | U12  |
|------|------|------|------|------|------|------|
| S1   | 26.0(3) | 21.8(3) | 16.7(3) | 1.2(2) | 2.3(2) | -1.9(3) |
| F1   | 39.9(9) | 33.8(10) | 30.9(9) | -2.9(8) | 9.1(7) | -13.8(8) |
| F2   | 46.7(11) | 44.8(12) | 31.9(9) | 11.2(8) | 8.8(8) | -11.4(9) |
| F3   | 41.3(10) | 43.8(12) | 28.5(9) | -6.7(8) | 0.0(7) | -15.1(9) |
| F4   | 39.4(9) | 29.7(9) | 26.7(8) | 1.0(7) | 4.7(7) | -11.5(8) |
| O1   | 33.9(10) | 30.5(13) | 29.8(10) | -7.1(9) | 0.4(8) | -6.0(9) |
| N1   | 31.4(12) | 27.1(14) | 21.0(11) | 5.1(9) | 9.5(9) | 2.8(10) |
| C1   | 26.5(12) | 26.7(16) | 20.4(12) | -1.1(11) | 5.5(9) | -3.4(11) |
| C5   | 21.2(11) | 27.5(16) | 18.7(12) | -0.2(11) | 4.8(9) | 1.3(10) |
| C6   | 23.0(12) | 26.3(18) | 25.6(13) | -1.1(10) | 6.3(10) | -1.4(10) |
| C7   | 28.1(13) | 33(2) | 25.2(13) | 7.1(11) | 8.3(10) | 1.2(11) |
| C8   | 29.0(13) | 40.3(18) | 20.3(13) | 1.8(12) | 4.0(10) | 1.4(12) |
| C9   | 24.4(13) | 32.0(17) | 24.4(13) | -5.4(12) | 1.7(10) | -2.8(11) |
| C10  | 22.9(12) | 25.7(15) | 23.2(13) | 0.8(10) | 4.4(10) | -0.4(10) |
| C2   | 24.6(12) | 37(2) | 24.3(12) | -0.9(12) | 2.3(10) | 1.2(12) |
| C3   | 25.5(13) | 41(2) | 28.9(15) | 3.0(12) | 3.1(11) | 1.4(11) |
| C4   | 36.4(16) | 52(2) | 27.8(15) | 4.0(14) | -0.1(12) | 1.6(15) |
| C11  | 27.4(13) | 22.7(15) | 19.8(12) | 0.5(10) | 5.3(10) | -2.1(11) |
| C12  | 38.8(15) | 31.2(16) | 20.1(12) | 4.7(11) | 9.5(11) | 2.0(13) |
| C13  | 32.4(14) | 32(2) | 34.6(14) | 4.1(12) | 10.2(11) | 3.4(12) |
| C14  | 34.5(15) | 30.1(18) | 29.7(14) | -1.8(12) | 2.3(12) | -8.5(13) |

Table S11 Bond Lengths for CCDC 2067817.

| Atom | Atom | Length/Å |
|------|------|----------|
| S1   | O1   | 1.491(2) |
| S1   | N1   | 1.664(3) |
| S1   | C11  | 1.849(3) |
| F1   | C6   | 1.347(3) |
| F2   | C7   | 1.346(3) |
| F3   | C9   | 1.345(3) |
| F4   | C10  | 1.343(3) |
| N1   | C1   | 1.473(3) |
| C1   | C5   | 1.514(3) |
| C1   | C2   | 1.545(4) |
| C5   | C6   | 1.390(4) |
### Table S12. Bond Angles for CCDC 2067817.

| Atom | Atom | Atom | Angle/° | Atom | Atom | Angle/° |
|------|------|------|---------|------|------|---------|
| O1   | S1   | N1   | 111.80(12) | C9   | C8   | C7   | 117.7(2) |
| O1   | S1   | C11  | 106.71(12) | F3   | C9   | C8   | 119.9(2) |
| N1   | S1   | C11  | 95.86(13)  | F3   | C9   | C10  | 118.5(3) |
| C1   | N1   | S1   | 117.3(2)   | C8   | C9   | C10  | 121.6(3) |
| N1   | C1   | C5   | 110.8(2)   | F4   | C10  | C5   | 120.5(2) |
| N1   | C1   | C2   | 107.4(2)   | F4   | C10  | C9   | 118.0(3) |
| C5   | C1   | C2   | 111.4(2)   | C9   | C10  | C5   | 121.5(3) |
| C6   | C5   | C1   | 121.1(3)   | C3   | C2   | C1   | 111.2(3) |
| C6   | C5   | C10  | 116.1(2)   | C4   | C3   | C2   | 176.6(4) |
| C10  | C5   | C1   | 122.8(3)   | C12  | C11  | S1   | 110.23(19) |
| F1   | C6   | C5   | 119.8(2)   | C13  | C11  | S1   | 105.0(2) |
| F1   | C6   | C7   | 118.14(18) | C12  | C11  | C12  | 110.9(2) |
| C7   | C6   | C5   | 122.1(3)   | C14  | C11  | S1   | 107.33(18) |
| F2   | C7   | C6   | 118.8(3)   | C14  | C11  | C12  | 112.2(3) |
| F2   | C7   | C8   | 120.2(2)   | C14  | C11  | C13  | 110.9(2) |
| C8   | C7   | C6   | 121.1(3)   |       |       |       |         |

### Table S13. Torsion Angles for CCDC 2067817.

| A   | B   | C   | D   | Angle/° | A   | B   | C   | D   | Angle/° |
|-----|-----|-----|-----|---------|-----|-----|-----|-----|---------|
| S1  | N1  | C1  | C5  | -75.3(3) | C1  | C5  | C6  | C7  | 179.3(3) |
| S1  | N1  | C1  | C2  | 162.84(18) | C1  | C5  | C10 | F4  | 1.0(4)  |
| F1  | C6  | C7  | F2  | -0.5(4)  | C1  | C5  | C10 | C9  | -179.5(3) |
| F1  | C6  | C7  | C8  | 178.8(3) | C5  | C1  | C2  | C3  | 169.2(2) |
| F2  | C7  | C8  | C9  | 178.8(3) | C5  | C6  | C7  | F2  | -179.2(2) |
| F3  | C9  | C10 | F4  | 0.1(4)   | C5  | C6  | C7  | C8  | 0.1(4)  |
| F3  | C9  | C10 | C5  | -179.5(3) | C6  | C5  | C10 | F4  | 179.6(2) |
| O1  | S1  | N1  | C1  | -78.4(2) | C6  | C5  | C10 | C9  | -0.9(4)  |
| O1  | S1  | C11 | C12 | -56.4(2) | C6  | C7  | C8  | C9  | -0.5(4)  |
| O1  | S1  | C11 | C13 | 63.1(2)  | C7  | C8  | C9  | F3  | -179.8(3) |
| O1  | S1  | C11 | C14 | -178.9(2) | C7  | C8  | C9  | C10 | 0.3(4)  |
| N1  | S1  | C11 | C12 | 58.5(2)  | C8  | C9  | C10 | F4  | -180.0(3) |
| N1  | S1  | C11 | C13 | 177.96(19) | C8  | C9  | C10 | C5  | 0.5(4)  |
| N1  | S1  | C11 | C14 | -64.0(2) | C10 | C5  | C6  | F1  | -178.1(2) |
| N1  | C1  | C5  | C6  | 126.9(3) | C10 | C5  | C6  | C7  | 0.6(4)  |
| N1  | C1  | C5  | C10 | -54.6(4) | C2  | C1  | C5  | C6  | -113.7(3) |
| N1  | C1  | C2  | C3  | -69.3(3) | C2  | C1  | C5  | C10 | 64.8(3)  |
| C1  | C5  | C6  | F1  | 0.5(4)  | C11 | S1  | N1  | C1  | 171.0(2) |
Table S14 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å²×103) for CCDC 2067817.

| Atom  | x     | y     | z     | U(eq) |
|-------|-------|-------|-------|-------|
| H1A   | 4220.77 | 1212.23 | 7595.31 | 29    |
| H8    | 1918.92 | -177.81 | 3852.08 | 36    |
| H2A   | 4033.17 | -3955.75 | 7635.3  | 35    |
| H2B   | 5470.56 | -2615.51 | 7364.99 | 35    |
| H1    | 2510(40) | -1210(70) | 8348(16) | 38    |
| H4    | 6358.76 | -1741.01 | 10072.09 | 48    |
| H12A  | 861.91  | -1997.97 | 9091.41 | 44    |
| H12B  | -561.45 | -951.47  | 9470.08 | 44    |
| H12C  | 991.46  | 573.53   | 9568.43 | 44    |
| H13A  | -870.71 | 3900.06  | 8784.8  | 49    |
| H13B  | -2284.86 | 2061.8   | 8612.87 | 49    |
| H13C  | -1804.17 | 3418.83  | 7782.83 | 49    |
| H14A  | -1445.88 | -322.49  | 6995.27 | 48    |
| H14B  | -1970.65 | -1886.65 | 7764.1  | 48    |
| H14C  | -348.34  | -2396.79 | 7493.96 | 48    |
VII. Computational details.

All DFT geometry optimizations were performed with the dispersion-corrected B97D functional\(^5\) and 6-311+G(2d,2p) basis set as implemented within the Gaussian 16 series of programs.\(^6\) Solvent effects were included with the conductor-like polarizable continuum model (CPCM)\(^7\) to mimic the solvent (CH\_2Cl\_2 or THF) during both geometry optimizations and vibrational analysis. All energies presented for the reactant complex (RC), transition state (TS), and product (P) are given in Hartree. All energies have been corrected with zero-point energies (ZPE). Vibrational frequency calculations were performed at the same level of theory used for optimization. All transition states were verified to have only one negative eigenvalue in the Hessian matrix, describing the motion along the reaction coordinate. In addition, intrinsic reaction coordinate (IRC)\(^8\) calculations were performed at the wB97D/6-311+G(2d,2p) level to verify the expected connections of the first-order saddle points with the local minima found on the potential energy surface. Natural bond orbital (NBO)\(^9\) analysis of charges was performed at TPSS-D3/def2-TZVPP level of theory.\(^10,11\) Optimized structures were illustrated using CYLview20.3.\(^12\)

VIII. Natural bond orbital (NBO) analysis of charges of the different atoms in sulfinyl imines.

![Sulfinyl imine structure](image)

**Table S15.** NBO charges on different atoms of experimentally studied sulfinyl imines based on TPSS-D3/def2-TZVPP calculations.

| Entry | R      | S      | O      | N      | C      |
|-------|--------|--------|--------|--------|--------|
| 1a    | C\_6F\_5 | 1.1809 | -0.8474| -0.5275| 0.0766 |
| 1b    | 2,3,5,6-C\_6H\_4F\_4 | 1.1808 | -0.8478| -0.5243| 0.0772 |
| 1c    | 2,6-C\_6H\_2F\_3 | 1.1805 | -0.8530| -0.5367| 0.0816 |
| 1d    | 2,6-C\_6H\_4F\_2 | 1.1802 | -0.8538| -0.5339| 0.0824 |
| 1e    | 2-C\_6H\_4F | 1.1868 | -0.8561| -0.5688| 0.1005 |
| 1f    | C\_6H\_5 | 1.1863 | -0.8569| -0.5658| 0.1016 |
### Sulfanyl imine 1a

![Structure of Sulfanyl imine 1a](image)

#### Summary of Natural Population Analysis:

| Atom | No | Natural Charge | Core | Valence | Rydberg | Total |
|------|----|----------------|------|---------|---------|-------|
| N    | 1  | -0.52755       | 1.99940 | 5.50854 | 0.01961 | 7.52755 |
| S    | 2  | 1.18094        | 9.99904 | 4.70637 | 0.11364 | 14.81906 |
| C    | 3  | -0.15636       | 1.99943 | 4.13596 | 0.02098 | 6.15636 |
| C    | 4  | -0.60940       | 1.99935 | 4.60103 | 0.00901 | 6.60940 |
| H    | 5  | 0.22397        | 0.00000 | 0.77454 | 0.00149 | 0.77603 |
| H    | 6  | 0.22779        | 0.00000 | 0.77047 | 0.00173 | 0.77221 |
| C    | 7  | 0.20369        | 0.00000 | 0.79457 | 0.00174 | 0.79631 |
| C    | 8  | -0.60653       | 1.99936 | 4.59962 | 0.00755 | 6.60653 |
| H    | 9  | 0.20244        | 0.00000 | 0.79555 | 0.00202 | 0.79756 |
| H    | 10 | 0.21865        | 0.00000 | 0.77967 | 0.00167 | 0.78135 |
| C    | 12 | -0.60605       | 1.99937 | 4.59853 | 0.00815 | 6.60605 |
| H    | 13 | 0.20997        | 0.00000 | 0.78826 | 0.00176 | 0.79003 |
| H    | 14 | 0.22317        | 0.00000 | 0.77532 | 0.00151 | 0.77683 |
| C    | 15 | 0.20350        | 0.00000 | 0.79484 | 0.00167 | 0.79650 |
| O    | 16 | -0.84736       | 1.99990 | 6.83647 | 0.01099 | 8.84736 |
| C    | 17 | 0.07656        | 1.99932 | 3.89635 | 0.02777 | 5.92344 |
| H    | 18 | 0.18011        | 0.00000 | 0.81322 | 0.00667 | 0.81989 |
| C    | 19 | -0.21310       | 1.99893 | 4.19613 | 0.01804 | 6.21310 |
| C    | 20 | 0.34252        | 1.99846 | 3.63559 | 0.02343 | 5.65748 |
| C    | 21 | 0.35462        | 1.99845 | 3.62306 | 0.02387 | 5.64538 |
| C    | 22 | 0.23930        | 1.99833 | 3.73755 | 0.02503 | 5.76070 |
| C    | 23 | 0.24104        | 1.99837 | 3.73551 | 0.02508 | 5.75896 |
| C    | 24 | 0.27950        | 1.99839 | 3.69661 | 0.02550 | 5.72050 |
| F    | 25 | -0.24398       | 1.99994 | 7.23662 | 0.00742 | 9.24398 |
| F    | 26 | -0.26552       | 1.99994 | 7.25872 | 0.00686 | 9.26552 |
| F    | 27 | -0.24256       | 1.99994 | 7.23531 | 0.00731 | 9.24256 |
| F    | 28 | -0.25102       | 1.99994 | 7.24404 | 0.00706 | 9.25102 |
| F    | 29 | -0.25102       | 1.99994 | 7.24399 | 0.00708 | 9.25102 |

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*S Total*  
-0.00000  
45.98582  
105.59778  
0.41640  
152.00000
**Sulfinyl imine 1b**

![Molecular structure of Sulfinyl imine 1b]

**Summary of Natural Population Analysis:**

| Atom No | Charge | Core   | Valence | Rydberg | Total |
|---------|--------|--------|---------|---------|-------|
| N 1     | -0.52432 | 1.99940 | 5.50552 | 0.01940 | 7.52432 |
| S 2     | 1.18080   | 9.99904 | 4.70662 | 0.11354 | 14.81920 |
| C 3     | -0.15635  | 1.99943 | 4.13594 | 0.02099 | 6.15635 |
| C 4     | -0.60951  | 1.99935 | 4.60115 | 0.00901 | 6.60951 |
| H 5     | 0.22460 | 0.00000 | 0.77391 | 0.00149 | 0.77540 |
| H 6     | 0.22765 | 0.00000 | 0.77062 | 0.00173 | 0.77235 |
| H 7     | 0.20328 | 0.00000 | 0.79498 | 0.00175 | 0.79672 |
| C 8     | -0.60652 | 1.99936 | 4.59964 | 0.00752 | 6.60652 |
| H 9     | 0.20231 | 0.00000 | 0.79568 | 0.00202 | 0.79769 |
| H 10    | 0.21907 | 0.00000 | 0.77928 | 0.00165 | 0.78093 |
| H 11    | 0.21231 | 0.00000 | 0.78589 | 0.00180 | 0.78769 |
| C 12    | -0.60601 | 1.99937 | 4.59849 | 0.00815 | 6.60601 |
| H 13    | 0.20965 | 0.00000 | 0.78857 | 0.00177 | 0.79035 |
| H 14    | 0.23303 | 0.00000 | 0.77545 | 0.00152 | 0.77697 |
| H 15    | 0.20334 | 0.00000 | 0.79499 | 0.00168 | 0.79666 |
| O 16    | -0.84778 | 1.99990 | 6.83690 | 0.01098 | 8.84778 |
| C 17    | 0.07725   | 1.99932 | 3.89577 | 0.02766 | 5.92275 |
| H 18    | 0.17984  | 0.00000 | 0.81349 | 0.00667 | 0.82016 |
| C 19    | -0.20065 | 1.99893 | 4.18410 | 0.01761 | 6.20056 |
| C 20    | 0.33312   | 1.99842 | 3.64586 | 0.02260 | 5.66688 |
| C 21    | 0.34220   | 1.99842 | 3.63418 | 0.02521 | 5.65780 |
| C 22    | 0.30021   | 1.99840 | 3.67778 | 0.02360 | 5.69979 |
| C 23    | 0.30231   | 1.99844 | 3.67545 | 0.02380 | 5.69769 |
| C 24    | -0.28618  | 1.99900 | 4.27453 | 0.01265 | 6.28638 |
| H 25    | 0.25047 | 0.00000 | 0.74807 | 0.00146 | 0.74953 |
| F 26    | -0.27038  | 1.99994 | 7.26376 | 0.00668 | 9.27038 |
| F 27    | -0.24710   | 1.99994 | 7.24010 | 0.00706 | 9.24710 |
| F 28    | -0.26823  | 1.99994 | 7.26161 | 0.00667 | 9.26823 |
| F 29    | -0.26841  | 1.99994 | 7.26172 | 0.00674 | 9.26841 |

* Total * | -0.00000 | 43.98657 | 99.62005 | 0.39338 | 144.00000
### Sulfinyl imine 1c

![Sulfinyl imine 1c](image)

#### Summary of Natural Population Analysis:

| Atom | No  | Charge | Core    | Valence | Rydberg | Total   |
|------|-----|--------|---------|---------|---------|---------|
| N    | 1   | -0.53669 | 1.99940 | 5.51790 | 0.01939 | 7.53669 |
| S    | 2   | 1.18053  | 9.99904 | 4.70635 | 0.11408 | 14.81947|
| C    | 3   | -0.15723 | 1.99943 | 4.13670 | 0.02110 | 6.15723 |
| C    | 4   | -0.60942 | 1.99936 | 4.60103 | 0.00903 | 6.60942 |
| H    | 5   | 0.22430  | 0.00000 | 0.77419 | 0.00151 | 0.77570 |
| H    | 6   | 0.22743  | 0.00000 | 0.77081 | 0.00176 | 0.77257 |
| H    | 7   | 0.20186  | 0.00000 | 0.79637 | 0.00177 | 0.79814 |
| C    | 8   | -0.60613 | 1.99936 | 4.59922 | 0.00756 | 6.60613 |
| H    | 9   | 0.20181  | 0.00000 | 0.79614 | 0.00205 | 0.79819 |
| H    | 10  | 0.21898  | 0.00000 | 0.77934 | 0.00168 | 0.78102 |
| H    | 11  | 0.21079  | 0.00000 | 0.78739 | 0.00182 | 0.78921 |
| C    | 12  | -0.60561 | 1.99937 | 4.59808 | 0.00816 | 6.60561 |
| H    | 13  | 0.20837  | 0.00000 | 0.78984 | 0.00179 | 0.79163 |
| H    | 14  | 0.22290  | 0.00000 | 0.77557 | 0.00153 | 0.77710 |
| H    | 15  | 0.20280  | 0.00000 | 0.79550 | 0.00169 | 0.79720 |
| O    | 16  | -0.85303 | 1.99990 | 6.84219 | 0.01093 | 8.85303 |
| C    | 17  | 0.08156  | 1.99932 | 3.89156 | 0.02757 | 5.91844 |
| H    | 18  | 0.17716  | 0.00000 | 0.81595 | 0.00689 | 0.82284 |
| C    | 19  | -0.24232 | 1.99887 | 4.22625 | 0.01719 | 6.24232 |
| C    | 20  | 0.42325  | 1.99855 | 3.55602 | 0.02217 | 5.57679 |
| C    | 21  | 0.43353  | 1.99854 | 3.54504 | 0.02288 | 5.56674 |
| C    | 22  | -0.34303 | 1.99893 | 4.33144 | 0.01265 | 6.34303 |
| C    | 23  | -0.33947 | 1.99896 | 4.32803 | 0.01249 | 6.33947 |
| C    | 24  | 0.40405  | 1.99854 | 3.57468 | 0.02273 | 5.59595 |
| H    | 25  | 0.24854  | 0.00000 | 0.75005 | 0.00141 | 0.75146 |
| H    | 26  | 0.24797  | 0.00000 | 0.75065 | 0.00137 | 0.75203 |
| F    | 27  | -0.27832 | 1.99994 | 7.27183 | 0.00655 | 9.27832 |
| F    | 28  | -0.28461 | 1.99994 | 7.27814 | 0.00653 | 9.28461 |
| F    | 29  | -0.25999 | 1.99994 | 7.25317 | 0.00688 | 9.25999 |

* Total *  
-0.00000  | 41.98740  | 93.63945  | 0.37314  | 136.00000
### Sulfynyl imine 1d

![Image of a chemical structure](image)

**Summary of Natural Population Analysis:**

| Atom | No. | Natural Charge | Core | Valence | Rydberg | Total     |
|------|-----|----------------|------|---------|----------|-----------|
| N    | 1   | -0.53394       | 1.99941 | 5.51543 | 0.01910  | 7.53394   |
| S    | 2   | 1.18025        | 9.99904 | 4.70671 | 0.11399  | 14.81975  |
| C    | 3   | -0.15723       | 1.99943 | 4.13668 | 0.02113  | 6.15723   |
| C    | 4   | -0.09454       | 1.99936 | 4.60116 | 0.00903  | 6.60954   |
| H    | 5   | 0.22500        | 0.00000 | 0.77349 | 0.00151  | 0.77500   |
| H    | 6   | 0.22724        | 0.00000 | 0.77099 | 0.00176  | 0.77276   |
| H    | 7   | 0.20131        | 0.00000 | 0.79691 | 0.00178  | 0.79869   |
| C    | 8   | -0.06111       | 1.99936 | 4.59922 | 0.00753  | 6.60611   |
| H    | 9   | 0.20166        | 0.00000 | 0.79630 | 0.00204  | 0.79834   |
| H    | 10  | 0.21948        | 0.00000 | 0.77886 | 0.00166  | 0.78052   |
| H    | 11  | 0.21029        | 0.00000 | 0.78788 | 0.00183  | 0.78971   |
| C    | 12  | -0.60553       | 1.99937 | 4.59800 | 0.00816  | 6.60553   |
| H    | 13  | 0.20792        | 0.00000 | 0.79027 | 0.00181  | 0.79208   |
| H    | 14  | 0.22275        | 0.00000 | 0.77572 | 0.00154  | 0.77725   |
| H    | 15  | 0.20259        | 0.00000 | 0.79570 | 0.00170  | 0.79741   |
| O    | 16  | -0.85383       | 1.99990 | 6.84301 | 0.01091  | 8.85383   |
| C    | 17  | 0.08242        | 1.99932 | 3.89086 | 0.02740  | 5.91758   |
| H    | 18  | 0.17701        | 0.00000 | 0.81614 | 0.00685  | 0.82299   |
| C    | 19  | -0.23216       | 1.99889 | 4.21566 | 0.01761  | 6.23216   |
| C    | 20  | 0.41033        | 1.99853 | 3.56952 | 0.02162  | 5.58967   |
| C    | 21  | 0.41863        | 1.99852 | 3.55915 | 0.02370  | 5.58137   |
| C    | 22  | -0.28274       | 1.99908 | 4.27033 | 0.01334  | 6.28274   |
| C    | 23  | -0.27862       | 1.99910 | 4.26610 | 0.01341  | 6.27862   |
| C    | 24  | -0.15005       | 1.99925 | 4.13767 | 0.01313  | 6.15005   |
| H    | 25  | 0.21752        | 0.00000 | 0.78145 | 0.00103  | 0.78248   |
| F    | 26  | -0.29127       | 1.99994 | 7.28505 | 0.00627  | 9.29127   |
| F    | 27  | -0.26628       | 1.99994 | 7.25966 | 0.00667  | 9.26628   |
| H    | 28  | 0.23176        | 0.00000 | 0.76697 | 0.00127  | 0.76824   |
| H    | 29  | 0.23114        | 0.00000 | 0.76756 | 0.00130  | 0.76886   |

* Total * 0.00000 39.98844 87.65247 0.35909 128.00000
Sulfinyl imine 1e

Summary of Natural Population Analysis:

| Atom | No | Charge | Core     | Valence | Rydberg | Total   |
|------|----|--------|----------|---------|---------|---------|
| N    | 1  | -0.56879| 1.99939  | 5.54981 | 0.01960 | 7.56879 |
| S    | 2  | 1.18683 | 9.99904  | 4.69913 | 0.11499 | 14.81317|
| C    | 3  | -0.15785| 1.99942  | 4.13724 | 0.02118 | 6.15785 |
| C    | 4  | -0.60803| 1.99936  | 4.59966 | 0.00901 | 6.60803 |
| H    | 5  | 0.21824 | 0.00000  | 0.78013 | 0.00163 | 0.78176 |
| H    | 6  | 0.22855 | 0.00000  | 0.76965 | 0.00180 | 0.77145 |
| H    | 7  | 0.20194 | 0.00000  | 0.79627 | 0.00179 | 0.79806 |
| C    | 8  | -0.60540| 1.99936  | 4.59846 | 0.00758 | 6.60540 |
| H    | 9  | 0.20211 | 0.00000  | 0.79583 | 0.00206 | 0.79789 |
| H    | 10 | 0.21684 | 0.00000  | 0.78148 | 0.00167 | 0.78316 |
| H    | 11 | 0.21040 | 0.00000  | 0.78777 | 0.00183 | 0.78960 |
| C    | 12 | -0.60567| 1.99937  | 4.59812 | 0.00817 | 6.60567 |
| H    | 13 | 0.20786 | 0.00000  | 0.79033 | 0.00181 | 0.79214 |
| H    | 14 | 0.22327 | 0.00000  | 0.77520 | 0.00153 | 0.77673 |
| H    | 15 | 0.20285 | 0.00000  | 0.79544 | 0.00171 | 0.79715 |
| O    | 16 | -0.85610| 1.99990  | 6.84528 | 0.01091 | 8.85610 |
| C    | 17 | 0.10053 | 1.99930  | 3.87314 | 0.02702 | 5.89947 |
| H    | 18 | 0.15530 | 0.00000  | 0.83757 | 0.00713 | 0.84470 |
| C    | 19 | -0.13575| 1.99909  | 4.11843 | 0.01823 | 6.13575 |
| C    | 20 | -0.14344| 1.99918  | 4.13158 | 0.01269 | 6.14344 |
| C    | 21 | -0.13538| 1.99915  | 4.12301 | 0.01322 | 6.13538 |
| C    | 22 | -0.26750| 1.99908  | 4.25523 | 0.01319 | 6.26750 |
| C    | 23 | -0.26039| 1.99909  | 4.24849 | 0.01281 | 6.26039 |
| C    | 24 | 0.37958 | 1.99853  | 3.60014 | 0.02175 | 5.62042 |
| H    | 25 | 0.21105 | 0.00000  | 0.78754 | 0.00141 | 0.78895 |
| H    | 26 | 0.23229 | 0.00000  | 0.76613 | 0.00158 | 0.76771 |
| H    | 27 | 0.22854 | 0.00000  | 0.77008 | 0.00137 | 0.77146 |
| H    | 28 | 0.22053 | 0.00000  | 0.77013 | 0.00134 | 0.77147 |
| F    | 29 | -0.29043| 1.99994  | 7.28417 | 0.00612 | 9.29043 |

* Total * | -0.00000 | 37.98921 | 81.66546 | 0.34532 | 120.00000
**Sulfinyl imine 1f**

Summary of Natural Population Analysis:

| Atom | No | Charge     | Core     | Valence  | Rydberg | Total    |
|------|----|------------|----------|----------|----------|----------|
| N    | 1  | -0.56578   | 1.99939  | 5.54678  | 0.01961  | 7.56578  |
| S    | 2  | 1.18627    | 9.99904  | 4.69976  | 0.11493  | 14.81373 |
| C    | 3  | -0.15787   | 1.99942  | 4.13724  | 0.02120  | 6.15787  |
| C    | 4  | -0.60817   | 1.99980  | 5.59980  | 0.00901  | 6.60817  |
| H    | 5  | 0.21388    | 0.00000  | 0.77948  | 0.00164  | 0.78112  |
| H    | 6  | 0.22839    | 0.00000  | 0.76981  | 0.00180  | 0.77161  |
| H    | 7  | 0.20138    | 0.00000  | 0.79682  | 0.00180  | 0.79862  |
| C    | 8  | -0.60547   | 1.99936  | 4.59853  | 0.00758  | 6.60547  |
| H    | 9  | 0.20193    | 0.00000  | 0.79601  | 0.00206  | 0.79807  |
| H    | 10 | 0.21732    | 0.00000  | 0.78100  | 0.00168  | 0.78268  |
| H    | 11 | 0.20988    | 0.00000  | 0.78828  | 0.00184  | 0.79012  |
| C    | 12 | -0.60559   | 1.99957  | 4.59804  | 0.00818  | 6.60559  |
| H    | 13 | 0.20742    | 0.00000  | 0.79076  | 0.00182  | 0.79258  |
| H    | 14 | 0.22310    | 0.00000  | 0.77536  | 0.00154  | 0.77690  |
| H    | 15 | 0.20265    | 0.00000  | 0.79564  | 0.00171  | 0.79735  |
| O    | 16 | -0.85690   | 1.99990  | 6.84611  | 0.01089  | 8.85690  |
| C    | 17 | 0.10165    | 1.99930  | 3.87201  | 0.02703  | 5.89835  |
| H    | 18 | 0.15432    | 0.00000  | 0.83850  | 0.00718  | 0.84568  |
| C    | 19 | -0.12263   | 1.99909  | 4.10481  | 0.01873  | 6.12263  |
| C    | 20 | -0.15928   | 1.99916  | 4.14746  | 0.01265  | 6.15928  |
| C    | 21 | -0.15193   | 1.99914  | 4.13971  | 0.01309  | 6.15193  |
| C    | 22 | -0.20418   | 1.99923  | 4.19164  | 0.01331  | 6.20418  |
| C    | 23 | -0.19908   | 1.99923  | 4.18677  | 0.01308  | 6.19908  |
| C    | 24 | -0.17726   | 1.99924  | 4.16492  | 0.01310  | 6.17726  |
| H    | 25 | 0.20605    | 0.00000  | 0.79248  | 0.00146  | 0.79395  |
| H    | 26 | 0.22724    | 0.00000  | 0.77116  | 0.00160  | 0.77276  |
| H    | 27 | 0.20982    | 0.00000  | 0.78895  | 0.00124  | 0.79018  |
| H    | 28 | 0.20979    | 0.00000  | 0.78899  | 0.00121  | 0.79021  |
| H    | 29 | 0.20804    | 0.00000  | 0.79078  | 0.00118  | 0.79196  |

* Total * -0.00000 35.99024 75.67760 0.33216 112.00000
### IX. Cartesian coordinates of optimized structures.

#### Sulfinyl imine 1a

| Center Number | Atomic Number | Atomic Type | Coordinates (Ångstroms) | X         | Y         | Z         |
|---------------|---------------|-------------|-------------------------|-----------|-----------|-----------|
| 1             | 7             | 0           | 0.342465                | -0.039253 | 0.216642  |
| 2             | 16            | 0           | 1.091084                | -0.723996 | -0.683629 |
| 3             | 6             | 0           | 2.345806                | 0.505719  | 0.064579  |
| 4             | 6             | 0           | 2.368183                | 0.307130  | 1.578933  |
| 5             | 1             | 0           | 1.422124                | 0.614701  | 2.031106  |
| 6             | 1             | 0           | 2.549447                | -0.744536 | 1.823001  |
| 7             | 1             | 0           | 3.180282                | 0.908737  | 2.006624  |
| 8             | 6             | 0           | 1.910076                | 1.912545  | -0.354711 |
| 9             | 1             | 0           | 1.805373                | 1.994725  | -1.443441 |
| 10            | 1             | 0           | 0.968721                | 2.193435  | 0.118813  |
| 11            | 1             | 0           | 2.680549                | 2.632838  | -0.042914 |
| 12            | 6             | 0           | 3.678828                | 0.099926  | -0.579581 |
| 13            | 1             | 0           | 4.474504                | 0.750836  | -0.197897 |
| 14            | 1             | 0           | 3.932422                | -0.935335 | -0.332647 |
| 15            | 9             | 0           | 3.650373                | 0.204705  | -1.670741 |
| 16            | 8             | 0           | 1.370382                | -2.076792 | -0.045401 |
| 17            | 6             | 0           | 1.419528                | -0.144100 | -0.485098 |
| 18            | 1             | 0           | 1.417911                | -0.536147 | -1.510179 |
| 19            | 6             | 0           | 2.739848                | 0.240098  | 0.019369  |
| 20            | 6             | 0           | 3.860698                | 0.050325  | -0.811943 |
| 21            | 6             | 0           | 2.988470                | 0.798512  | 1.288986  |
| 22            | 6             | 0           | 5.153378                | 0.381092  | -0.419795 |
| 23            | 6             | 0           | 4.276195                | 1.136736  | 1.700281  |
| 24            | 6             | 0           | 5.360584                | 0.929166  | 0.846262  |
| 25            | 9             | 0           | 6.596086                | 1.255385  | 1.241394  |
| 26            | 9             | 0           | 3.697723                | -0.477046 | -2.042556 |
| 27            | 9             | 0           | -1.991418               | 1.030196  | 2.150208  |
| 28            | 9             | 0           | -6.193821               | 0.179686  | -1.242935 |
| 29            | 9             | 0           | -4.482311               | 1.667347  | 2.915486  |

#### Sulfinyl imine 1b

| Center Number | Atomic Number | Atomic Type | Coordinates (Ångstroms) | X         | Y         | Z         |
|---------------|---------------|-------------|-------------------------|-----------|-----------|-----------|
| 1             | 7             | 0           | -3.40409                | -0.052449 | 0.221949  |
| 2             | 16            | 0           | 1.094104                | -0.731373 | -0.680845 |
| 3             | 6             | 0           | 2.344526                | 0.504962  | 0.065041  |
| 4             | 6             | 0           | 2.370003                | 0.306907  | 1.579111  |
| 5             | 1             | 0           | 1.422610                | 0.608704  | 2.032364  |
| 6             | 1             | 0           | 2.557382                | -0.743647 | 1.823005  |
| 7             | 1             | 0           | 3.179076                | 0.913445  | 2.005681  |
| 8             | 6             | 0           | 1.905363                | 1.909606  | -0.354118 |
| 9             | 1             | 0           | 1.792608                | 1.990492  | -1.442566 |
| 10            | 1             | 0           | 0.960401                | 2.186866  | 0.122308  |
| 11            | 1             | 0           | 2.669819                | 2.633444  | -0.045490 |
| 12            | 6             | 0           | 3.678275                | 0.105312  | -0.581442 |
| 13            | 1             | 0           | 4.471814                | 0.759362  | -0.200588 |
| 14            | 1             | 0           | 3.938414                | -0.929013 | -0.335423 |
| 15            | 1             | 0           | 3.647734                | 0.210472  | -1.672520 |
| 16            | 8             | 0           | 1.380839                | -2.082096 | -0.041484 |
| 17            | 6             | 0           | -1.409375               | -0.147200 | -0.483455 |
| 18            | 1             | 0           | -1.412214               | -0.530412 | -1.511802 |
| 19            | 6             | 0           | -2.737324               | 0.237810  | 0.020676  |
| 20            | 6             | 0           | -3.855051               | 0.048683  | -0.815544 |
| 21            | 6             | 0           | -2.984974               | 0.795495  | 1.290735  |
| 22            | 6             | 0           | -5.142972               | 0.385287  | -0.410659 |
| 23            | 6             | 0           | -4.279972               | 1.129573  | 1.685257  |
| 24            | 6             | 0           | -5.369498               | 0.931157  | 0.846083  |
| 25            | 1             | 0           | -6.371570               | 1.194430  | 1.166138  |
| 26            | 9             | 0           | -3.686005               | -0.478424 | -2.047419 |
| 27            | 9             | 0           | -1.986097               | 1.025533  | 2.152651  |
| 28            | 9             | 0           | -6.176594               | 0.177965  | -1.252141 |
| 29            | 9             | 0           | -4.471986               | 1.661075  | 2.910214  |
### Sulfinyl imine 1c

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 7             | 0           | -0.335417   | -0.056567   | 0.238513    |
| 2             | 16            | 0           | 1.090869    | -0.741536   | -0.660484   |
| 3             | 6             | 0           | 2.344662    | 0.505690    | 0.061514    |
| 4             | 6             | 0           | 2.377625    | 0.328195    | 1.578062    |
| 5             | 1             | 0           | 1.431417    | 0.634705    | 2.030696    |
| 6             | 1             | 0           | 2.567026    | -0.719102   | 1.834659    |
| 7             | 1             | 0           | 3.188024    | 0.940971    | 1.993324    |
| 8             | 6             | 0           | 1.902911    | 1.904778    | -0.373087   |
| 9             | 1             | 0           | 1.786017    | 1.971803    | -1.462068   |
| 10            | 1             | 0           | 0.958734    | 2.185719    | 0.102697    |
| 11            | 1             | 0           | 2.667424    | 2.633583    | -0.076080   |

### Sulfinyl imine 1d

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 7             | 0           | -0.332951   | -0.069477   | 0.242257    |
| 2             | 16            | 0           | 1.094187    | -0.747044   | -0.660177   |
| 3             | 6             | 0           | 2.343379    | 0.505381    | 0.061810    |
| 4             | 6             | 0           | 2.378251    | 0.326514    | 1.578141    |
| 5             | 1             | 0           | 1.430699    | 0.627606    | 2.031486    |
| 6             | 1             | 0           | 2.572956    | -0.720184   | 1.833294    |
| 7             | 1             | 0           | 3.185902    | 0.942839    | 1.993648    |
| 8             | 6             | 0           | 1.894987    | 1.902937    | 0.089081    |
| 9             | 1             | 0           | 1.775074    | 1.970211    | -1.459571   |
| 10            | 1             | 0           | 0.950468    | 2.173930    | 0.106871    |
| 11            | 1             | 0           | 2.656935    | 2.634854    | -0.074740   |
| 12            | 6             | 0           | 3.676109    | 0.105700    | -0.586196   |
| 13            | 1             | 0           | 4.468967    | 0.766962    | -0.216134   |
| 14            | 1             | 0           | 3.941324    | -0.925127   | -0.330910   |
| 15            | 1             | 0           | 3.639603    | 0.199034    | -1.677236   |
| 16            | 8             | 0           | 3.185902    | 0.942839    | 1.993648    |
| 17            | 6             | 0           | 1.894987    | 1.902937    | -0.370830   |
| 18            | 1             | 0           | 1.775074    | 1.970211    | -1.459571   |
| 19            | 1             | 0           | 0.950468    | 2.173930    | 0.106871    |
| 20            | 1             | 0           | 2.656935    | 2.634854    | -0.074740   |
| 21            | 1             | 0           | 3.676109    | 0.105700    | -0.586196   |
| 22            | 1             | 0           | 4.468967    | 0.766962    | -0.216134   |
| 23            | 1             | 0           | 3.941324    | -0.925127   | -0.330910   |
| 24            | 1             | 0           | 3.639603    | 0.199034    | -1.677236   |
| 25            | 1             | 0           | 1.401596    | -2.089152   | 0.000960    |
| 26            | 8             | 0           | 1.401596    | -2.089152   | 0.000960    |
| 27            | 9             | 0           | 1.997057    | 1.007648    | 2.156461    |
| 28            | 1             | 0           | 5.966015    | 0.215000    | -1.131261   |
| 29            | 1             | 0           | -4.430854   | 1.555804    | 2.693991    |
### Sulfinyl imine 1e

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X     | Y     | Z     |
| 1             | 7             | 0           | -0.364759 | -0.130948 | 0.260239 |
| 2             | 16            | 0           | 1.086566 | -0.823530 | -0.567465 |
| 3             | 6             | 0           | 2.303938 | 0.507253 | 0.067891 |
| 4             | 6             | 0           | 2.335404 | 0.438640 | 1.593080 |
| 5             | 1             | 0           | 1.382815 | 0.760513 | 2.021360 |
| 6             | 1             | 0           | 2.540388 | -0.584825 | 1.923470 |
| 7             | 1             | 0           | 3.133426 | 1.092819 | 1.967033 |
| 8             | 6             | 0           | 1.831012 | 1.860122 | -0.467321 |
| 9             | 1             | 0           | 1.719108 | 1.845479 | -1.558766 |
| 10            | 1             | 0           | 0.867482 | 2.151359 | -0.018969 |
| 11            | 1             | 0           | 2.574922 | 2.627972 | -0.220498 |
| 12            | 6             | 0           | 3.648597 | 0.089086 | -0.542762 |
| 13            | 1             | 0           | 4.425854 | 0.791958 | -0.219149 |
| 14            | 1             | 0           | 3.932884 | -0.914596 | -0.211324 |
| 15            | 1             | 0           | 4.613322 | 0.101034 | -1.638801 |
| 16            | 8             | 0           | 1.424641 | -2.106184 | 0.180088 |
| 17            | 6             | 0           | -1.417594 | -0.211875 | -0.475184 |
| 18            | 1             | 0           | -1.387202 | -0.596464 | -1.507055 |
| 19            | 6             | 0           | -2.741808 | 0.199482 | 0.002132 |
| 20            | 6             | 0           | -3.856070 | 0.136732 | -0.877470 |
| 21            | 6             | 0           | -2.943646 | 0.655334 | 1.318804 |
| 22            | 6             | 0           | -5.109732 | 0.522786 | -0.465194 |
| 23            | 6             | 0           | -4.207501 | 1.041744 | 1.746309 |
| 24            | 6             | 0           | -5.267131 | 0.969040 | 0.842232 |
| 25            | 1             | 0           | -3.686933 | -0.219222 | -1.894502 |
| 26            | 1             | 0           | -2.095338 | 0.692768 | 1.995489 |
| 27            | 1             | 0           | -5.965603 | 0.480781 | -1.130940 |
| 28            | 1             | 0           | -4.386514 | 1.392236 | 2.757842 |
| 29            | 9             | 0           | -6.503151 | 1.347440 | 1.258240 |

### Sulfinyl imine 1f

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X     | Y     | Z     |
| 1             | 7             | 0           | -0.361295 | -0.143824 | 0.268626 |
| 2             | 16            | 0           | 1.090122 | -0.832038 | -0.562295 |
| 3             | 6             | 0           | 2.303043 | 0.506255 | 0.066830 |
| 4             | 6             | 0           | 2.339212 | 0.440426 | 1.592060 |
| 5             | 1             | 0           | 1.386001 | 0.757608 | 2.022399 |
| 6             | 1             | 0           | 2.550576 | -0.581443 | 1.923420 |
| 7             | 1             | 0           | 3.134791 | 1.099522 | 1.962728 |
| 8             | 6             | 0           | 1.821888 | 1.855921 | -0.469062 |
| 9             | 1             | 0           | 1.705913 | 1.838677 | -1.560064 |
| 10            | 1             | 0           | 0.867482 | 2.143455 | -1.642870 |
| 11            | 1             | 0           | 2.563149 | 2.627737 | -0.226473 |
| 12            | 6             | 0           | 3.648017 | 0.093814 | -0.546894 |
| 13            | 1             | 0           | 4.423032 | 0.800439 | -0.225934 |
| 14            | 1             | 0           | 3.937605 | -0.908328 | -0.215311 |
| 15            | 1             | 0           | 3.617274 | 0.104548 | -1.642870 |
| 16            | 8             | 0           | 1.437211 | -2.111178 | 0.187450 |
| 17            | 6             | 0           | -1.413277 | -0.217076 | -0.468448 |
| 18            | 1             | 0           | -1.382079 | -0.596646 | -1.502258 |
| 19            | 6             | 0           | -2.738996 | 0.197632 | 0.007830 |
| 20            | 6             | 0           | -3.827056 | 0.142711 | -0.879361 |
| 21            | 6             | 0           | -2.944897 | 0.646644 | 1.325215 |
| 22            | 6             | 0           | -5.099163 | 0.533289 | -0.462605 |
| 23            | 6             | 0           | -4.215300 | 1.032830 | 1.738217 |
| 24            | 6             | 0           | -5.294196 | 0.978995 | 0.846338 |
| 25            | 1             | 0           | -3.669473 | -0.208842 | -1.897191 |
| 26            | 1             | 0           | -2.098938 | 0.677265 | 2.005536 |
| 27            | 1             | 0           | -5.935832 | 0.488219 | -1.154525 |
| 28            | 1             | 0           | -4.372241 | 1.375620 | 2.757858 |
| 29            | 1             | 0           | -6.285100 | 1.281930 | 1.174751 |
### RC for Si attack in DCM of 1a with 2a

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 12            | 0           | X 1.752059   Y 0.993972   Z 1.338645 |
| 2             | 6             | 0           | X 0.168084   Y 0.976086   Z 2.770136 |
| 3             | 6             | 0           | X -0.508465  Y -0.099134  Z 2.991829 |
| 4             | 6             | 0           | X -1.144228  Y -1.244342  Z 3.141462 |
| 5             | 6             | 0           | X -0.464268  Y -1.365487  Z 0.052405 |
| 6             | 7             | 0           | X 0.694645   Y -0.824521  Z 0.013671 |
| 7             | 1             | 0           | X -0.593773  Y -2.414239  Z 0.308682 |
| 8             | 16            | 0           | X 2.004027   Y -1.808736  Z 0.482680 |
| 9             | 8             | 0           | X 2.804406   Y -0.775112  Z 1.253745 |
| 10            | 6             | 0           | X -1.687624  Y -0.640647  Z -0.252089 |
| 11            | 6             | 0           | X -2.908015  Y -1.284560  Z -0.032947 |
| 12            | 6             | 0           | X -1.737088  Y 0.662058   Z -0.753997 |
| 13            | 6             | 0           | X -4.118286  Y -0.669696  Z -0.274392 |
| 14            | 6             | 0           | X -2.939964  Y 1.292082   Z -1.006002 |
| 15            | 6             | 0           | X -4.130850  Y 0.626986   Z -0.762093 |
| 16            | 35            | 0           | X 2.984442   Y 2.860563   Z 0.251230 |
| 17            | 6             | 0           | X 2.845665   Y -2.002998  Z -1.153502 |
| 18            | 6             | 0           | X 3.046930   Y -0.651062  Z -1.818994 |
| 19            | 1             | 0           | X 3.605494   Y 0.029918   Z -1.177971 |
| 20            | 1             | 0           | X 3.621608   Y -0.802819  Z -2.733265 |
| 21            | 1             | 0           | X 2.099500   Y -1.853932  Z -2.083553 |
| 22            | 6             | 0           | X 1.960228   Y -2.934008  Z -1.976311 |
| 23            | 1             | 0           | X 1.758235   Y -3.871048  Z -1.455633 |
| 24            | 1             | 0           | X 1.014943   Y -2.462675  Z -2.243370 |
| 25            | 1             | 0           | X 2.483257   Y -3.174884  Z -2.901885 |
| 26            | 6             | 0           | X 4.179822   Y -2.663355  Z -0.804593 |
| 27            | 1             | 0           | X 4.039726   Y -3.618937  Z -0.297716 |
| 28            | 1             | 0           | X 4.722853   Y -2.850674  Z -1.730925 |
| 29            | 1             | 0           | X 4.789025   Y -2.014336  Z -0.177321 |
| 30            | 1             | 0           | X -0.769050  Y -2.007781  Z 3.811315 |
| 31            | 1             | 0           | X -2.095398  Y -1.429544  Z 2.660040 |
| 32            | 1             | 0           | X -0.041888  Y 1.826008   Z 3.419160 |
| 33            | 9             | 0           | X -5.256914  Y -1.302805  Z -0.043301 |
| 34            | 9             | 0           | X -5.278246  Y 1.228102   Z -0.999210 |
| 35            | 9             | 0           | X -2.924366  Y -2.525256  Z 0.438106 |
| 36            | 9             | 0           | X -0.632691  Y 1.333327   Z -1.031033 |
| 37            | 9             | 0           | X -2.962142  Y 2.525526   Z -1.483921 |

### TS for Si attack in DCM of 1a with 2a

**Imaginary frequency: -362.8069**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 12            | 0           | X 1.935766   Y 0.978448  Z 1.031645 |
| 2             | 6             | 0           | X 0.807175   Y 0.950552  Z 2.953043 |
| 3             | 6             | 0           | X -0.075306  Y 0.058769  Z 3.020668 |
| 4             | 6             | 0           | X -0.928905  Y -0.969125  Z 2.822759 |
| 5             | 6             | 0           | X -0.473307  Y -1.183641  Z 0.600035 |
| 6             | 7             | 0           | X 0.720036   Y -0.722492  Z 0.271613 |
| 7             | 1             | 0           | X -0.609878  Y -2.242822  Z 0.776230 |
| 8             | 16            | 0           | X 2.012215   Y -1.770958  Z 0.523472 |
| 9             | 8             | 0           | X 3.064002   Y -0.758491  Z 0.971005 |
| 10            | 6             | 0           | X -1.685083  Y -0.490808  Z 0.129041 |
| 11            | 6             | 0           | X -2.879861  Y -1.206445  Z 0.080273 |
| 12            | 6             | 0           | X -1.733346  Y 0.832060   Z -0.297301 |
| 13            | 6             | 0           | X -4.058501  Y -0.653717  Z -0.377023 |
| 14            | 6             | 0           | X -2.903404  Y 1.408759   Z -0.757673 |
| 15            | 6             | 0           | X -4.069076  Y 0.664835   Z -0.800020 |
| 16            | 35            | 0           | X 2.752482   Y 2.860665   Z -0.352488 |
| 17            | 6             | 0           | X 2.454561   Y -2.199635  Z -1.22586 |
| 18            | 6             | 0           | X 2.655936   Y -0.936672  Z -2.043990 |
| 19            | 1             | 0           | X 3.437770   Y -0.307977  Z -1.619939 |
| 20            | 1             | 0           | X 2.961162   Y -1.224264  Z -3.050788 |
| 21            | 1             | 0           | X 1.738444   Y -0.355316  Z -2.117334 |
| Center | Atomic Number | Atomic Type | X           | Y           | Z           |
|--------|---------------|-------------|-------------|-------------|-------------|
| 1      | 12            | 0           | 2.221079    | 0.606913    | 1.256903    |
| 2      | 6             | 0           | 0.679391    | 1.482991    | 3.341757    |
| 3      | 6             | 0           | 0.081226    | 0.488502    | 3.032821    |
| 4      | 6             | 0           | -0.620642   | -0.746915   | 2.693747    |
| 5      | 6             | 0           | -0.463193   | -1.180705   | 1.206702    |
| 6      | 7             | 0           | 0.820327    | -0.796832   | 0.661370    |
| 7      | 1             | 0           | -0.568945   | -2.264982   | 1.216033    |
| 8      | 16            | 0           | 1.939639    | -1.957246   | 0.468345    |
| 9      | 8             | 0           | 3.204152    | -1.156817   | 0.867364    |
| 10     | 6             | 0           | -1.582275   | -0.669652   | 0.313139    |
| 11     | 6             | 0           | -2.516304   | -1.545714   | -0.217455   |
| 12     | 6             | 0           | -1.694017   | 0.658234    | -0.071792   |
| 13     | 6             | 0           | -3.510355   | -1.137811   | -1.090690   |
| 14     | 6             | 0           | -2.675107   | 1.096940    | -0.941737   |
| 15     | 6             | 0           | -3.589857   | 0.193077    | -1.454204   |
| 16     | 35            | 0           | 3.115901    | 2.876001    | 0.948192    |
| 17     | 6             | 0           | 2.119627    | -2.142623   | -1.366917   |
| 18     | 6             | 0           | 2.381984    | -0.790856   | -2.008459   |
| 19     | 1             | 0           | 3.324784    | -0.365676   | -1.665598   |
| 20     | 1             | 0           | 2.440363    | -0.914244   | -3.090821   |
| 21     | 1             | 0           | 1.574287    | -0.091359   | -1.791136   |
| 22     | 6             | 0           | 0.796000    | -2.737878   | -1.890057   |
| 23     | 1             | 0           | 0.549146    | -3.656446   | -1.303070   |
| 24     | 1             | 0           | -0.020390   | -2.026956   | -1.710730   |
| 25     | 1             | 0           | 0.869124    | -2.980861   | -2.899717   |
| 26     | 6             | 0           | 3.279421    | -3.110342   | -1.583244   |
| 27     | 1             | 0           | 3.097287    | -4.069029   | -1.094462   |
| 28     | 1             | 0           | 3.400674    | -3.297050   | -2.651229   |
| 29     | 1             | 0           | 4.211072    | -2.694699   | -1.200844   |
| 30     | 1             | 0           | -0.203028   | -1.540002   | 3.315576    |
| 31     | 1             | 0           | -1.673406   | -0.652707   | 2.961404    |
| 32     | 1             | 0           | 1.161332    | 2.385254    | 3.637837    |
| 33     | 9             | 0           | -2.467073   | -2.844561   | 0.091762    |
| 34     | 9             | 0           | -4.379012   | -2.014081   | -1.581330   |
| 35     | 9             | 0           | -4.535205   | 0.602640    | -2.287553   |
| 36     | 9             | 0           | -2.746767   | 2.376849    | -1.286663   |
| 37     | 9             | 0           | -0.836669   | 1.567775    | 0.392115    |

**PRODUCT for Si attack in DCM of 1a with 2a**
RC for Re attack in DCM of 1a with 2a

| Center| Atomic Number| Atomic Type | Coordinates (Angstroms) |
|-------|---------------|-------------|-------------------------|
|       |               |             | X | Y | Z |
| 1     | 12            | 0           | -2.095113 | 1.332956 | 0.402503 |
| 2     | 6             | 0           | -1.080424 | 1.065005 | 2.257687 |
| 3     | 6             | 0           | -0.245928 | 0.104134 | 2.480627 |
| 4     | 6             | 0           | 0.578434  | -0.909065 | 2.643881 |
| 5     | 6             | 0           | 0.169037  | -1.194897 | -1.135451 |
| 6     | 7             | 0           | -0.894131 | -0.609008 | -0.756357 |
| 7     | 1             | 0           | 0.159116  | -2.053101 | -1.803639 |
| 8     | 16            | 0           | -2.419814 | -1.091634 | -1.346055 |
| 9     | 8             | 0           | -3.236096 | 0.053696  | -0.780086 |
| 10    | 6             | 0           | 1.480768  | -0.774374 | -0.650833 |
| 11    | 6             | 0           | 2.463196  | -1.743153 | -0.471756 |
| 12    | 6             | 0           | 1.798657  | 0.539053  | -0.314621 |
| 13    | 6             | 0           | 3.702737  | -1.437583 | 0.053102 |
| 14    | 6             | 0           | 3.037719  | 0.868719  | 0.197345 |
| 15    | 6             | 0           | 3.987001  | -0.123814 | 0.388943 |
| 16    | 35            | 0           | -2.665424 | 3.631879  | -0.397325 |
| 17    | 6             | 0           | -2.813948 | -2.570840 | -0.281662 |
| 18    | 6             | 0           | -2.742421 | -2.206267 | 1.190624 |
| 19    | 1             | 0           | -3.439059 | -1.405902 | 1.434677 |
| 20    | 1             | 0           | -3.024992 | -3.085235 | 1.771181 |
| 21    | 1             | 0           | -1.738244 | -1.906800 | 1.487430 |
| 22    | 6             | 0           | -1.838779 | -3.682944 | -0.649222 |
| 23    | 1             | 0           | -1.781415 | -3.845778 | -1.726813 |
| 24    | 1             | 0           | -0.840450 | -3.498179 | -0.255390 |
| 25    | 1             | 0           | -2.196743 | -4.607935 | -0.196962 |
| 26    | 6             | 0           | -4.240654 | -2.922204 | -0.709045 |
| 27    | 1             | 0           | -4.295100 | -3.184950 | -1.765839 |
| 28    | 1             | 0           | -4.565649 | -3.786104 | -0.129228 |
| 29    | 1             | 0           | -4.928190 | -2.101539 | -0.509431 |
| 30    | 1             | 0           | 1.628591  | -0.829046 | 2.390286 |
| 31    | 1             | 0           | 0.239665  | -1.842714 | 3.076280 |
| 32    | 1             | 0           | -1.201858 | 1.780006  | 3.072896 |
| 33    | 9             | 0           | 2.195931  | -3.009626 | -0.772111 |
| 34    | 9             | 0           | 4.610869  | -2.382064 | 0.239217 |
| 35    | 9             | 0           | 5.168277  | 0.185970  | 0.884702 |
| 36    | 9             | 0           | 3.327666  | 2.123445  | 0.498998 |
| 37    | 9             | 0           | 0.934220  | 1.519829  | -0.519746 |

TS for Re attack in DCM of 1a with 2a

Imaginary frequency: -346.1914
| Center Number | Atomic Number | Atomic Type | X           | Y           | Z           |
|---------------|---------------|-------------|-------------|-------------|-------------|
| 1             | 12            | 0           | -2.024246   | 0.209499    | -0.219732   |
| 2             | 6             | 0           | 0.480012    | 2.361783    | -1.081365   |
| 3             | 6             | 0           | -0.944980   | 2.679260    | -1.029076   |
| 4             | 6             | 0           | -2.121675   | 2.907204    | -0.955783   |
| 5             | 6             | 0           | 0.847290    | 1.442630    | 0.107109    |
| 6             | 7             | 0           | 0.050877    | 0.217641    | 0.171443    |
| 7             | 1             | 0           | 0.563471    | 1.953696    | 1.002319    |
| 8             | 16            | 0           | 0.297441    | -0.895894   | 0.999033    |
| 9             | 8             | 0           | -1.163621   | -1.130240   | -1.478646   |
| 10            | 6             | 0           | 2.341260    | 1.193021    | 0.247696    |
| 11            | 6             | 0           | 2.865299    | 1.059980    | 1.528047    |
| 12            | 6             | 0           | 3.234225    | 1.007692    | -0.797218   |
| 13            | 6             | 0           | 4.191844    | 0.760280    | 1.769794    |
| 14            | 6             | 0           | 4.570559    | 0.706827    | 0.587392    |
| 15            | 6             | 0           | 5.052647    | 0.580950    | 0.701230    |
| 16            | 35            | 0           | -4.313261   | 0.441874    | 0.669293    |
| 17            | 6             | 0           | 0.686473    | -2.459737   | -0.081321   |
| 18            | 6             | 0           | -0.402944   | -2.770371   | 0.930774    |
| 19            | 1             | 0           | -1.365754   | -2.920228   | 0.443234    |
| 20            | 1             | 0           | -0.144229   | -3.689658   | 1.457988    |
| 21            | 1             | 0           | -0.492716   | -1.972611   | 1.668142    |
| 22            | 6             | 0           | 2.030289    | -2.232088   | 0.602518    |
| 23            | 1             | 0           | 2.797494    | -1.907225   | 0.103168    |
| 24            | 1             | 0           | 1.942909    | -1.491218   | 1.395033    |
| 25            | 1             | 0           | 2.364553    | -3.169683   | 1.048158    |
| 26            | 6             | 0           | 0.786815    | -3.543381   | -1.152570   |
| 27            | 1             | 0           | 1.555790    | -3.306708   | 1.889697    |
| 28            | 1             | 0           | 1.054557    | -4.489450   | -0.680263   |
| 29            | 1             | 0           | -0.163575   | -3.675595   | -1.667949   |
| 30            | 1             | 0           | -3.155975   | 3.155301    | -0.905517   |
| 31            | 1             | 0           | 1.058650    | 3.285792    | -1.038958   |
| 32            | 1             | 0           | 0.699627    | 1.883191    | -2.033530   |
| 33            | 9             | 0           | 6.327408    | 0.292150    | 0.912550    |
| 34            | 9             | 0           | 4.640908    | 0.635191    | 3.012120    |
| 35            | 9             | 0           | 2.065105    | 1.193564    | 2.586473    |
| 36            | 9             | 0           | 5.387184    | 0.555182    | -1.619454   |
| 37            | 9             | 0           | 2.837156    | 1.094738    | -2.069103   |
### RC for Si attack in THF of 1a with 2a

| Center Number | Atomic Number | Atomic Type | X          | Y          | Z          |
|---------------|---------------|-------------|------------|------------|------------|
| 1             | 16            | 0           | -1.305457  | 1.969138   | -1.216155  |
| 2             | 7             | 0           | -0.164330  | 0.737919   | -0.639880  |
| 3             | 8             | 0           | -0.660448  | 2.682255   | -2.344182  |
| 4             | 6             | 0           | 1.020257   | 0.951419   | -1.054390  |
| 5             | 1             | 0           | 1.204419   | 1.807815   | -1.703601  |
| 6             | 6             | 0           | 2.199201   | 0.180738   | -0.664814  |
| 7             | 6             | 0           | 2.208941   | -1.175937  | -0.372722  |
| 8             | 6             | 0           | 3.401541   | 0.869354   | -0.526474  |
| 9             | 6             | 0           | 3.343603   | -1.822900  | 0.067265   |
| 10            | 6             | 0           | 4.551391   | 0.248544   | -0.079122  |
| 11            | 6             | 0           | 4.518827   | -1.103130  | 0.221743   |
| 12            | 12            | 0           | -1.119260  | -1.057832  | 0.301214   |
| 13            | 8             | 0           | -2.984338  | -0.270746  | 0.781290   |
| 14            | 6             | 0           | -4.114626  | -0.097815  | -0.094298  |
| 15            | 6             | 0           | -5.173172  | -1.076663  | 0.417642   |
| 16            | 6             | 0           | -4.712359  | -1.422227  | 1.851330   |
| 17            | 6             | 0           | -3.539858  | -0.482477  | 2.092429   |
| 18            | 1             | 0           | -5.201758  | -1.967794  | -0.204500  |
| 19            | 1             | 0           | -2.751237  | -0.878890  | 2.724806   |
| 20            | 1             | 0           | -5.495502  | -1.278172  | 2.591721   |
| 21            | 1             | 0           | -4.378807  | -2.456494  | 1.906602   |
| 22            | 1             | 0           | -6.159793  | -0.619661  | 0.402058   |
| 23            | 1             | 0           | -4.444404  | 0.940262   | -0.011644  |
| 24            | 1             | 0           | -3.866464  | 0.483217   | 2.485735   |
| 25            | 1             | 0           | -3.778457  | -0.297768  | -1.106285  |
| 26            | 6             | 0           | -1.165209  | 3.144654   | 0.242758   |
| 27            | 6             | 0           | -2.069854  | 4.303506   | -0.181798  |
| 28            | 1             | 0           | -2.099717  | 5.032023   | 0.628822   |
| 29            | 1             | 0           | -1.692250  | 4.797186   | -1.075408  |
| 30            | 1             | 0           | -3.091460  | 3.968027   | -0.367896  |
| 31            | 6             | 0           | 0.274938   | 3.604110   | 0.404540   |
| 32            | 1             | 0           | 0.286809   | 4.450615   | 1.092349   |
| 33            | 1             | 0           | 0.903884   | 2.824724   | 0.833516   |
| 34            | 1             | 0           | 0.695061   | 3.940181   | -0.543103  |
| 35            | 6             | 0           | -1.699031  | 2.479080   | 1.502455   |
| 36            | 1             | 0           | -2.737386  | 2.176139   | 1.382200   |
| 37            | 1             | 0           | -1.105459  | 1.615584   | 1.799054   |
| 38            | 1             | 0           | -1.655769  | 3.208886   | 2.312605   |
| 39            | 35            | 0           | -1.901979  | -2.497354  | -1.610212  |
| 40            | 6             | 0           | 1.598259   | 0.699781   | 2.697453   |
| 41            | 1             | 0           | 1.290858   | 1.616093   | 3.191568   |
| 42            | 1             | 0           | 2.629946   | 0.599063   | 2.413886   |
| 43            | 6             | 0           | 0.728338   | -0.273495  | 2.486622   |
| 44            | 6             | 0           | -0.136478  | -1.187383  | 2.191079   |
| 45            | 1             | 0           | -0.285214  | -1.967542  | 2.973983   |
| 46            | 9             | 0           | 1.111556   | -1.905935  | -0.561627  |
| 47            | 9             | 0           | 3.448037   | 2.170793   | -0.784476  |
| 48            | 9             | 0           | 5.673448   | 0.933831   | 0.070059   |
| 49            | 9             | 0           | 5.609183   | -1.709201  | 0.647260   |
| 50            | 9             | 0           | 3.320888   | -3.117686  | 0.333766   |

### TS for Si attack in THF of 1a with 2a

**Imaginary frequency:** -355.8269

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 16            | 0           | -1.101403 1.938963 -1.312504 |
| 2             | 7             | 0           | -0.099495 0.802764 -0.493841 |
| 3             | 8             | 0           | -0.215086 2.729292 -2.211897 |
| 4             | 6             | 0           | 1.040362 1.258378 -0.009311 |
| 5             | 1             | 0           | 1.242377 2.320915 -0.060906 |
| 6             | 6             | 0           | 2.276497 0.450167 -0.013085 |
| 7             | 6             | 0           | 2.359642 -0.897582 -0.327698 |
| 8             | 6             | 0           | 3.485870 1.089670 0.257808 |
| Center | Atomic Number | Atomic Type | Coordinates (Ångstroms) |
|--------|---------------|-------------|------------------------|
|        |               |             | X                      | Y                      | Z                      |
| 1      | 6             | 0           | 3.558147               | -1.584397              | -0.365931              |
| 10     | 6             | 0           | 4.698785               | 0.432915               | 0.228786               |
| 11     | 6             | 0           | 4.735640               | -0.916146              | -0.083665              |
| 12     | 6             | 0           | -0.967432              | -1.077293              | 0.027058               |
| 13     | 8             | 0           | -2.963672              | -0.507837              | 0.075989               |
| 14     | 6             | 0           | -3.836899              | -0.505429              | -1.082288              |
| 15     | 6             | 0           | -5.171907              | -1.026695              | -0.582146              |
| 16     | 6             | 0           | -5.170294              | -0.578481              | 0.878690               |
| 17     | 6             | 0           | -3.724565              | -0.804782              | 1.272739               |
| 18     | 1             | 0           | -5.200030              | -2.114406              | -0.644285              |
| 19     | 1             | 0           | -3.539500              | -1.844818              | 1.547054               |
| 20     | 1             | 0           | -5.426622              | 0.478840               | 0.957235               |
| 21     | 1             | 0           | -5.854363              | -1.147911              | 1.502800               |
| 22     | 1             | 0           | -6.003614              | -0.623722              | -1.154602              |
| 23     | 1             | 0           | -3.900130              | 0.521585               | -1.441489              |
| 24     | 1             | 0           | -3.362916              | -0.149498              | 2.061456               |
| 25     | 1             | 0           | -3.385349              | -1.131960              | -1.848468              |
| 26     | 6             | 0           | -1.711336              | 3.189113               | -0.054083              |
| 27     | 6             | 0           | -2.771788              | 3.951966               | -0.895814              |
| 28     | 1             | 0           | -3.248252              | 4.683053               | -0.201247              |
| 29     | 1             | 0           | -2.326189              | 4.484039               | -1.695431              |
| 30     | 1             | 0           | -3.547784              | 3.285255               | -1.235325              |
| 31     | 6             | 0           | -0.600896              | 4.142009               | 0.366276               |
| 32     | 1             | 0           | -1.050921              | 5.018101               | 0.836024               |
| 33     | 1             | 0           | 0.077709               | 3.696227               | 1.088477               |
| 34     | 1             | 0           | -0.031516              | 4.475483               | -0.500392              |
| 35     | 6             | 0           | -2.355535              | 2.469760               | 1.121068               |
| 36     | 1             | 0           | -3.213598              | 1.883996               | 0.792766               |
| 37     | 1             | 0           | -1.660737              | 1.804627               | 1.630776               |
| 38     | 1             | 0           | -2.707259              | 3.213321               | 1.838024               |
| 39     | 35            | 0           | -1.429826              | -3.455952              | -0.637949              |
| 40     | 6             | 0           | 0.983167               | 1.333264               | 2.305229               |
| 41     | 1             | 0           | 0.485830               | 2.263053               | 2.551968               |
| 42     | 1             | 0           | 2.048526               | 1.308633               | 2.483974               |
| 43     | 6             | 0           | 0.268312               | 0.187181               | 2.386681               |
| 44     | 6             | 0           | -0.437656              | -0.830451              | 2.181745               |
| 45     | 1             | 0           | -0.866230              | -1.529807              | 2.883450               |
| 46     | 9             | 0           | 1.261901               | -1.607055              | -0.634441              |
| 47     | 9             | 0           | 3.485492               | 2.382128               | 0.573837               |
| 48     | 9             | 0           | 5.821774               | 1.080428               | 0.499426               |
| 49     | 9             | 0           | 5.888362               | -1.559976              | -0.111597              |
| 50     | 9             | 0           | 3.582267               | -2.871833              | -0.671281              |

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PRODUCT for Si attack in THF of 1a with 2a
| Center | Atomic Number | Atomic | Type | X     | Y     | Z     |
|--------|----------------|--------|------|-------|-------|-------|
| 1      | 16             | 0      | -1.587562 | 2.185817 | -0.689007 |
| 2      | 7              | 0      | -0.300648  | 1.100072  | -0.159539 |
| 3      | 8              | 0      | -0.944492  | 3.314874  | -1.406107 |
| 4      | 6              | 0      | 0.853655   | 1.513225  | -0.512054 |
| 5      | 1              | 0      | 0.931858   | 2.440484  | -1.080774 |
| 6      | 6              | 0      | 2.105187   | 0.828234  | -0.210463 |
| 7      | 6              | 0      | 3.211118   | 1.061568  | -1.025662 |
| 8      | 6              | 0      | 2.281250   | -0.030531 | 0.869826 |
| 9      | 6              | 0      | 4.426387   | 0.445552  | -0.799848 |
| 10     | 6              | 0      | 3.485829   | -0.650927 | 1.121900 |
| 11     | 6              | 0      | 4.560417   | -0.414907 | 0.277474 |
| 12     | 12             | 0      | -0.789307  | -1.122237 | 0.183258 |
| 13     | 35             | 0      | -1.768029  | -1.961444 | 2.328130 |
| 14     | 8              | 0      | -2.421677  | -0.956797 | -1.058505 |
| 15     | 6              | 0      | -3.722878  | -1.514116 | -0.734991 |
| 16     | 6              | 0      | -4.512772  | -1.444497 | -2.027802 |
| 17     | 6              | 0      | -3.421433  | -1.627600 | -3.081344 |
| 18     | 6              | 0      | -2.277908  | -0.824268 | -2.495561 |
| 19     | 1              | 0      | -4.987182  | -0.468618 | -2.134603 |
| 20     | 1              | 0      | -2.355997  | 0.235231  | -2.742152 |
| 21     | 1              | 0      | -3.135773  | -2.676674 | -3.158922 |
| 22     | 1              | 0      | -3.709362  | -1.266329 | -4.065550 |
| 23     | 1              | 0      | -5.282961  | -2.210627 | -2.06970 |
| 24     | 1              | 0      | -3.574263  | -2.540338 | -0.400590 |
| 25     | 1              | 0      | -1.295619  | -1.201259 | -2.769245 |
| 26     | 1              | 0      | -4.141314  | -0.928941 | 0.079578 |
| 27     | 6              | 0      | 0.732667   | -2.189890 | -0.909195 |
| 28     | 1              | 0      | 1.475983   | -2.609218 | -0.227008 |
| 29     | 1              | 0      | 1.255608   | -1.564906 | -1.637452 |
| 30     | 6              | 0      | -2.067474  | 2.839352  | 0.990244 |
| 31     | 6              | 0      | -3.074627  | 3.940961  | 0.654354 |
| 32     | 1              | 0      | -3.457918  | 4.351375  | 1.588789 |
| 33     | 1              | 0      | -2.610109  | 4.746086  | 0.088121 |
| 34     | 1              | 0      | -3.922022  | 3.552950  | 0.086850 |
| 35     | 6              | 0      | -0.848418  | 3.400007  | 1.701040 |
| 36     | 1              | 0      | -1.181484  | 3.967653  | 2.573200 |
| 37     | 1              | 0      | -0.180523  | 2.616304  | 2.045209 |
| 38     | 1              | 0      | -0.297833  | 4.084699  | 1.051024 |
| 39     | 6              | 0      | -2.737763  | 1.711929  | 1.761985 |
| 40     | 1              | 0      | -3.536536  | 1.245938  | 1.829434 |
| 41     | 1              | 0      | -2.033427  | 0.941749  | 2.068502 |
| 42     | 1              | 0      | -3.184926  | 2.126743  | 2.666280 |

RC for Re attack in THF of 1a with 2a
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X                       |
|               |               |             | Y                       |
|               |               |             | Z                       |

TS for Re attack in THF of 1a with 2a

Imaginary frequency: -378.6744

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43  6  0  0.010556  -3.242064  -1.576214
44  6  0  -0.677488  -4.081346  -2.105582
45  1  0  -1.244904  -4.841182  -2.584847
46  9  0  3.620971  -1.469744  2.151352
47  9  0  1.272204  -0.264466  1.706479
48  9  0  3.102100  1.877270  -2.064971
49  9  0  5.713626  -1.010271  0.503035
50  9  0  5.455361  0.668645  -1.608014

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-543-
### PRODUCT for Re attack in THF of 1b with 2a

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 16            | 0           | -1.493695, -1.787799, -0.890716 |
| 2             | 7             | 0           | -0.639590, -0.700378, -0.014670 |
| 3             | 8             | 0           | -1.478148, -3.126434, -0.207258 |
| 4             | 6             | 0           | 0.553866, -1.154841, 0.668070 |
| 5             | 1             | 0           | 0.664397, -2.231483, 0.544631 |
| 6             | 6             | 0           | 1.840697, -0.511780, 0.166614 |
| 7             | 6             | 0           | 3.009244, -1.260607, 0.132304 |
| 8             | 6             | 0           | 1.950103, 0.799083, -0.268200 |
| 9             | 6             | 0           | 4.211390, -0.759544, -0.331555 |
| 10            | 6             | 0           | 3.136337, 1.333539, -0.739633 |
| 11            | 6             | 0           | 4.274560, 0.549482, -0.773959 |
| 12            | 12            | 0           | -1.604622, 1.024482, 0.362375 |
| 13            | 35            | 0           | -2.247511, 3.052248, -0.868504 |
| 14            | 8             | 0           | -3.248015, 0.434110, 1.413391 |
| 15            | 6             | 0           | -4.572755, 1.018362, 1.310797 |
| 16            | 6             | 0           | -5.390643, 0.317841, 2.378965 |
| 17            | 6             | 0           | -4.751722, -1.072394, 2.412463 |
| 18            | 6             | 0           | -3.282870, -0.761003, 2.237889 |
| 19            | 1             | 0           | -6.448773, 0.300669, 2.130339 |
| 20            | 1             | 0           | -2.724321, -1.540179, 1.724788 |
| 21            | 1             | 0           | -4.949181, -1.608748, 3.338330 |
| 22            | 1             | 0           | -5.116878, -1.677126, 1.580093 |
| 23            | 1             | 0           | -5.267971, 0.816824, 3.340440 |
| 24            | 1             | 0           | -4.474479, 2.091100, 1.452801 |
| 25            | 1             | 0           | -2.798618, -0.522086, 3.185369 |
| 26            | 1             | 0           | -4.950949, 0.818987, 0.308277 |
| 27            | 6             | 0           | 0.405545, -0.934463, 2.193119 |
| 28            | 1             | 0           | 1.338876, -1.158500, 2.710951 |
| 29            | 1             | 0           | -0.353501, -1.626037, 2.559038 |
| 30            | 6             | 0           | -0.542664, -2.076530, -2.475661 |
| 31            | 6             | 0           | -1.511929, -2.877544, -3.346072 |
| 32            | 1             | 0           | -1.064760, -3.049616, -4.326644 |
| 33            | 1             | 0           | -1.733301, -3.845184, -2.896521 |
| 34            | 1             | 0           | -2.450732, -2.340952, -3.494396 |
| 35            | 6             | 0           | 0.728509, -2.873463, -2.224576 |
| 36            | 1             | 0           | 1.119715, -3.243236, -3.174450 |
| 37            | 1             | 0           | 1.504403, -2.262072, -1.769386 |
| 38            | 1             | 0           | 0.524426, -3.729001, -1.581288 |
| 39            | 6             | 0           | -0.259150, -0.714773, -3.095237 |
| 40            | 1             | 0           | -1.173471, -0.128040, -3.206982 |
| 41            | 1             | 0           | 0.440076, -0.140508, -2.489524 |
| 42            | 1             | 0           | 0.174403, -0.847868, -4.088298 |
| 43            | 6             | 0           | -0.007840, 0.430989, 2.505285 |
| 44            | 6             | 0           | -0.364532, 1.556588, 2.723579 |
| 45            | 1             | 0           | -0.644405, 2.556173, 2.963545 |
| 46            | 9             | 0           | 2.988462, -2.529655, 0.547334 |
| 47            | 9             | 0           | 5.296717, -1.522064, -0.357518 |
| 48            | 9             | 0           | 5.416687, 1.049989, -1.220035 |
| 49            | 9             | 0           | 0.895888, 1.630116, -0.254745 |
| 50            | 9             | 0           | 3.187107, 2.593327, -1.351500 |

### RC for Re attack in DCM of 1a with 2b

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 12            | 0           | 1.807659, 0.815041, 1.294378 |
| 2             | 6             | 0           | 0.094691, 0.763026, 2.612256 |
| 3             | 6             | 0           | -0.517636, -0.537733, 2.693562 |
| 4             | 6             | 0           | -0.989892, -1.650533, 2.707015 |
| 5             | 6             | 0           | -0.540527, -1.218928, -0.272330 |
| 6             | 7             | 0           | 0.653413, -0.761220, -0.324605 |
| 7             | 1             | 0           | -0.633209, 1.515930, 2.298253 |
| 8             | 1             | 0           | 0.470615, 1.063458, 3.594621 |
| Center Number | Atomic Number | Atomic Type | X (Angstroms) | Y (Angstroms) | Z (Angstroms) |
|---------------|---------------|-------------|---------------|---------------|---------------|
| 1             | 12            |             | -1.195957     | -1.072022     | 1.186858      |
| 2             | 6             | 0           | 0.286690      | -0.941042     | 2.833340      |
| 3             | 6             | 0           | 1.283999      | 0.007394      | 2.591112      |
| 4             | 6             | 0           | 2.068530      | 0.868136      | 2.215407      |
| 5             | 6             | 0           | 1.043296      | 1.057439      | 0.019568      |
| 6             | 6             | 0           | -0.175394     | 0.593812      | 0.012236      |
| 7             | 7             | 0           | 0.661466      | -1.961773     | 2.912485      |
| 8             | 1             | 0           | -0.362582     | -0.687118     | 3.672162      |
| 9             | 1             | 0           | 1.233967      | 2.111679      | 0.184229      |
| 10            | 16            | 0           | -1.375651     | 1.669892      | 0.526791      |
| 11            | 8             | 0           | -2.285647     | 0.692423      | 1.258696      |
| 12            | 6             | 0           | 2.138089      | 0.313709      | -0.612599     |
| 13            | 6             | 0           | 3.202560      | 1.022211      | -1.161726     |
| 14            | 6             | 0           | 2.185064      | -1.072725     | -0.714976     |
| 15            | 6             | 0           | 4.261855      | 0.393617      | -1.788112     |
| 16            | 6             | 0           | 3.233762      | -1.723584     | -1.332742     |
| 17            | 6             | 0           | 4.276621      | -0.987215     | -1.872530     |
| 18            | 35            | 0           | -2.328426     | -2.983072     | 0.086442      |
| 19            | 6             | 0           | -2.212781     | 2.013108      | -1.087895     |
| 20            | 6             | 0           | -2.598580     | 0.710626      | -1.770563     |
| 21            | 1             | 0           | -3.241033     | 0.103687      | -1.134031     |
| 22            | 1             | 0           | -3.151189     | 0.949223      | -2.680096     |
| 23            | 1             | 0           | -1.722848     | 0.125943      | -2.045804     |
| 24            | 6             | 0           | -1.227027     | 2.833184      | -1.914748     |
| 25            | 1             | 0           | -0.865687     | 3.721488      | -1.380583     |
| 26            | 1             | 0           | -0.360913     | 2.242863      | -2.211779     |
| 27            | 1             | 0           | -1.730141     | 3.165955      | -2.822844     |
| 28            | 6             | 0           | -3.443286     | 2.836198      | -0.707218     |
| 29            | 1             | 0           | -3.170116     | 3.758146      | -0.192133     |
| 30            | 1             | 0           | -3.976988     | 3.106122      | -1.618716     |
| 31            | 1             | 0           | -4.119007     | 2.263484      | -0.073514     |
| 32            | 6             | 0           | 3.218368      | 1.780277      | 2.215076      |

**TS for Re attack in DCM of 1a with 2b**

**Frequency**  
-214.275
### PRODUCT for Re attack in DCM of 1a with 2b

| Center Number | Atomic Number | Atomic Type | Coordinates (Ångstroms) | X     | Y     | Z     |
|---------------|---------------|-------------|-------------------------|-------|-------|-------|
|               |               |             |                         |       |       |       |
| 1             | 12            | 0           | -1.962037               | -0.328538 | 0.494381 |
| 2             | 6             | 0           | -1.436526               | -2.674506 | 1.868483 |
| 3             | 6             | 0           | -0.228755               | -2.175052 | 1.826008 |
| 4             | 6             | 0           | 0.971725                | -1.681959 | 1.770249 |
| 5             | 6             | 0           | 1.223969                | -0.323419 | 1.119953 |
| 6             | 7             | 0           | 0.025679                | 0.284873  | 0.586754 |
| 7             | 1             | 0           | -1.795521               | -3.339335 | 1.091681 |
| 8             | 1             | 0           | -2.093437               | -2.485456 | 2.710547 |
| 9             | 1             | 0           | 1.662118                | 0.301391  | 1.903926 |
| 10            | 16            | 0           | -0.386678               | 1.738056  | 1.183912 |
| 11            | 8             | 0           | -1.926021               | 1.564987  | 1.251220 |
| 12            | 6             | 0           | 2.285379                | -0.453161 | 0.034727 |
| 13            | 6             | 0           | 3.519991                | 0.161616  | 0.149201 |
| 14            | 6             | 0           | 2.039071                | -1.147006 | -1.140877 |
| 15            | 6             | 0           | 4.470996                | 0.109782  | -0.855887 |
| 16            | 6             | 0           | 2.968128                | -1.217177 | -2.162184 |
| 17            | 6             | 0           | 4.191535                | -0.583908 | -2.018307 |
| 18            | 35            | 0           | -3.747362               | -1.403638 | -0.801111 |
| 19            | 6             | 0           | -0.174512               | 2.927300  | -0.222369 |
| 20            | 6             | 0           | -0.937309               | 2.441901  | -1.443061 |
| 21            | 1             | 0           | -2.008781               | 2.399283  | -1.249967 |
| 22            | 1             | 0           | -0.770982               | 3.138438  | -2.266201 |
| 23            | 1             | 0           | -0.588064               | 1.458980  | -1.760408 |
| 24            | 6             | 0           | 1.326548                | 2.984735  | -0.489947 |
| 25            | 1             | 0           | 1.894698                | 3.191778  | 0.420342 |
| 26            | 1             | 0           | 1.683044                | 2.049413  | -0.918679 |
| 27            | 1             | 0           | 1.534432                | 3.784629  | -1.200520 |
| 28            | 6             | 0           | -0.703414               | 4.268304  | 0.279426 |
| 29            | 1             | 0           | -0.167967               | 4.601731  | 1.170004 |
| 30            | 1             | 0           | -0.565183               | 5.022784  | -0.496341 |
| 31            | 1             | 0           | -1.765915               | 4.207942  | 0.512055 |
| 32            | 6             | 0           | 2.162350                | -2.392832 | 2.355558 |
| 33            | 1             | 0           | 2.682179                | -1.737991 | 3.057280 |
| 34            | 1             | 0           | 1.866269                | -3.298899 | 2.877374 |
| 35            | 1             | 0           | 2.870647                | -2.661089 | 1.570015 |
| 36            | 9             | 0           | 3.822218                | 0.853736  | 1.251000 |
| 37            | 9             | 0           | 5.640619                | 0.721481  | -0.711666 |
| 38            | 9             | 0           | 5.090080                | -0.645905 | -2.990378 |
| 39            | 9             | 0           | 2.699377                | -1.889007 | -3.275234 |
| 40            | 9             | 0           | 0.876679                | -1.774066 | -1.317745 |
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XI. $^1$H, $^{13}$C and $^{19}$F NMR spectra of new compounds.

$^1$H NMR spectrum of compound 1a (300 MHz, CDCl$_3$)

$^{19}$F NMR spectrum of compound 1a (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound 1a (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound 1b (300 MHz, CDCl$_3$)
$^{19}$F NMR spectrum of compound 1b (282 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of compound 1b (75 MHz, CDCl$_3$)
$^1$H NMR spectrum of compound 1c (300 MHz, CDCl$_3$)

$^{19}$F NMR spectrum of compound 1c (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound 1c (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound 1d (300 MHz, CDCl$_3$)
$^{19}$F NMR spectrum of compound 1d (282 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of compound 1d (75 MHz, CDCl$_3$)
$^1$H NMR spectrum of compound 1e (300 MHz, CDCl$_3$)

$^{19}$F NMR spectrum of compound 1e (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound 1e (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound 3a (300 MHz, CDCl$_3$)
$^{19}$F NMR spectrum of compound 3a (282 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of compound 3a (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound 3'a (300 MHz, CDCl$_3$)
$^{19}$F NMR spectrum of compound 3'a (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound 3'a (75 MHz, CDCl₃)

$^1$H NMR spectrum of compound 3'b (300 MHz, CDCl₃)
$^{19}$F NMR spectrum of compound 3b (282 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of compound 3b (300 MHz, CDCl$_3$)
$^1$H NMR spectrum of compound 3'b (300 MHz, CDCl$_3$)

$^{19}$F NMR spectrum of compound 3'b (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound $3'b$ (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound $3'c$ (300 MHz, CDCl$_3$)
$^{19}$F NMR spectrum of compound 3’c (282 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of compound 3’c (75 MHz, CDCl$_3$)
$^1$H NMR spectrum of compound 3'd (300 MHz, CDCl₃)

$^{19}$F NMR spectrum of compound 3'd (282 MHz, CDCl₃)
$^{13}$C NMR spectrum of compound $3'd$ (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound $3'e$ (300 MHz, CDCl$_3$)
$^{19}$F NMR spectrum of compound 3'e (282 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of compound 3'e (75 MHz, CDCl$_3$)
$^1$H NMR spectrum of compound 4ab (300 MHz, CDCl₃)

$^1$F NMR spectrum of compound 4ab (282 MHz, CDCl₃)
$^{13}$C NMR spectrum of compound 4ab (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound 4ac (300 MHz, CDCl$_3$)
$^1$H NMR spectrum of compound 4ac (282 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of compound 4ab (75 MHz, CDCl$_3$)

$^{19}$F NMR spectrum of compound 4ac (282 MHz, CDCl$_3$)
$^1$H NMR spectrum of compound 4bb (300 MHz, CDCl$_3$)

19$^F$ NMR spectrum of compound 4bb (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound 4bb (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound 4bc (300 MHz, CDCl$_3$)
$^{19}$F NMR spectrum of compound 4bc (282 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of compound 4bc (75 MHz, CDCl$_3$)
$^1$H NMR spectrum of compound 4cb (300 MHz, CDCl$_3$)

$^{19}$F NMR spectrum of compound 4cb (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound 4cb (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound 4cc (300 MHz, CDCl$_3$)
\(^{19}\text{F}\) NMR spectrum of compound 4cc (282 MHz, CDCl\(_3\))

\[ \text{Diagram of compound 4cc with its \(^{19}\text{F}\) NMR spectrum} \]

\(^{13}\text{C}\) NMR spectrum of compound 4cc (75 MHz, CDCl\(_3\))

\[ \text{Diagram of compound 4cc with its \(^{13}\text{C}\) NMR spectrum} \]

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$^1$H NMR spectrum of compound 4db (300 MHz, CDCl$_3$)

$^{19}$F NMR spectrum of compound 4db (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound 4db (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound 4dc (300 MHz, CDCl$_3$)
$^{19}$F NMR spectrum of compound 4dc (282 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of compound 4dc (75 MHz, CDCl$_3$)
$^1$H NMR spectrum of compound 4eb (300 MHz, CDCl$_3$)

$^{19}$F NMR spectrum of compound 4eb (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound $4eb$ (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound $4ec$ (300 MHz, CDCl$_3$)
\[ ^{19}F \text{NMR spectrum of compound 4ec (282 MHz, CDCl}_3) \]

\[ ^{13}C \text{NMR spectrum of compound 4ec (75 MHz, CDCl}_3) \]
$^1$H NMR spectrum of compound 4fb (300 MHz, CDCl$_3$)

$^{19}$F NMR spectrum of compound 4fb (282 MHz, CDCl$_3$)
$^{13}$C NMR spectrum of compound 4fb (75 MHz, CDCl$_3$)

$^1$H NMR spectrum of compound 4fc (300 MHz, CDCl$_3$)
\( ^{19}F \text{ NMR spectrum of compound 4fc (282 MHz, CDCl}_3 \)