Supporting Information

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Bimolecular Cross-Metathesis of a Tetrasubstituted Alkene with Allylic Sulfones

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Supporting Information

SUPPORTING INFORMATION

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^{13}C NMR of **1d** 54

^{1}H NMR of **2d** 55

^{19}F NMR of **2d** 55

^{13}C NMR of **2d** 56

^{1}H NMR of **4b** 56

^{19}F NMR of **4b** 57

^{1}H NMR of **4c** 57

^{19}F NMR of **4c** 58

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^{1}H NMR of **4d** 60

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^{1}H NMR of **5d** 62

^{13}C NMR of **5d** 62

^{19}F NMR of **5d** 63

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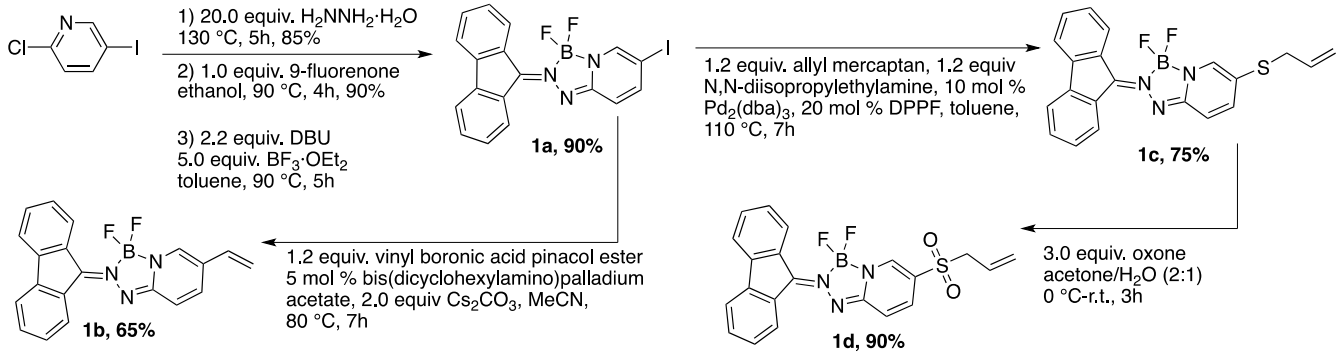
Experimental Procedures

General Considerations

Unless otherwise noted, all operations were performed in a fume hood using oven-dried (135 ˚C) glassware with distilled and degassed solvents under an atmosphere of purified dry nitrogen gas. Deuterated NMR solvents were purchase from Cambridge Isotope Laboratories. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded on a 300 MHz Oxford NMR spectrometer. ^{1}H NMR chemical shifts are reported in ppm from tetramethylsilane referenced to added internal standard tetramethylsilane (δ = 0.00 ppm) or with the solvent resonance resulting from incomplete deuterium incorporation as the internal standard ($CDCl_3$: δ 7.27 ppm, DMSO-d6 δ 2.50 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constants (Hz), and integration. ^{13}C NMR chemical shifts are reported referenced in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ = 77 ppm, DMSO-d6: δ = 39.5). ^{19}F NMR chemical shifts are reported with respect to added internal standard C_6F_6 (δ -164.9 ppm). Preparative column chromatography was carried out using pre-packed silica cartridges (4g) in a Combiflash chromatograph. High performance liquid chromatography was conducted using an Agilent 1100 LC system (Agilent Technologies, Santa Clara, CA) equipped with a diode array detector (DAD). High resolution mass spectrometry was performed on a hybrid linear ion trap 7 Tesla Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometer (Thermo Fisher, San Jose, CA), or an Orbitrap Fusion Mass Spectrometer (Thermo Fisher, San Jose, CA) at the New Mexico State University Chemical Analysis and Instrumentation Laboratory.



Scheme 1: Synthesis of the metathesis probes

Synthesis of 2-(9*H*-fluoren-9-ylidene)-3,3-difluoro-6-iodo-2,3-dihydro-[1,2,4,3]triazaborolo[4,5-*a*]pyridin-2-ium-3-uide (1a)

2-Hydrazinyl-5-iodopyridine[1] (1.17g, 5 mmol) was combined with 9-fluorenone (0.9 g, 5 momol) in ethanol and refluxed for 4h to yield the hydrazine as yellow colored solid (1.78g, 4.56 mmol, 90%) . The hydrazone ((Z)-2-((9H-fluoren-9-ylidene) hydrazono)-5-iodo-1,2-dihydropyridine) was used directly without further purification. To a mixture of hydrazone: (Z)-2-((9H-fluoren-9-ylidene) hydrazono)-5-iodo-1,2-dihydropyridine (0.397 g, 1 mmol) and BF_3•Et_2O (0.705 g, 5 mmol) in dry toluene (5 mL) was added DBU (0.33 g, 2.2 mmol) and heated at about 90 ˚C for 8h. Volatiles were removed *in vacuo*. The residue was dissolved in dichloromethane (25 mL), washed with water, the organic layer was separated, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel column chromatography using hexanes/EtOAc (70:30) eluent to isolate the product **1a** (0.426 g, 96 %) as a red solid. Rf = 0.39 (20:80, EtOAc: Hexane); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.98 (d, J =7.78 Hz, 1H), 8.37 (d, J =7.78 Hz, 1H), 7.79 (s, 1H), 7.60 (dd, J = 9.24, 1.91 Hz, 1H), 7.61-7.56 (m, 2H), 7.44 (dt, J = 7.48, 7.48, 1.17 Hz, 1H), 7.38 (dt, J = 7.48, 7.48, 1.03 Hz, 1H), 7.32 (dt, J =7.63, 7.63, 1.32 Hz, 1H), 7.28 (dt, J =5.72, 5.72, 1.17 Hz, 1H), 6.73 (d, J =9.39 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) 159. 2, 156.3, 150.7, 148.4, 141.84, 141.71, 141.09, 132.6, 132.1, 131.6, 131.1, 128.6, 128.5, 126.6 (t, J =8.98 Hz, 1C), 120.1, 119.7, 115.2, 70.2; ^{19}F NMR (300 MHz, $CDCl_3$); δ -149.09 (q, J =28 Hz, 2F). FT-IR (solid): 3058.6, 2923.68, 1630.59, 1608.41, 1520.63, 1471.48, 1443.52, 1407.84, 1358.66, 1299.84, 1153.27, 1100.24, 1074.20, 1034.67, 1016.35; UV-Vis (octanol) λ_{max}: 537 nm, €= 40,100 $M^{-1}cm^{-1}$; λ_{em}: 572nm; Φ_f = 0.80. Log $P_{o/w}$ = 0.79. HRMS (m/z): calcd for $[M+H]+$ $C_{18}H_{12}BF_2IN3$: 446.0167; found: 446.0162.

Synthesis of 2-(9*H*-fluoren-9-ylidene)-3,3-difluoro-6-vinyl-2,3-dihydro-[1,2,4,3]triazaborolo[4,5-*a*]pyridin-2-ium-3-uide (1b)

To bis(dicyclohexylamino)palladium acetate (7 mg, 0.04 mmol), 0.5 mL of dioxane was added, followed by vinyl pinacolboronate (135 µL, 0.8 mmol), **1a** (178mg, 0.4 mmol) and cesium carbonate (260mg, 0.8 mmol)[2]. The reaction mixture was heated at 80 °C for 7h. The reaction mixture was diluted with 20 mL of diethyl ether and washed with 20 mL of 20% HCl and 20 mL of water, the organic layer was separated, dried over Na_2SO_4, and concentrated *in vacuo*. The residue was purified by flash chromatography eluting with EtOAc /hexane (5:95) to obtain the product **1b** as a red solid (106 mg, 75%). Rf = 0.48 (10:90, EtOAc: hexane); ^{1}H NMR (300 MHz,

$CDCl_3$): δ 8.98 (d, J = 7.80 Hz, 1H), 8.40 (d, J = 7.81 Hz, 1H), 7.68 (dd, J = 9.18, 1.95 Hz, 1H), 7.59-7.54 (m, 4H), 7.43-7.25 (m, 4H), 6.9(d, J = 9.18Hz, 1H), 6.50(dd, J = 17.57, 10.93 Hz, 1H), 5.56 (d, J = 17.57 Hz, 1H), 5.2 (d, J = 11.13 Hz, 1H; ^{13}C NMR (75 MHz, $CDCl_3$) 160. 3, 149.8, 141.8, 141.7, 138.3, 134.9, 134.2, 132.5, 132.0, 131.7, 131.5, 128.7, 128.6, 126.6 (t, J = 9.21 Hz, 1C), 124.5, 122.2, 120.2, 119.9, 113.8, 112.9; ^{19}F NMR (282 MHz, $CDCl_3$); δ -149.89 (q, J =31.21 Hz, 2F). FT-IR (solid); 2921.75, 1718.34, 1640.23, 1624.80, 1608.41, 1536.09, 1484.02, 1399.16, 1157.13, 1117.59, 1099.27, 1080.95; UV-Vis (octanol) λ_{max}: 537 nm, € = 33,500 $M^{-1}cm^{-1}$; λ_{em}: 601nm; Φf = 0.18. Log $P_{o/w}$ = 0.70. HRMS/(m/z): calcd for [M+H]+ $C_{20}H_{14}BF_2N_3$: 346.13271; found: 346.13223.

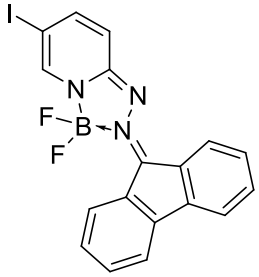
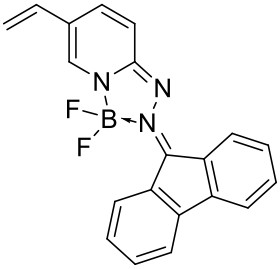
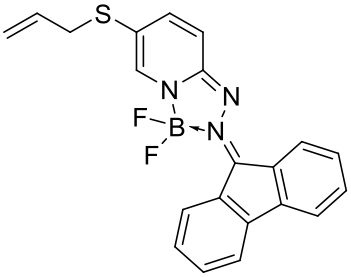
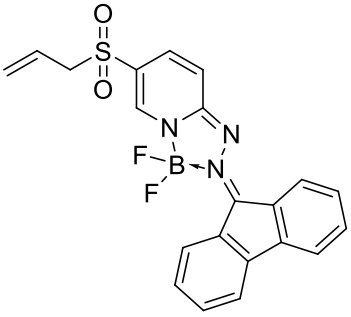
Synthesis of 6-(allylthio)-2-(9*H*-fluoren-9-ylidene)-3,3-difluoro-2,3-dihydro-[1,2,4,3]triazaborolo[4,5-*a*]pyridin-2-ium-3-uide (1c)

Following the literature procedure the C-S coupling was carried out as follows.[3]The iodide 1a (178 mg, 0.4 mmol), $Pd_2(dba)_3$ (36 mg, 10 mol%), DPPF (44 mg, 20 mol%), allyl mercaptan (96 µL, 1.2 mmol) and N,N-diisopropyl amine (76 µL, 0.44 mmol) were combined in a sealed tube under an atmosphere of nitrogen. The reaction mixture was heated at 110 °C in toluene (0.1 M) for 7h. The reaction was cooled to room temperature and diluted with 20 mL of ether, washed with 20 mL of water and 20 mL of 1 M HCl solution. The organic layer was separated, dried over Na_2SO_4, and concentrated *in vacuo*. The residue was purified by column chromatography eluting with EtOAc/hexane (1:99) to obtain the product 1c as a red solid (106 mg, 72%). Rf = 0.48 (30:70, EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.97 (d, J = 7.78 Hz, 1H), 8.39 (d, J = 7.78 Hz, 1H), 7.68 (s, 1H), 7.58-7.24 (m, 7H), 6.82 (d, J = 9.39 Hz, 1H), 5.82 (dd, J = 17.02, 9.98 Hz, 1H), 5.08 (d, J = 10.56 Hz, 1H), 4.96 (d, J = 17.02 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) 159.9, 150.2, 147.2, 141.7, 141.6, 140.5, 133.2, 132.4, 132.2, 132.0, 131.5, 131.1, 128.6, 128.4, 126.5 (t, J = 9.21 Hz, 1C), 120.0, 119.7, 118.5, 116.2, 113.4, 40.0; ^{19}F NMR (282 MHz, $CDCl_3$); δ -149.45 (q, J = 30.34 Hz, 2F). FT-IR (solid); 3068.32,2918.86, 1761.41, 1608.41, 1628.66, 1531.27, 1443.52, 1452.20, 1466.66, 1399.16, 1303.70; UV-Vis (octanol) λ_{max}: 531 nm, €= 34,200 $M^{-1}cm^{-1}$; λ_{em}: 618nm; Φ_f = 0.06. Log $P_{o/w}$ = 1.43. HRMS/(m/z): calcd for [M+H]+ $C_{21}H_{17}BF_2N_3S$: 392.12043; found: 392.11995.

Synthesis of 6-(allylsulfonyl)-2-(9H-fluoren-9-ylidene)-3,3-difluoro-2,3-dihydro-[1,2,4,3]triazaborolo[4,5-a]pyridin-2-ium-3-uide (1d)

Oxone (230 mg, 0.75 mmol) in water (1.5 mL) was added to a cooled (0 °C) solution of the allylic sulfide **1c** (98 mg, 0.25 mmol) in acetone (3.0 mL). The reaction mixture was stirred at room temperature for 3h.[4] The reaction mixture was diluted with dichloromethane (15 mL), washed with water, the organic layer was separated, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography eluting with dichloromethane to isolate the product **1d** as a red solid (75 mg, 0.177 mmol, 71%). Rf = 0.18 (30:70, EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.88 (d, J = 7.61 Hz, 1H), 8.34 (d, J = 8.36 Hz, 1H), 8.09 (bs, 1H), 7.63-7.27 (m, 7H), 6.82 (dd, J = 9.39, 3.37 Hz, 1H), 5.96-5.81 (m, 1H), 5.47 (dd, J = 10.12, 2.93 Hz, 1H), 5.30-5.29 (m, 1H), 3.84 (dd J = 7.68, 2.64 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) 159.9, 154.0, 142.4, 142.4, 140.3, 137.8, 133.7, 132.9, 132.8, 131.9, 130.5, 128.8, 128.7, 127.3 (t, J = 9.21 Hz, 1C), 125.4, 124.4, 120.7, 120.2, 119.9, 113.3, 61.0; ^{19}F NMR (282 MHz, $CDCl_3$); δ -148.45 (q, J = 28.61 Hz, 2F). FT-IR (solid); 3078.93, 2926.57, 1636.37, 1609.37, 1528.38, 1500.41, 1422.30, 1454.13, 1161.95,1139.77, 1016.35; UV-Vis (octanol) λ_{max}: 507 nm, €= 24,615 $M^{-1}cm^{-1}$; λ_{em}: 531 nm; Φ_f = 0.13. Log $P_{o/w}$ = 2.00. HRMS/(m/z): calcd for [M+H]+ $C_{21}H_{17}BF_2N_3O_2S$: 424.11026; found: 424.10981.

Table S1 Photophysical properties of the compounds

SN	λ_{max}	λ_{emis}	Stoke's shift	Absorptivity ε	Quantum Yield	Brightness
 1a	537	**560**	23	38,250	0.87	33,277
 1b	537	**601**	64	33,500	0.18	6,030
 1c	531	**618**	87	34,200	0.06	2,200
 1d	507	**531**	24	24,600	0.13	3,200

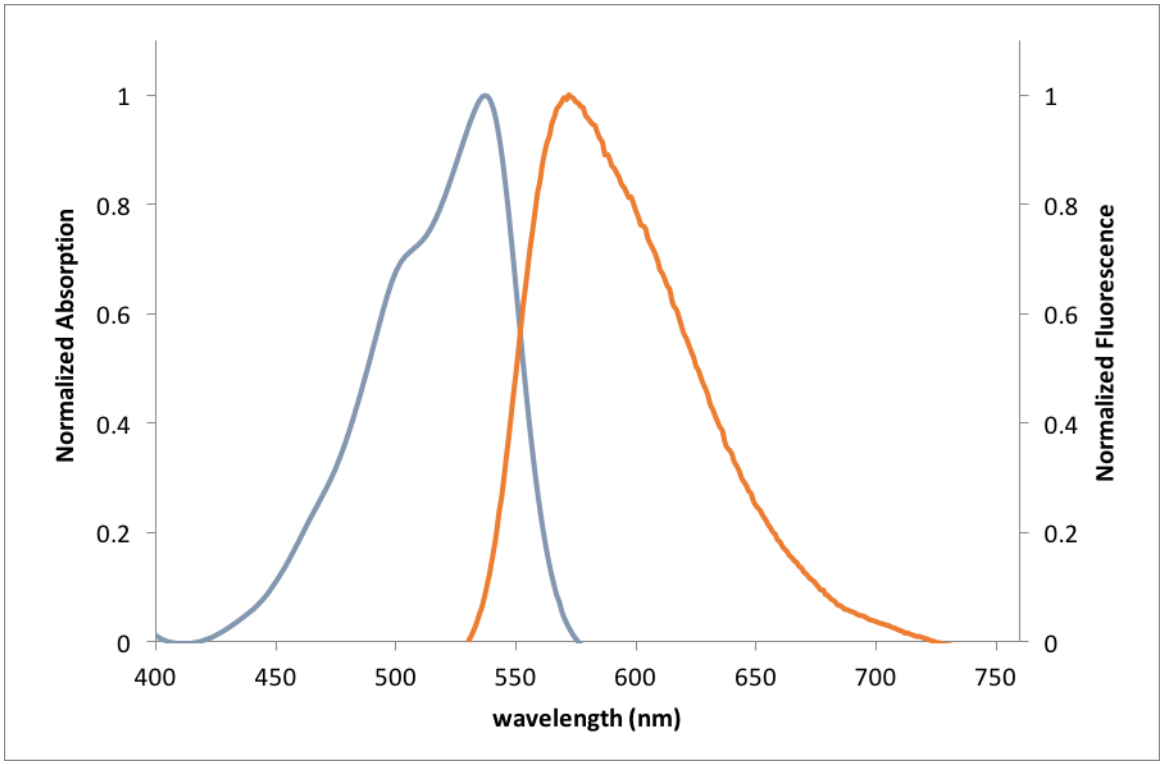
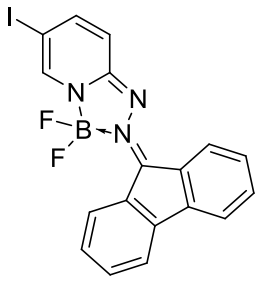


Figure S1. Normalized fluorescence and absorption spectra of **1a** in 1-octanol solution. **1a** has a Stoke's shift of 35 nm and a Φ_f = 0.80 when excited at 520 nm. A calculated ε = 40,100 $M^{-1}cm^{-1}$, with a λ_{max} = 537 nm, λ_{em} = 570 nm with brightness = 32,100.



1a

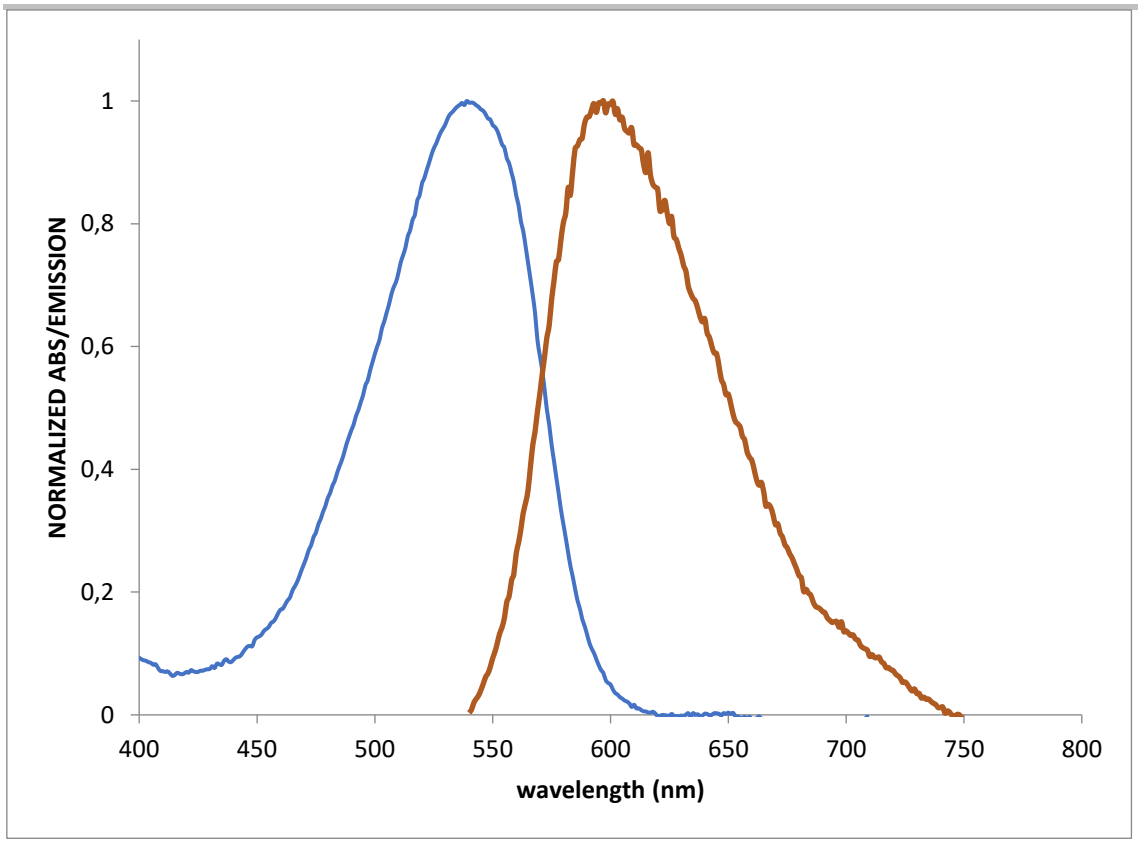
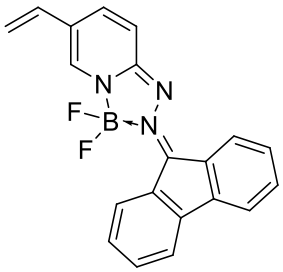


Figure S2. Normalized fluorescence/absorption spectra of **1b** in 1-octanol reveal a Stokes shift of 58nm, λ_{max} = 539nm and λ_{em} = 601nm. F_f = 0.18 when excited at 530nm.



1b

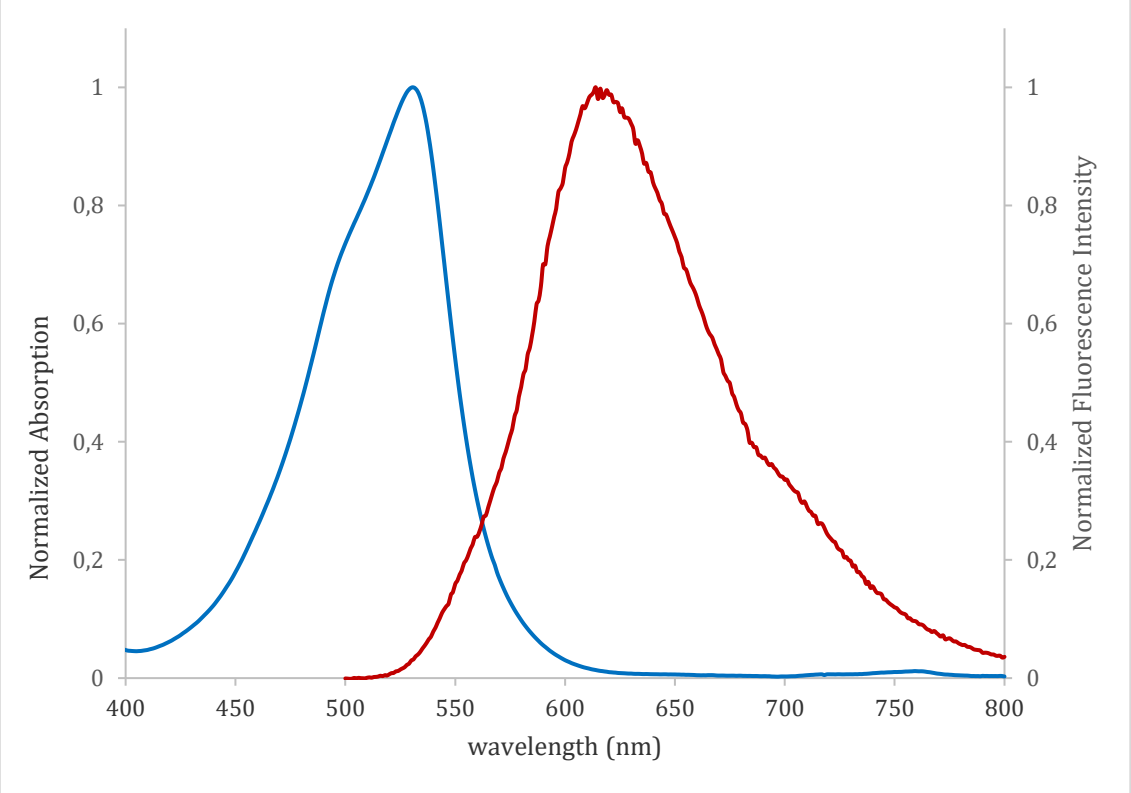
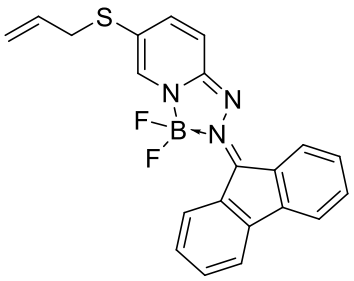


Figure S3. Normalized absorption/fluorescence spectra of 1c 1-octanol. Stoke's shift is 86nm with Φf of 0.06, when excited at 520nm. A calculated ε = 34,200M-1cm-1, with a λmax = 531nm and λem = 617nm.



1c

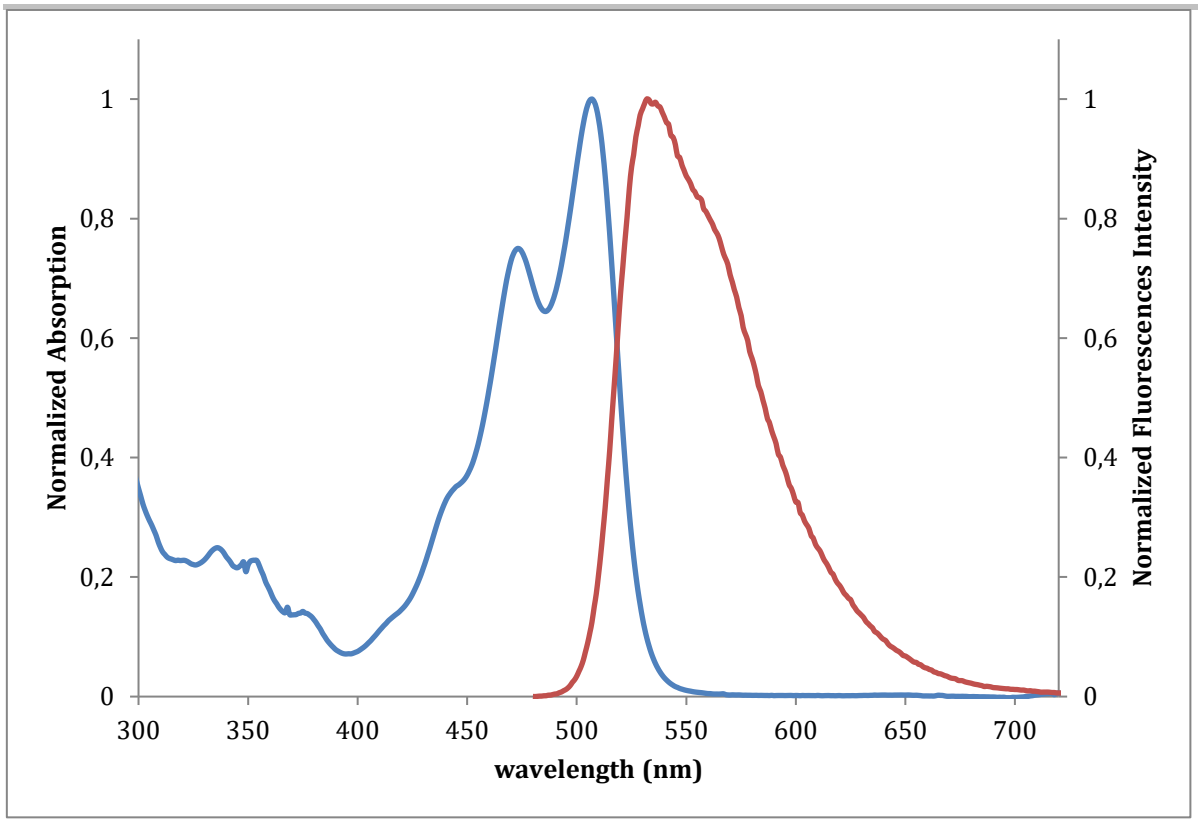
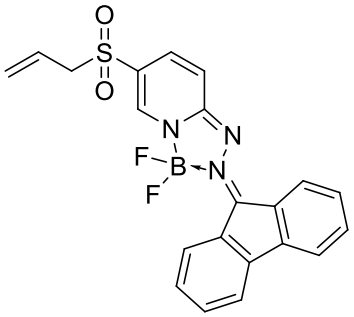


Figure S4. Normalized absorption/fluorescence spectra of **1d** in 1-octanol. The Stoke's shift is 24 nm with Φ_f = 0.13, when excited at 490 nm. A calculated ε =24,600 $M^{-1}cm^{-1}$, with a λ_{max} = 507 nm and λ_{em} = 531 nm.



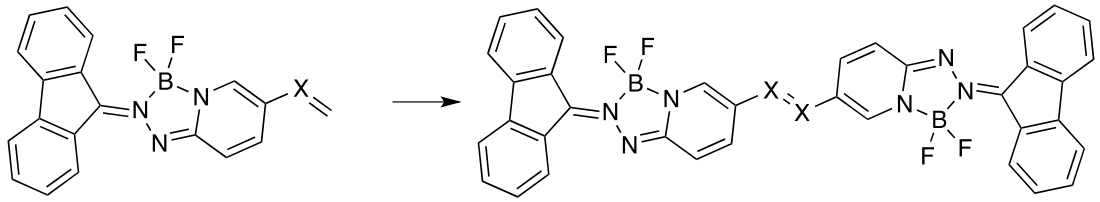
1d

Table S2. RP-LC gradients for separation of metathesis probes reaction products.

	Time	A H_2O 0.1% formic acid	B CH_3CN 0.1% formic acid
Citral	0	50	50
	5	30	70
	25	25	75
	30	1	99
Geranyl Acetone	0	50	50
	5	20	80
	25	1	99
	35	1	99
Q10	0	50	50
	5	20	80
	15	10	90
	50	1	99
	200	1	99
RS-VII-133 RS-VII-144 RS-VII-145	0	50	50
	10	30	70
	55	10	90
	55.1	1	99
	60	1	99
RS-VII-118	0	50	50
	5	20	80
	30	10	90
RS-VII-58	0	50	50
	5	20	80
	35	10	90
	40	1	99

General procedure (I) for homodimerization of 1b, 1c and 1d*:*

The metathesis probe (0.05 mmol), HG(II) catalyst (1.5 mg, 0.0025 mmol) and dichloromethane (1 mL, 0.5M) were combined in a flask under an atmosphere of nitrogen and heated to reflux for the specified time. The reaction progress was monitored by TLC. The product distributions were analyzed by HPLC-MS and NMR.



X = -CH, **1b**
X = -S-CH_2-CH, **1c**
X = -SO_2-CH_2-CH, **1d**

X = -CH, **2b**, trace
X = -S-CH_2-CH, **2c**, 84%
X = -SO_2-CH_2-CH, **2d**, 95%

Scheme 2: Homodimerization reaction of the metathesis probe

Homodimerization of 1b:

Following the general procedure **(I)**, homodimerization of the vinyl probe **(1b)** was attempted but only trace amounts of the homodimer **2b,** were observed. Extending the reaction time to 12 h resulted in decomposition of **1b** that produced uncharacterized oligomeric products.

Homodimerization of 1c:

Following the general procedure **(I)**, allylic sulfide probe **(1c)** was heated for 2h, resulting in a dark solution and fine precipitate. The solids were filtered to afford the homodimer **2c** (17 mg, **0.022 mmol,** 90%). Due to very poor solubility of **1c** we were unable to obtain a high resolution ^{13}C NMR spectrum. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.35 (d, *J* = 1.17 Hz, 4 H), 5.42 (d, *J* = 6.46 Hz, 2 H), 6.88 (s, 1 H), 6.83 (s, 1 H), 7.31 - 7.53 (m, 7 H), 7.53 - 7.67 (m, 5 H), 8.41 (s, 1 H), 8.37 (s, 1 H), 8.98 (d, *J* = 8.22 Hz, 2 H); HRMS/(m/z): calcd for $[M+H]^+$ $C_{40}H_{29}N_6S_2B_2F_4$: 755.2017; found: 755.2009

Homodimerization of 1d:

Following the general procedure **(I)**, **1d** was heated for 2h, resulting in a dark solution with orange precipitate. The solids were filtered to afford the homodimer **2d (**18 mg, **0.022 mmol,** 91%). Due to very poor solubility of **1d** we were unable to obtain a high resolution ^{13}C NMR spectrum.^{1}H NMR (300 MHz, DMSO-d_6) δ 8.88 (d, *J* = 7.7 Hz, 2H), 8.31 – 8.18 (m, 3H), 7.85 (dd, *J* = 10.6, 8.5 Hz, 5H), 7.53 (q, *J* = 7.8 Hz, 4H), 7.35 (td, *J* = 8.0, 3.5 Hz, 4H), 7.14 (d, *J* = 9.5 Hz, 2H), 5.88 – 5.76 (m, 2H), 4.45 – 4.27 (m, 4H); ^{13}C NMR (50 MHz, DMSO-d_6) δ 160.03, 152.59, 141.79, 141.66, 139.78, 139.34, 134.20, 133.22, 132.33, 131.01, 129.76, 129.15, 128.74, 126.82, 126.36, 122.55, 121.32, 120.91, 113.54, 57.86; ^{19}F NMR (282 MHz, DMSO-d_6) δ -147.18, -147.37. HRMS/(m/z): calcd for $[M+Na]^+$ $C_{40}H_{28}N_6O_4S_2B_2F_4N$: 841.16257; found: 841.16334.

General procedure (II) for cross metathesis reactions of 1b, 1c, 1d with 2-methyl-2-butene (1S):

The compound (**1b**, **1c**, **1d**: 0.05 mmol), HG(II) catalyst (1.5 mg, 0.0025 mmol) was combined with 2-methyl-2-butene (**1S,** 5 mmol, 100 equivalents**)** in dichloromethane and heated at 40 °C. The product distributions were analyzed at 30 minutes and 8h, respectively. An aliquot (50 μL) of the reaction mixture was passed through a short column of silica gel (800 mg) eluted with dichloromethane and the colored fractions were collected and analyzed as a mixture by LC-MS. The respective quantification histogram and the LC chromatogram are shown for each product mixture. The trisubstituted products (**4b**) were isolated and characterized by HPLC-MS, NMR spectroscopy and mass spectrometry.

Vinyl probe (1b) and 2-methyl-2-butene (1S) cross metathesis:

Following the general procedure **II**, after 8h reaction time compound **4b** was isolated by column chromatography eluting with EtOAc/hexane (1:99) to yield a red colored solid (15 mg, 0.04mmol, 40%).. R_f = 0.25 (5:95, EtOAc/hexane); ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.05 (d, *J* = 7.63 Hz, 1H), 8.43 (d, *J* = 7.63 Hz, 1H), 7.69-7.60 (m, 2H), 7.52-7.29 (m, 6H), 6.92 (d, *J* = 9.10 Hz, 1H), 6.01(s, 1H), 1.92 (d, *J* = 1.17 Hz, 3H), 1.88(d, *J* = 1.17 Hz, 3H); ^{13}C NMR (50 MHz, $CDCl_3$) δ 19.5, 26.76, 112.84, 119.58, 119.78, 119.95,

126.16, 128.25, 128.47, 129.08, 130.83, 131.53, 131.91, 133.03, 133.77, 134.57, 137.19, 141.23, 143.03, 159.20; ^{19}F NMR (282 MHz, $CDCl_3$); δ -149.89 (q, *J* = 31.21 Hz, 2F). HRMS/(m/z): calcd for $[M+H]^+$ $C_{22}H_{18}BF_2N_3$: 374.16401; found: 374.16340.
Based on the LC-MS UV detection, at 30 min **3b** was formed as major product (66%) and **4b** as minor (27%). The products at 8h are **3b** 52% and **4b** 40 % respectively and traces of homodimer **2b** were detected.

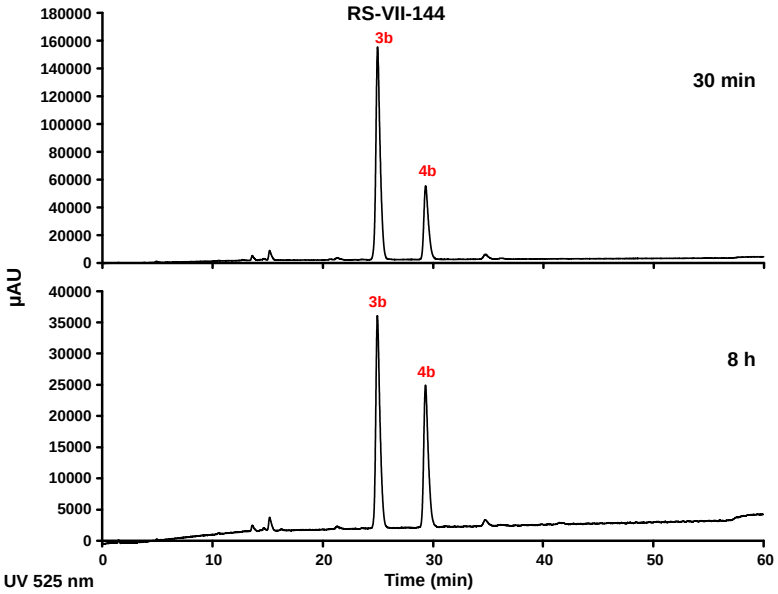


Figure S5 HPLC-UV-MS chromatogram of **(1b)** and 2-methyl-2-butene **(1S)** cross reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products.

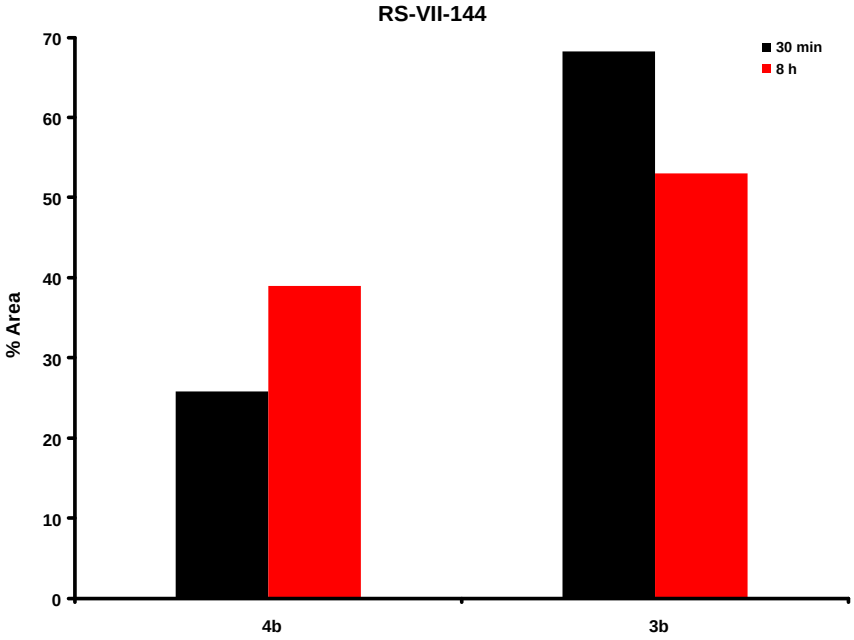


Figure S6 Relative abundance of total peak area for **(1b)** and 2-methyl-2-butene **(1S)** cross- metathesis reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products.

Sulfide probe (1c) and 2-methyl-2-butene(1S) cross-metathesis:

Following the general procedure **II**, after 8h reaction time compound **4c** was isolated by column chromatography eluting with EtOAc/hexane (10:90) to yield a dark red solid (25 mg, 0.059 mmol, 61%). R_f = 0.59 (30:70, EtOAc/ hexane); ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.03 (d, *J* = 6.75 Hz, 1H), 8.41 (d, *J* = 7.78 Hz, 1H), 8.0 (s, 1H), 7.69-7.28 (m, 8H), 6.85 (d, J = 8.80 Hz, 1H), 5.25 (tt, *J* = 7.48, 1.32 Hz, 1H), 3.35 (d, *J* = 7.34 Hz, 2H), 1.75 (s, 3H), 1.42(s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) 159.8,150.0, 147.6, 141.7, 141.5, 140.9, 137.3, 134.6, 131.4, 131.9, 131.4, 128.5, 128.4, 126.4 (t, *J* = 9.02 Hz, 1C), 124.3, 120.0, 119.7, 119.0, 116.5, 113.1, 34.7, 25.5, 17.4; ^{19}F NMR (282 MHz, $CDCl_3$); δ -149.45 (q, *J* =30.34 Hz, 2F). HRMS/(m/z): calcd for $[M+H]^+$ $C_{23}H_{21}BF_2N_3S$: 420.15173; found: 420.15155. Based on the HPLC-MS UV detection, at 30 minutes **3c** was formed as a minor product (24%) and **4c** as major product (57%). The product ratio at 8h was found **3c** (17%) and **4c** (61 %) respectively. Trace amounts of the homodimerization product **2c** were observed at 8h (7%).

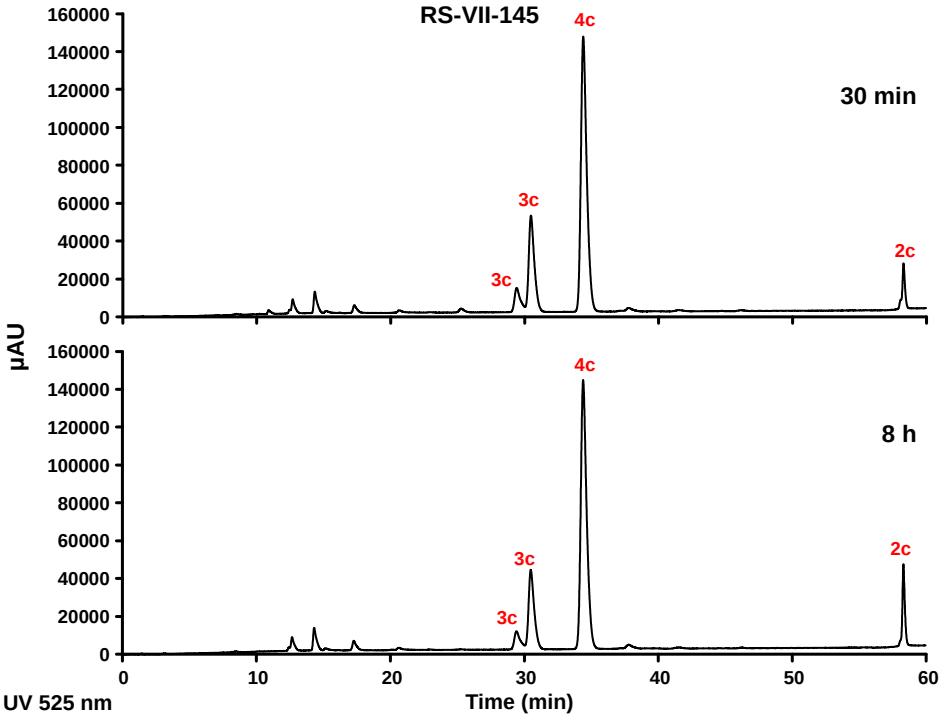


Figure S7 HPLC-UV-MS chromatogram of **(1c)** and 2-methyl-2-butene **(1S)** cross-metathesis reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products.

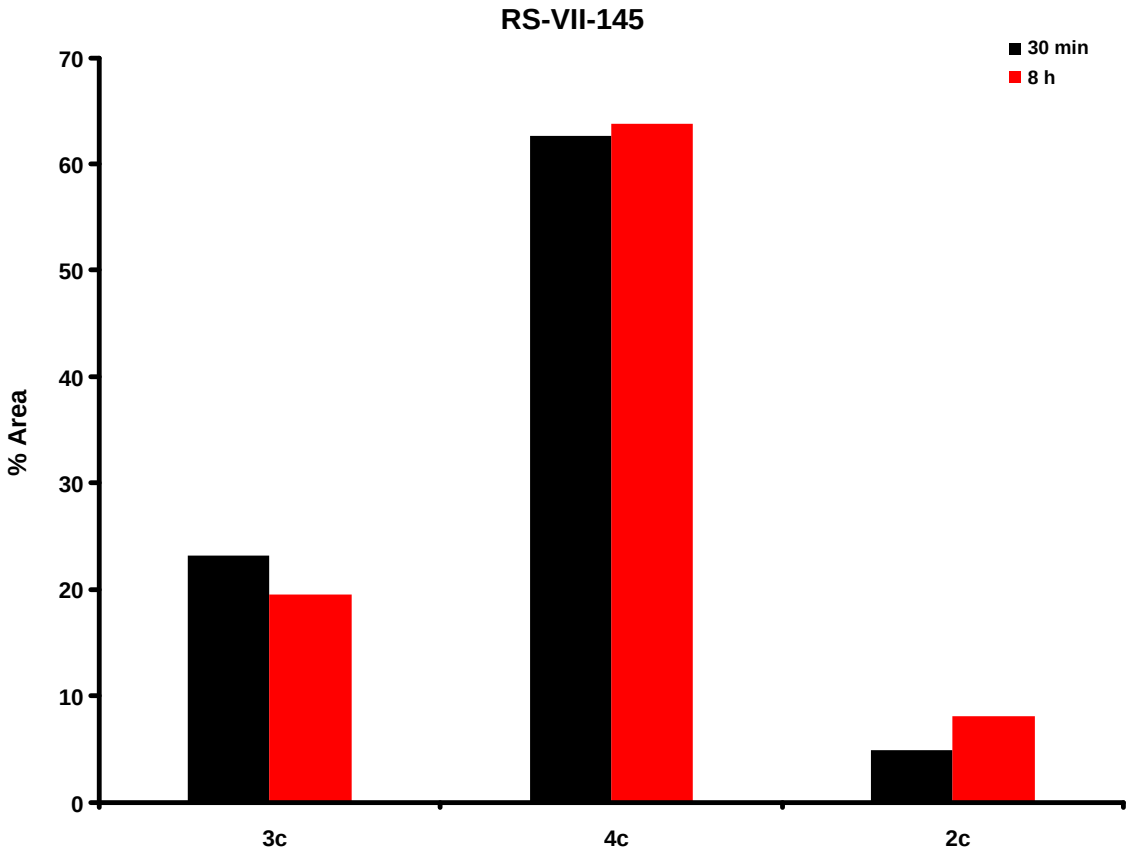


Figure S8 Relative abundance of total peak area for **(1c)** and 2-methyl-2-butene **(1S)** cross metathesis reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products.

Sulfone (1d) and 2-methyl-2-butene (1S) cross-metathesis:

Following the general procedure **II**, after 8h reaction time compound **4d** was isolated by column chromatography eluting with EtOAc/hexane (15:85) to yield an orange solid (44 mg, 0.098 mmol, 98%). R_f = 0.22 (30:70, EtOAc/ hexane); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.94 (d, *J* =7.78 Hz, 1H), 8.38 (d, *J* = 7.63 Hz, 1H), 8.06 (d, *J* = 1.32 Hz, 1H), 7.66 (dd, *J* = 9.54, 2.05 Hz,1H), 7.59-7.55 (m, 2H), 7.50-7.30 (m, 4H), 6.87 (d, *J* = 9.54Hz, 1H), 5.28 (tt, *J* = 7.78, 1.47 Hz, 1H), 3.81 (d, *J* = 8.07 Hz, 2H), 1.81 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) 160.0, 154.9, 143.9, 142.5, 142.4, 140.3, 137.9, 133.7, 132.9, 132.0, 130.6, 128.9, 128.8, 127.3 (t, *J* = 9.26 Hz, 1C), 124.5, 120.8, 120.3, 120.0, 113.2, 110.3, 56.3, 25.8, 18.0; ^{19}F NMR (282 MHz, $CDCl_3$); δ -148.55 (q, *J* = 28.61 Hz, 2F). UV-Vis (octanol) λ_{max}: 537 nm, €= 40100 $M^{-1}cm^{-1}$; λ_{em}: 572 nm; Φ_f = 0.80. Log Po/w = 0.79. HRMS/(m/z): calcd for $[M+H]^+$ $C_{23}H_{20}BF_2N_3O_2S$: 452.14156; found: 452.14091. Based on the HPLC-MS UV detection, at 30 minutes **3d** was formed as a minor product (25%) and **4d** as major (72%). The product distribution at 8h contained trace amounts of **3d** (1%) and the major produce **4d** (98 %) respectively. No homodimerization product **2d** was detected at 8h.

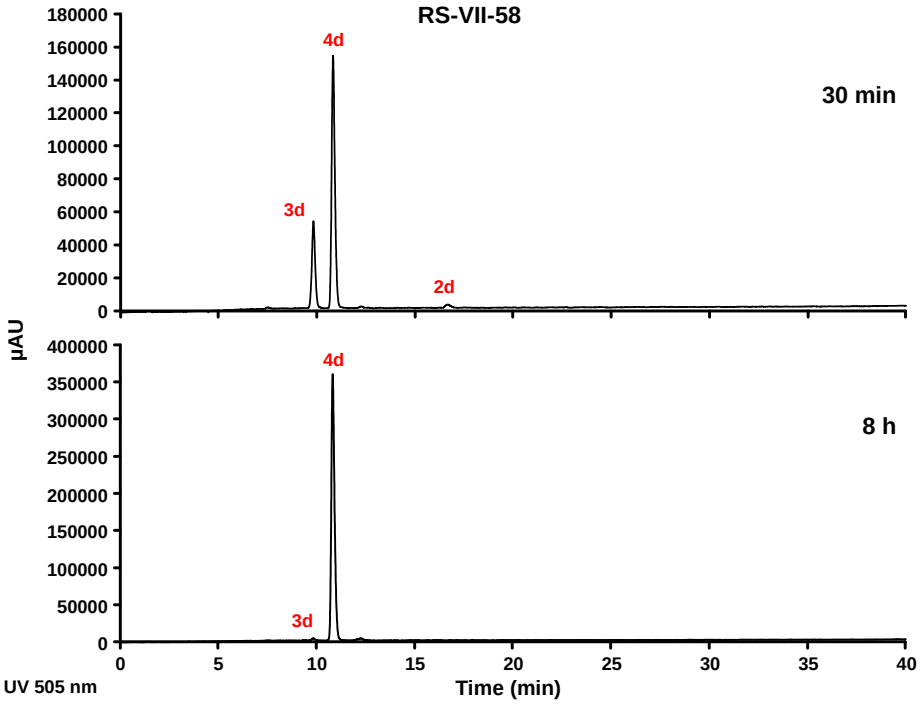


Figure S9. HPLC-UV-MS chromatogram of allyl sulfone (1d) and 2-methyl-2-butene (1S) cross- metathesis reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products.

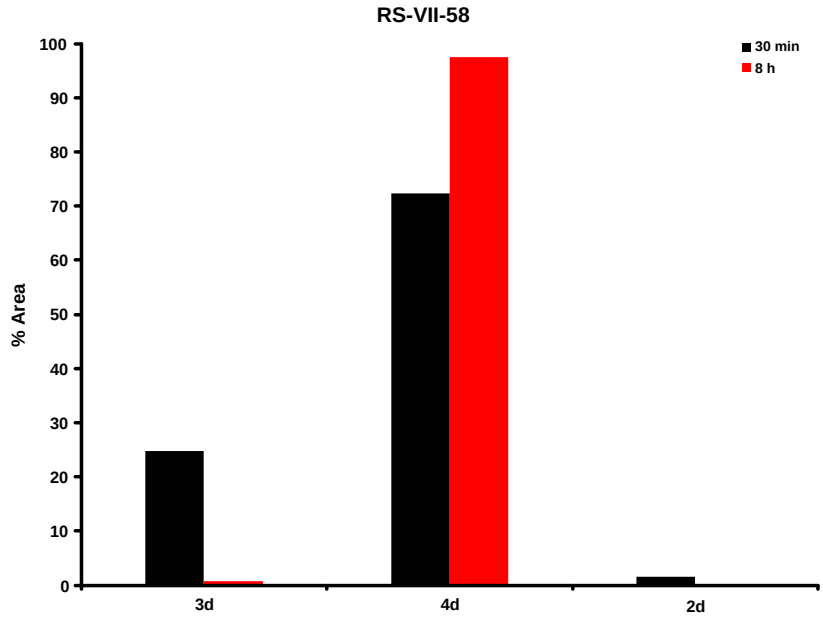


Figure S10. Relative abundance of total peak area for allylic sulfone (**1d)** and 2-methyl-2-butene **(1S)** cross-metathesis reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products.

Secondary cross-metathesis of sulfone homodimer (2d) with 2-methyl-2-butene(2S)

The homodimer 2d (10 mg, 0.012 mmol), 2-methyl-2-butene 2S (142 μL, 1.22 mmol), HG(II) catalyst (0.4 mg, 0.0006 mmol) and dichloromethane (2 mL, 0.006M) were combined and heated at 40 °C. The aliquot at 30 min and 8h were analyzed.

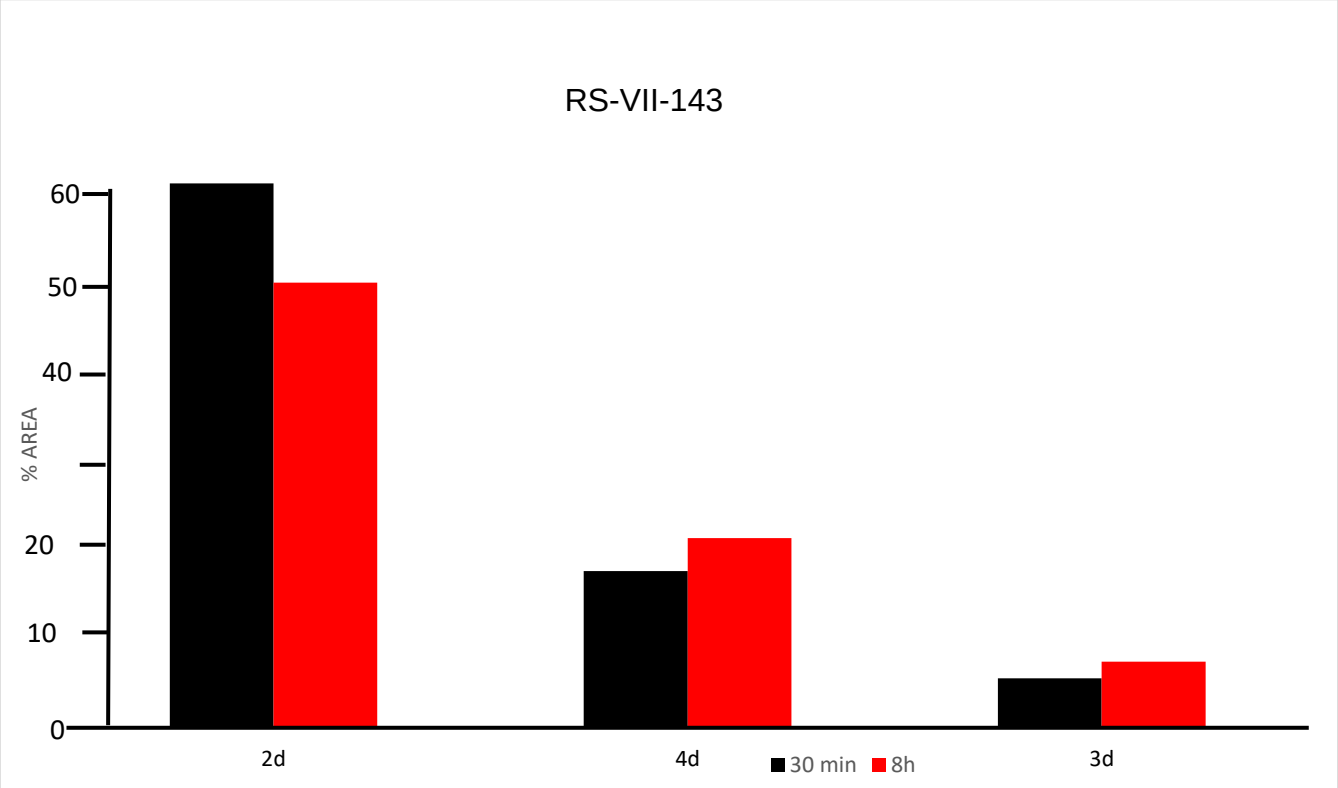


Figure S11. Relative abundance of total peak area for allylic sulfone homodimer (2d) and 2-methyl-2-butene (1S) cross-metathesis reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products

Sulfone (1d) and citral (2S) cross-metathesis:

The allylic sulfone **1d** (21 mg, 0.05 mmol), citral (94 μL, 0.05 mmol), HG(II) catalyst (1.5 mg, 0.0025 mmol) and dichloromethane (1 mL, 0.05M) were combined and heated to reflux at 40 °C for 1h. An aliquot of the reaction mixture was passed through a short column of silica gel (800 mg) and the colored fractions were collected and analyzed by HPLC-MS. The product distribution was quantified as shown in the Scheme 4. The remaining reaction mixture was purified by flash chromatography to isolate **5d** (11 mg, 43%), **4d (**7.5 mg, 33 %) and **2d** (6.7 mg, 24 %) as orange solids. The spectral properties of **5d** are as follows: R_f = 0.44 (5:95, MeOH:DCM); ^{1}H NMR (300 MHz ,$CDCl_3$): δ 9.98 (d, *J* = 7.8 Hz, 1 H), 8.94 (d, *J* = 7.8 Hz, 1 H), 8.36 (d, *J* = 7.9 Hz, 1 H), 8.19 - 7.98 (m, 1 H), 7.65 - 7.25 (m, 6 H), 6.88 (d, *J* = 9.5 Hz, 1 H), 5.87 (dd, *J* = 8.0, 12.8 Hz, 1 H), 5.79 - 5.49 (m, 2 H), 3.78 (d, *J* = 7.0 Hz, 2 H), 2.65 (t, *J* = 7.8 Hz, 1 H), 2.42 - 2.19 (m, 3 H), 2.19 - 2.10 (m, 2 H), 1.96 (s, 1 H); ^{19}F NMR (282 MHz, $CDCl_3$) δ = -149.83-149.52(m, 2F); ^{13}C NMR (50 MHz ,$CDCl_3$) δ 191.1, 190.3, 162.1, 162.0, 160.0, 155.2, 142.6, 142.5, 140.5, 140.2, 139.9, 138.2, 137.7, 137.6, 133.9, 133.0, 132.0, 130.6, 128.9, 128.9, 128.7, 127.4(t, *J* = 8.83Hz, 1C), 120.6, 120.3, 120.0, 117.7, 117.3, 116.2, 113.5, 60.0, 59.9, 39.2, 31.6, 31.4, 29.9, 29.7, 24.9, 17.5.

None of the possible cross-metathesis products from reaction at the electron deficient α-β unsaturated alkene were detected. For comparison, an authentic sample of **6d** was synthesized by an alternative route. The allylic sulfone **1d** (21 mg, 0.05 mmol), acrolein (16.6 μL, 0.25 mmol), HG(II) catalyst (1.5 mg, 0.0025 mmol) and dichloromethane (1 mL, 0.05M) were heated to refluxed at 40 °C for 2h. The reaction mixture was passed through a pad of celite, volatiles were removed under reduced pressure, and the residue was purified by column chromatography. The compound **6d** (17 mg, 75%) was isolated as an orange solid. R_f = 0.51 (5:95, MeOH:DCM); ^{1}H NMR (200 MHz ,$CDCl_3$) δ = 9.68 - 9.58 (m, 1 H), 8.97 - 8.83 (m, 1 H), 8.35 (d, *J* = 7.8 Hz, 1 H), 8.20 - 8.07 (m, 1 H), 7.64 - 7.22 (m, 9 H), 6.91 - 6.70 (m, 2 H), 6.37 - 6.18 (m, 1 H), 4.11 (d, *J* = 7.4 Hz, 2 H) ; ^{19}F NMR (282 MHz ,$CDCl_3$) δ = -150.05-149.74 (m, 2F) ; ^{13}C NMR (50MHz ,$CDCl_3$) δ = 191.7, 159.9, 156.0, 142.6, 142.6, 142.5, 140.7, 139.7, 139.3, 137.6, 137.0, 134.0, 133.8, 133.2, 133.2, 131.9, 130.5, 128.9, 128.9, 127.7, 127.5, 127.3, 126.8, 120.5, 120.4, 120.0, 113.9, 59.6

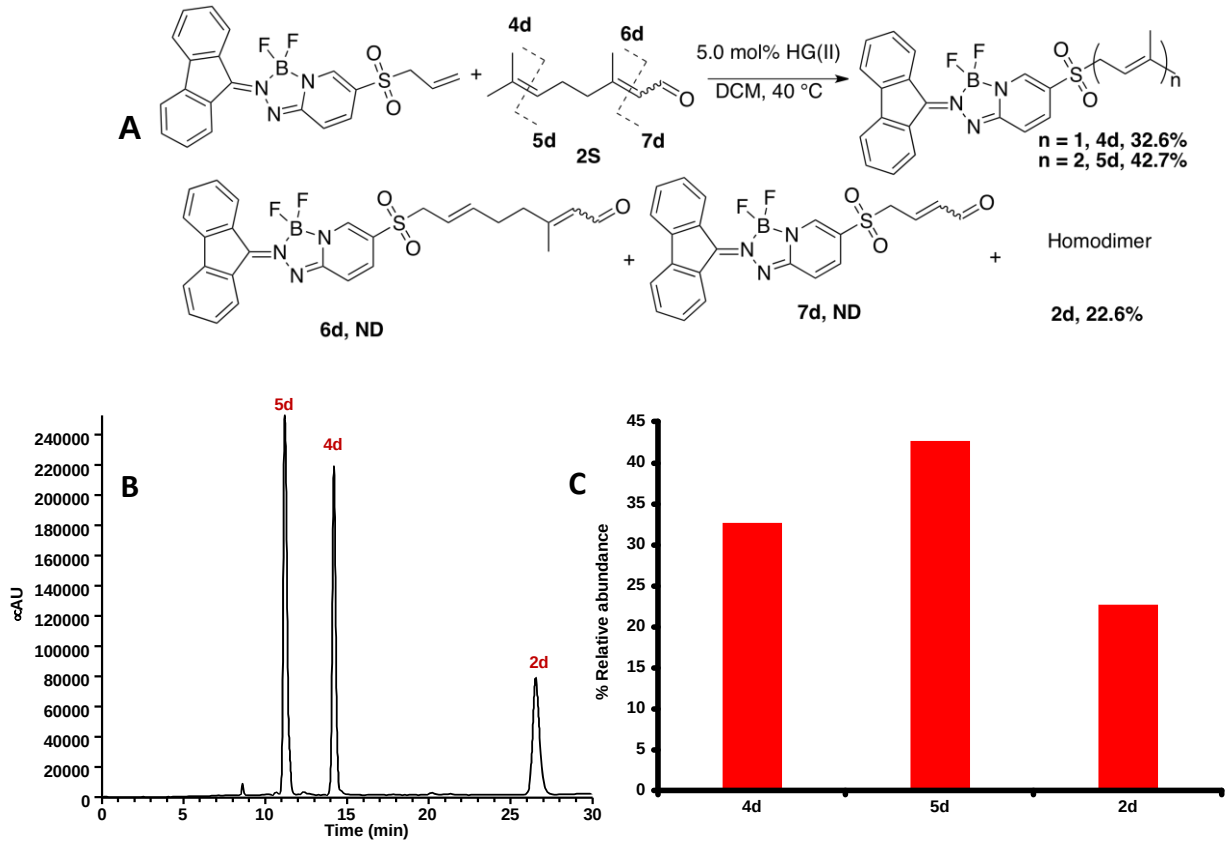


Figure S12. Cross-metathesis of **1d** with citral. A) Cross-metathesis reactions were conducted using 1.0 equiv citral (**2S**), 1.0 equiv of **1d** in dichloromethane (0.05M), 5 mol% HG(II) at 40 °C, monitored for 1h; B) HPLC chromatogram of reaction mixture; C) quantification of product distribution (%) by integration of UV chromatographic peaks at 505 nm. Product identities for chromatographic peaks were determined by accurate mass measurement and isotopic fine structure analysis provided by in-line high resolution mass spectrometry after UV detection.

Sulfone (1d) and squalene (3S) cross-metathesis:

The allylic sulfone **(1d)** (21 mg, 0.05 mmol), squalene (120 μL, 0.25 mmol), HG(II) catalyst (1.5 mg, 0.0025 mmol) and dichloromethane (1 mL, 0.05M) were combined and heated to refluxed at 40 °C for one hour. An aliquot of the reaction mixture was passed through a short column of silica gel and the colored fractions were collected and analyzed by HPLC-MS. The products were quantified as shown in Scheme 5. The remaining reaction mixture was concentrated and purified by column chromatography to isolate **4d** (9 mg, 0.02 mmol, 40%).

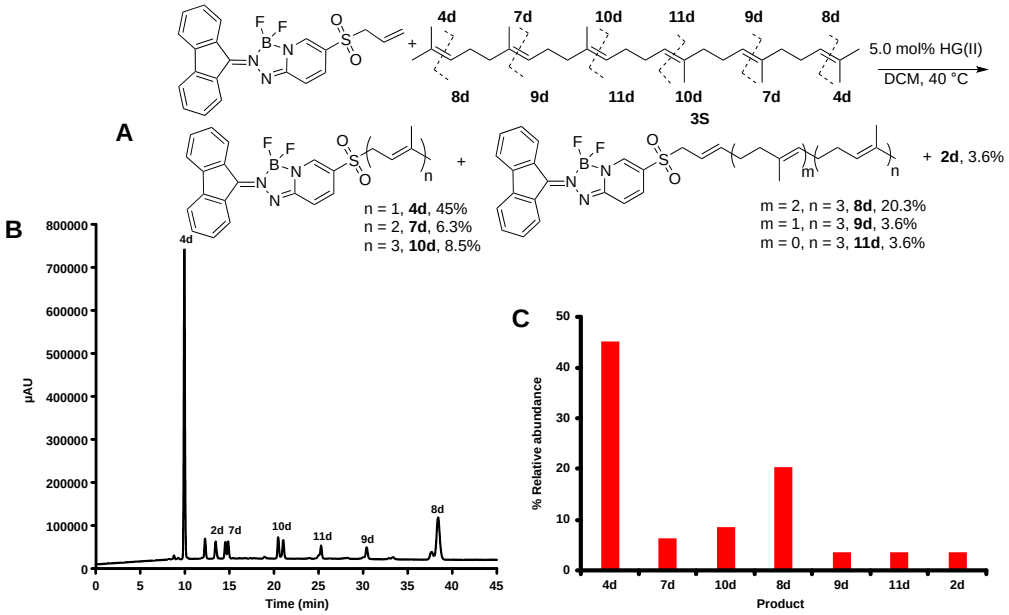


Figure S13. Cross-metathesis of **1d** with squalene. A) Cross-metathesis reactions were conducted using 5.0 equiv squalene **(3S),** 1.0 equiv of **1d** in dichloromethane (0.05M), 5 mol% HG(II) at 40 °C monitored for 1h; B) HPLC chromatogram of reaction mixture; C) quantification of product distribution (%) by integration of UV chromatographic peaks at 505 nm. Product identities for chromatographic peaks were determined by accurate mass measurement and isotopic fine structure analysis provided by in-line high resolution mass spectrometry after UV detection

General procedure (III) for cross-metathesis reactions with tetrasubstituted alkene 4S:

Each of the metathesis probes (0.05 mmol) were treated with 2,3-dimethyl-2-butene **(4S)** (177 μL, 1.5 mmol), HG(II) catalyst (1.5 mg, 0.0025 mmol), in 1,2-dichloroethane and heated at 60 °C for 4h. An aliquot of the reaction mixture was passed through a short column of silica gel and the colored fractions were collected and analyzed by HPLC-MS. The respective quantification histogram and the HPLC chromatogram are shown below.

Sulfide probe (1c) and 2,3-dimethyl-2-butene (4S) cross-metathesis:

Following the general procedure **(III)**, the reaction of **1c** and tetrasubstituted alkene **4S** was carried out and the product **4c** (5 mg, 0.011 mmol, 24.4%) and homodimer **2c** (6 mg, 0.007 mmol, 31.3%) were detected.

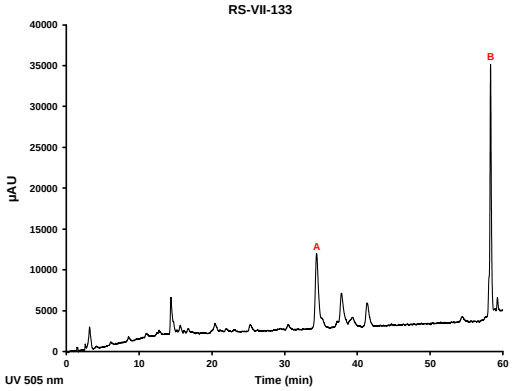


Figure S14. HPLC- MS chromatogram of allylic sulfide **(1c)** and 2,3-dimethyl-2-butene **(4S)** cross-metathesis reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products.

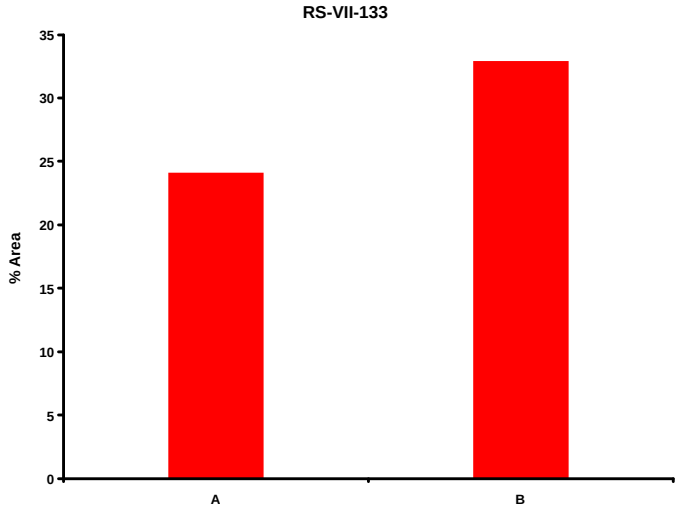


Figure S15. Relative abundance of total peak area for allyllic sulfide **(1c)** and 2,3-dimethyl-2-butene **(4S)** cross-metathesis reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products.

Sulfone probe (1d) and 2,3-dimethyl-2-butene (4S) cross-metathesis:

Following the general procedure **(III)**, the reaction of **1d** and **4S** was carried out and the product **4d** (59%) and homodimer **2d** (31%) were detected. The reaction mixture was purified by flash chromatography to isolate **4d** (12 mg, 0.027 mmol, 54%), and **2d** (5 mg, 0.006 mmol, 30%) respectively. The chromatogram and the histogram associated with the products are shown below.

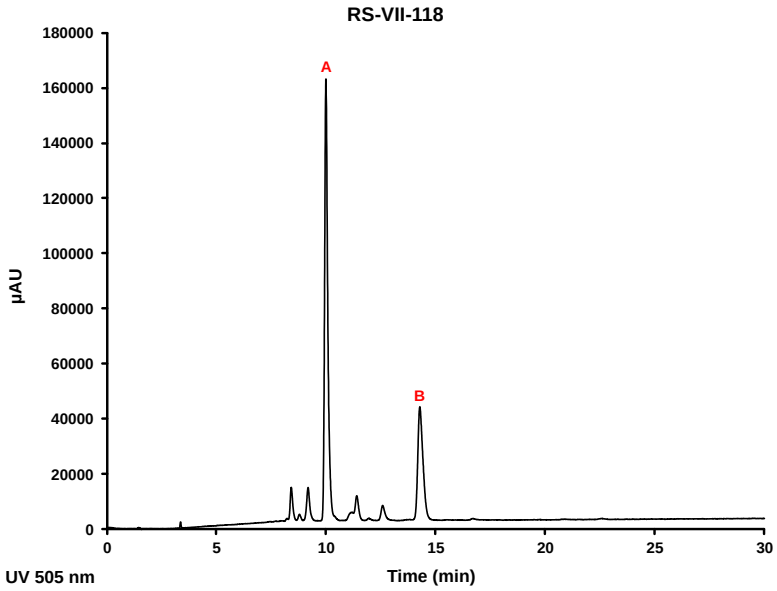


Figure S16. HPLC-MS chromatogram of the cross-metathesis reaction products from allylic sulfone **(1d)** and 2,3-dimethyl-2-butene **(4S)** after 30 min and 8h reaction times. UV detection at 525 nm was used for quantitation of reaction products and HRMS detection was used to identify the reaction products.

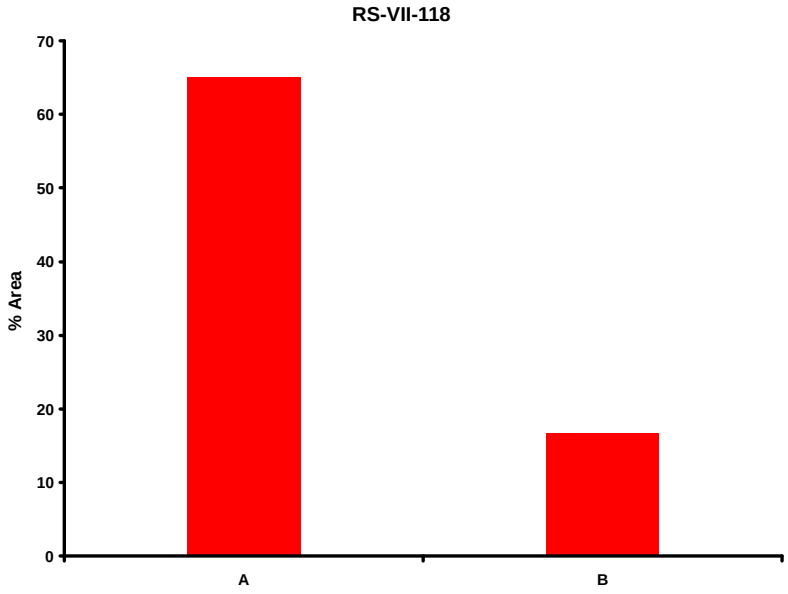


Figure S17. Relative abundance of total peak area for allylic sulfone **(1d)** and 2,3-dimethyl-2-butene **(4S)** cross-metathesis reaction products after 30 min and 8h reaction times. UV detection at 525 nm was used for relative quantitation of reaction products and HRMS detection was used to identify the reaction products.

Methyl allyl sulfone (12) and 2,3-dimethyl-2-butene (4S) cross-metathesis:

Following the general procedure **(III)**, the methyl allyl sulfone **(12)** and the tetrasubstituted alkene (**4S**) cross-metathesis was carried out and the products **13** (3.7 mg, 0.025 mmol, 50%) and **14** (2.1 mg, 0.01mmol, 40%) were isolated. The spectral data for each product are shown below.

3-methyl-1-(methylsulfonyl)but-2-ene (13)

^{1}H NMR (300 MHz, $CDCl_3$): δ 5.41 – 5.27 (m, 1H), 3.71 (ddt, *J* = 8.1, 1.7, 0.9 Hz, 2H), 2.81 (t, *J* = 0.8 Hz, 3H), 1.84 (q, *J* = 1.1 Hz, 3H), 1.75 (t, *J* = 1.0 Hz, 3H); ^{13}C NMR (50 MHz, $CDCl_3$) δ 142.98, 110.92, 65.99, 39.30, 26.16, 18.50.

1,4-bis(methylsulfonyl)but-2-ene (14)

^{1}H NMR (300 MHz, DMSO-d_6): δ 5.97 – 5.88 (m, 2H), 4.03 – 3.95 (m, 4H), 2.93 (s, 6H); ^{13}C NMR (50 MHz, DMSO-d_6) δ 126.96, 57.06, 39.52.

Phenyl allyl sulfone (15) and 2,3-dimethyl-2-butene (4S) cross-metathesis:

Following the general procedure **(III)**, the phenyl allyl sulfone (**15)** and the tetrasubstituted alkene (**4S**) cross-metathesis was carried out and the products **16** (5.2 mg, 0.025 mmol, 50%) and **17** (3.3 mg, 0.01mmol, 40%) were isolated.

((3-methylbut-2-en-1-yl)sulfonyl)benzene (16)

^{1}H NMR (200 MHz,$CDCl_3$): δ 7.87 (dd, *J* = 1.1, 7.9 Hz, 2 H), 7.75 - 7.45 (m, 3 H), 5.20 (t, *J* = 7.6 Hz, 1 H), 3.79 (d, *J* = 8.0 Hz, 2 H), 1.72 (s, 3 H), 1.31 (s, 3 H)
^{13}C NMR (50 MHz,$CDCl_3$): δ = 142.9, 138.7, 133.5, 128.9, 128.5, 110.4, 56.2, 25.8, 17.7.

1,4-bis(phenylsulfonyl)but-2-ene (17)

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.4 Hz, 4H), 7.62 (dt, *J* = 32.5, 7.4 Hz, 6H), 5.62 (d, *J* = 5.0 Hz, 2H), 3.82 – 3.73 (m, 4H). The spectral properties of compound **17** were identical to the published values.[2]

Phenylvinyl sulfone (18) and 2,3-dimethyl-2-butene (4S) cross-metathesis:

Following the general procedure (III), phenylvinyl sulfone **18** and tetrasubstituted alkene (4S) were subjected to the cross-metathesis reaction conditions and monitored over an extended 12 h period. Analysis of the composition of the reaction mixture by 300 MHz ^{1}H-NMR showed only unreacted **18**, and no trisubstituted cross metathesis product was detected.

1-(allyloxy)-4-methoxybenzene (19) and 2,3-dimethyl-2-butene (4S) cross-metathesis:

The allylic ether 1-(allyloxy)-4-methoxybenzene (19) was synthesized following the reported procedure,[5] and used as an additional model chalcogenide substrate for the cross methatheis with 2,3-dimethyl-2-butene (4S). The reaction was conducted following the general procedure III. The reaction mixture was purified by silica gel chromatography eluted with hexanes to remove the homodimerization product, catalyst and other impurities. The resulting major fraction consisted of unreacted **19** and trace amounts (~7%) of the trisubstituted cross metathesis product determined by integration of the characteristic peak for the methyl groups that appear as singlet at δ1.8 in the 300 MHz ^{1}H-NMR ($CDCl_3$) (see spectrum page 70).[6]

Computational details

Electronic structure calculations were performed with the Gaussian 09 package, revision D01 or E01.[7] For the density functional theory (DFT) calculations, we used M06-L functional[8] and def2-SV(P) basis set[9] (for Ru, the 28 core electrons were treated using the effective core potential approach).[10] Solvent effects were evaluated using the implicit integral equation formalism polarizable continuum model (IEF-PCM, referred in the text as PCM)[11] with the dichloromethane solvent parameters. In all DFT calculations, ultrafine Lebedev's grid was used with 99 radial shells per atom and 590 angular points in each shell. The wave function stability tests[12] were performed to ensure that the closed-shell singlet states were the solutions with the lowest energy. Tight cutoffs on forces and atomic displacement were used to determine convergence in geometry optimization procedure. Hessian matrices were calculated for the optimized structures to confirm absence of imaginary frequencies or presence of a single imaginary frequency for minima and transition states, respectively. The M06-L functional with def2-SV(P) basis was found to be effective for the HG(II) catalyst as shown by the small differences between the computed and X-ray data shown in Figure S15 and Table S3.
Results from the DFT calculations were further refined by the single-point calculations at the DLPNO-CCSD(T)/def2-TZVP level[13] using Orca v4.0 program[14] according to the following scheme[15]:

$$H^{DLPNO-CCSD(T)} = E_{gas}^{DLPNO-CCSD(T)} + (E_{solv}^{M06L} - E_{gas}^{M06L}) + H_{corr}^{M06L} \quad \text{(Eq. S1)}$$

$$G^{DLPNO-CCSD(T)} = E_{gas}^{DLPNO-CCSD(T)} + (E_{solv}^{M06L} - E_{gas}^{M06L}) + G_{corr}^{M06L} \quad \text{(Eq. S2)}$$

where E_{gas} and E_{solv} are the electronic energies in gas- and solvent phase from the DFT calculations, and enthalpic/entropic corrections H_{corr} and G_{corr} were calculated by DFT using the standard approximations of quantum harmonic oscillator (for the vibrational component of the partition functions), rigid rotor (for the rotational component), and particle-in-the box (for the translational component) for T = 298.15 K and P = 1 atm.
The reaction complex approach was used for the evaluation of the enthalpy/free energy changes along reaction coordinate in order to minimize the error in the calculated entropy contribution.[15,16]

Validation of the computational model

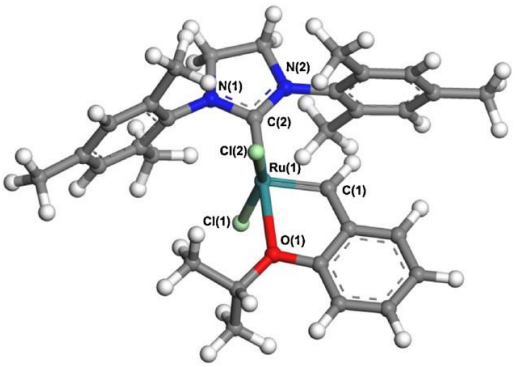


Figure S18. Equilibrium geometry of the HG(II) catalyst, calculated at the M06-L/def2-SV(P)+PCM(Dichloromethane) level of theory

Table S3. Comparison of the structural parameters of HG(II) pre-catalyst, obtained by X-ray crystallography and DFT calculations

Structural parameter	X-ray [a]	DFT [b]	% Error
Bond lengths (A˚)			
Ru(1) C(1)	1.82	1.84	1.09
Ru(1) C(2)	1.98	1.97	0.50
Ru(1) O(1)	2.26	2.34	3.50
Ru(1) Cl(1)	2.32	2.4	3.40
Ru(1) Cl(2)	2.34	2.41	2.90
C(2) N(1)	1.35	1.35(6)	0.44
C(2) N(2)	1.35	1.36	0.74
Bond angles (°)			
C(1) Ru(1) O(1)	79.3	77.9	1.7
C(1) Ru(1) C(2)	101.6	102.7	1.1
C(2) Ru(1) O(1)	176.2	179	1.5
C(1) Ru(1) Cl(1)	100.16	99.9	0.3
C(1) Ru(1) Cl(2)	100.16	97.5	2.6
O(1) Ru(1) Cl(1)	86.8	85.4	1.7
O(1) Ru(1) Cl(2)	85.3	84.2	1.3
C(2) Ru(1) Cl(1)	90.9	93.7	3.1
C(2) Ru(1) Cl(2)	96.6	96.5	0.0

Cl(1) Ru(1) Cl(2)	156.4	157.4	0.6
N(1) C(2) N(2)	106.9	106.7	0.2

[a] Crystallographic data obtained from Garber et al.[17]

[b] Calculated at the M06-L/def2-SV(P)+PCM(MeCN) level of theory.

Archive entries from the calculation files

The archive entries, formerly intended for the Browse Quantum Chemistry Database System, are organized as a simple list of data fields separated by backslash symbols, which is wrapped in 70-char text lines. The script 'Parse.Archive.pl', written in Perl, converts archive entry into human readable format. To use this script,
Check if Perl interpreter is installed on the system. To do this, run the command 'perl –v' in console. If console returns a message like 'command not found', please obtain and install a Perl interpreter (www.perl.org/get.html; Perl is Open Source software licensed under GNU GPL).
Save the script code, listed below, as a file named 'Parse.Archive.pl'.
Select an archive entry of interest and save it as another file (e.g. 'B-Xb.txt').
Run the command 'perl Parse.Archive.pl B-Xb.txt > B-Xb-parsed.txt' in console. The parsed archive entry will be stored in the file 'B-Xb-parsed.txt' in this example. In some cases, absolute path to the Perl interpreter might need to be provided.

```
# --- Parse.Archive.pl ---

# Merge all strings in one line
my $s='';
while (<>) {chomp;$s .= $_}
$_ = $s;

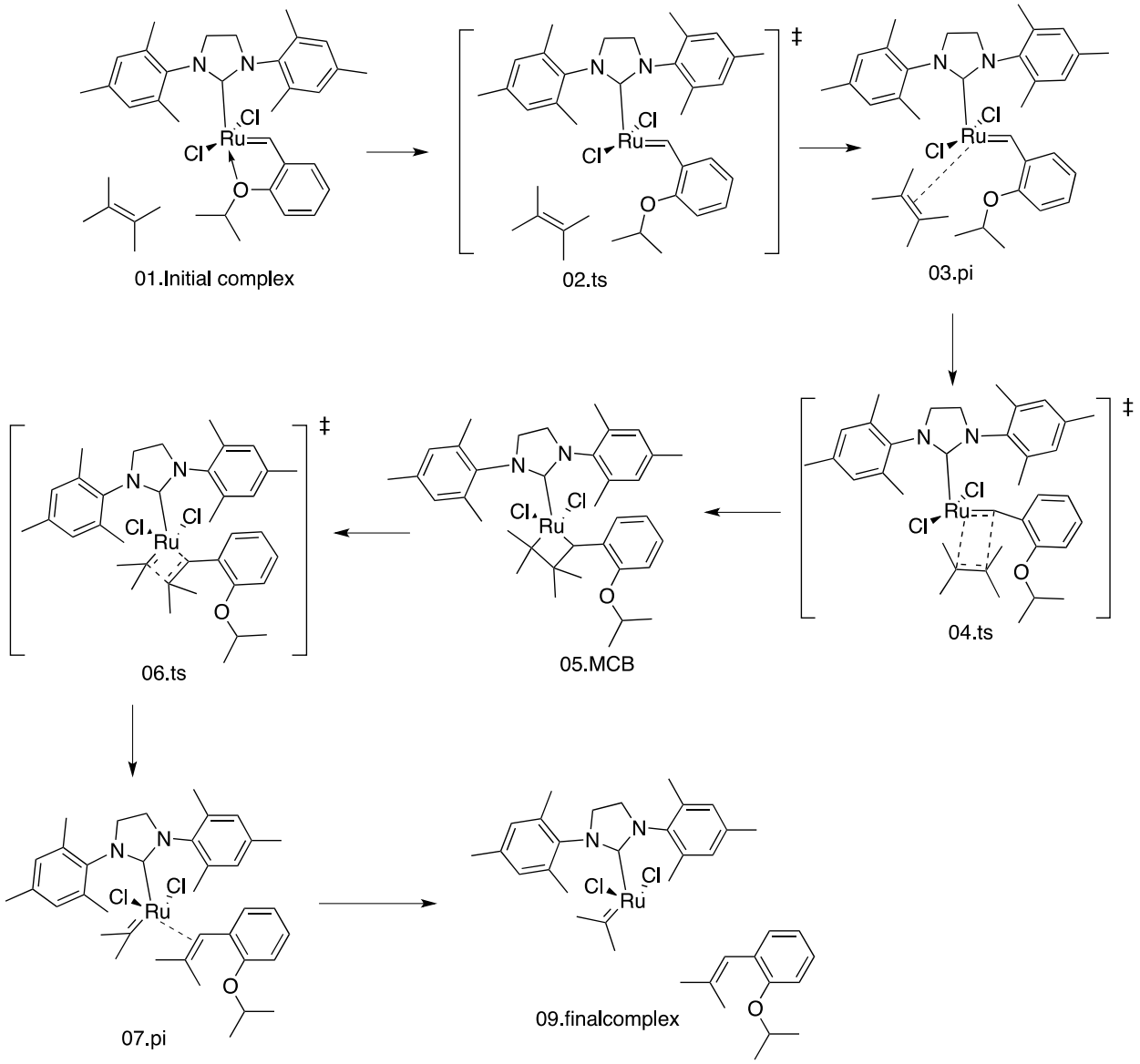
# Some PDF viewers (like Mac OS's Preview) might substitute
# 'end of line' symbols by the white space symbols,
# To remove these extra white spaces, please uncomment the following lines:
# my $str_length = 70;
# my $index = $str_length;
# while (length($_) > $index) {
#     substr $_,$index,1,'';
#     $index += $str_length;
# }

# Replace all backslashes by new-line symbols
s:\\:\n:g;

# Print the resulting output
print;

# --- END ---
```

HG(II) –2,3-dimethyl-2-butene (4S) initiation reaction evaluation



Scheme 3 Reaction of HG(II) and 2,3-dimethyl-2-butene(4S) (tetrasubstituted alkene)

01.initialcmplex

```
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7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
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02.ts

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,0,-3.668977649,-5.7220758462,1.3112488616\H,0,-2.6964209237,-7.207378
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\Dipole=0.6661541,2.2409087,0.5076577\Quadrupole=4.9805473,-15.4220904
,10.4415431,-24.7337412,-12.3254765,10.4199567\PG=C01 [X(C37H50Cl2N2O1
Ru1)]\\@

03.pi

1\1\GINC-C02\Stability\RM06L\Gen\C37H50Cl2N2O1Ru1\RISHIRAMT\17-Jul-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
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0,-7.5500706748,-3.8380304123,6.4382160745\C,0,-6.7353599576,-4.110025
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7405700668,-1.0195729243,4.8309273946\C,0,-4.7995213888,-1.2227822802,
3.8714865464\N,0,-4.6192137517,-0.041923146,3.2258764277\C,0,-5.546408
5836,0.9949654917,3.6902477517\C,0,-6.1473505871,0.3777581262,4.946094
4439\Ru,0,-4.0497344581,-3.0223423527,3.5499921531\C,0,-3.8808189981,-
5.8174185057,4.0372990298\C,0,-3.1443401526,-5.6564476472,2.8924981641
\C,0,-3.6346372396,0.2625815828,2.2417021718\C,0,-2.3218918032,0.53705
69698,2.6646494597\C,0,-1.358445671,0.8099551932,1.6877642317\C,0,-1.6
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\H,0,-3.2584651917,-7.080685285,5.6362100829\H,0,-3.7894340554,-5.4767
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21.9671805,-8.6102177,7.0956034\PG=C01 [X(C37H50Cl2N2O1Ru1)]\\@

04.ts

1\1\GINC-C01\Stability\RM06L\Gen\C37H50Cl2N2O1Ru1\RISHIRAMT\16-Jul-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
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,0.1581425728,3.2413723781\C,0,-1.8361709688,0.9117497514,-1.734944574
6\C,0,-6.1803538824,0.3696137037,0.7321005741\C,0,-7.6621326264,-2.869
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9537272,3.9149801932\H,0,-3.3848736307,-3.358884938,0.9093889398\C,0,-
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,-2.9849223349,3.5619885056\H,0,-2.8700189591,-5.2882729192,5.38559802
82\H,0,-3.9496369442,-6.681977212,5.0811306336\H,0,-4.6068033884,-5.16
36547397,5.7348496796\H,0,-5.9138982356,-5.3325795896,2.2528324742\H,0
,-6.3003570954,-5.3229275349,3.9888804025\H,0,-5.5474953052,-6.7602585
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3748754124\H,0,-0.988063163,-5.4287040792,2.2774118837\H,0,-1.76416735
22,-6.6504278862,3.3201893859\H,0,-1.4146651671,-5.0119087427,3.955392
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5,-16.5675446,-10.5951427,2.0048837\PG=C01 [X(C37H50Cl2N2O1Ru1)]\\@

05.MCB

1\1\GINC-JOKER-C13\Stability\RM06L\Gen\C37H50Cl2N2O1Ru1\RISHIRAM\19-Ma
y-2017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read
) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\
Title\\0,1\C,0,-5.1886375614,-1.9983905639,7.1708294112\C,0,-5.8294089
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672165565\C,0,-6.2164961556,0.4941196129,0.8580693242\C,0,-7.631336026
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,-6.5749284576,-4.7962887263,9.7911779957\H,0,-7.8327121171,-5.4209349
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295947415,1.5256854719\C,0,-3.88657112,-5.4016751015,5.0812477853\C,0,
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\Dipole=0.4267255,1.3297858,0.9500823\Quadrupole=-0.7678928,-7.0062311
,7.774124,-14.4051946,-14.4726112,1.4096941\PG=C01 [X(C37H50Cl2N2O1Ru1
)]\\@

06.ts

1\1\GINC-C10\Stability\RM06L\Gen\C37H50Cl2N2O1Ru1\RISHIRAMT\15-Jul-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
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C,0,-7.2329441287,-3.8707116693,6.4857833497\C,0,-6.6040785891,-3.9712
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3.7994218816\N,0,-4.600998067,-0.0678112883,3.1422658624\C,0,-5.236513
1544,1.0325883812,3.8774795684\C,0,-5.935680079,0.3157823342,5.0221771
56\Ru,0,-3.7876354054,-3.0134942212,3.2458084463\C,0,-4.3413537501,-4.
7429026058,3.9053171338\C,0,-2.7395500387,-5.052222142,2.6367226978\C,
0,-3.9215457474,0.2122793158,1.9174356015\C,0,-2.5264614573,0.38857013
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,0.2096350891,3.1639794621\C,0,-1.9338757478,1.2973705313,-1.740963261
4\C,0,-6.1813078989,0.3392391929,0.7655774485\C,0,-7.5847405575,-2.775
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,1.5831237269\H,0,-0.7403855903,0.7181621114,3.0726149243\H,0,-2.22610
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9,-2.9028172906,3.369577741\H,0,-2.9806351353,-4.9744799521,5.62358059
22\H,0,-4.0257442195,-6.3963541644,5.2566415449\H,0,-4.7148561942,-4.9
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87,-10.5788053,-17.3530572,-3.6988343\PG=C01 [X(C37H50Cl2N2O1Ru1)]\\@

07.pi

1\1\GINC-C11\Stability\RM06L\Gen\C37H50Cl2N2O1Ru1\RISHIRAMT\15-Jul-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
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8797349,1.5725832083\C,0,-2.5657228725,1.1888746751,0.2873007068\C,0,-
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,-0.5806748642\C,0,-5.1114103623,0.1033203792,0.696357372\C,0,-1.95369
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\C,0,-1.4657637133,-5.5845145364,3.5997277274\C,0,-3.044628294,-6.1360
254699,1.7224713597\C,0,-3.9162052271,-4.3126679077,5.688549606\C,0,-5
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7979159543\H,0,-8.4387380876,-3.4341644482,3.887073504\H,0,-6.83912007
7,-2.953832332,3.2480231934\H,0,-3.4564214096,-3.426601431,6.141086067
6\H,0,-3.1611130047,-5.1249310177,5.7271293055\H,0,-4.7688505762,-4.65
84201503,6.3073925486\H,0,-5.4773619777,-5.2687163755,2.7604499704\H,0
,-6.2216307086,-5.1120508106,4.3800814522\H,0,-4.8750820427,-6.2202606
747,4.173970408\H,0,-2.4176813879,-6.8343885026,1.1313949746\H,0,-3.77
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4593434354\H,0,-0.5938243379,-6.2139100608,3.3417366728\H,0,-2.1510105
545,-6.2324446146,4.1763990207\H,0,-1.1126510741,-4.7638452962,4.23845
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81,-8.838495,-22.8232037,-13.8331636\PG=C01 [X(C37H50Cl2N2O1Ru1)]\\@

09.finalcomplex

1\1\GINC-COMET-16-70\Stability\RM06L\Gen\C37H50Cl2N2O1Ru1\RISHIRAM\24-
Oct-2017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(re
ad) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)
\\Title\\0,1\C,0,-5.0407255839,-1.840538934,6.7865509857\C,0,-5.547053
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16,-3.6813047267,3.6682534173\C,0,-0.8157388639,-6.1538331663,1.902417
384\C,0,-3.8822653927,0.790380562,1.6225562255\C,0,-2.5982649491,1.362
4430344,1.5051111125\C,0,-2.1496483104,1.7195923528,0.2309330289\C,0,-
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2222\C,0,-6.1730031477,0.2814462597,0.6413277778\C,0,-7.1762864259,-2.
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573,-4.5449204889,9.2155074648\H,0,-8.0428445429,-5.0830989368,7.97540
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1.0954166751,-0.541567728\H,0,3.3788124802,-2.6310023012,4.0213800497\
H,0,2.0567023437,-3.8000826668,4.3053506099\H,0,1.7098661944,-2.243955
6948,3.5114202464\H,0,-1.2605721779,-5.8333145664,-0.1198991192\C,0,-0
.4515470075,-5.6464600259,3.2604016431\C,0,-1.1510688532,-7.6096821706
,1.8261284344\C,0,-3.3293083611,-3.8218385002,5.1127009785\C,0,-4.0077
978481,-4.964941711,2.9850853684\H,0,-7.5628434691,-1.4827239918,3.536
17525\H,0,-8.0200283889,-3.2058390311,3.5567235715\H,0,-6.4531426948,-
2.6885010818,2.8720820448\H,0,-3.0476210281,-2.8853363266,5.6081440264
\H,0,-2.4678176504,-4.5174890993,5.1933846295\H,0,-4.1645420996,-4.302
7200277,5.6621481451\H,0,-3.5240007141,-5.0760393006,1.9977518249\H,0,
-5.0980488662,-4.9741057826,2.7841889608\H,0,-3.7646243184,-5.85291958
19,3.6008570185\H,0,-0.3083132942,-8.2329497434,2.1841705779\H,0,-1.39
80463197,-7.9330128246,0.8008533825\H,0,-2.00889973,-7.8607343771,2.48
0611368\H,0,0.5836093901,-5.9302543896,3.5326489118\H,0,-1.1074880188,
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8\\Version=ES64L-G16RevA.03\HF=-2638.4765317\RMSD=3.389e-09\Dipole=-0.
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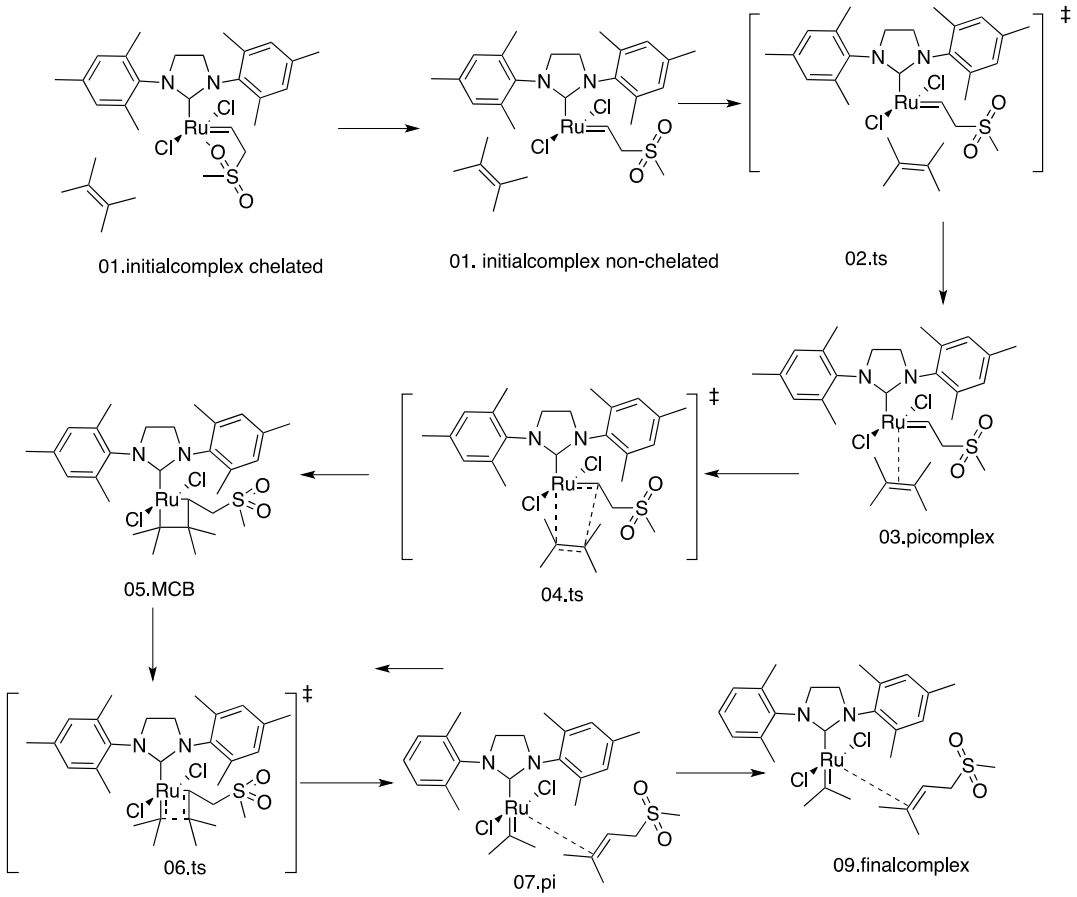
-7.5716287,-24.8385331,-10.8490368\PG=C01 [X(C37H50Cl2N2O1Ru1)]\\@

Reaction of allylsulfone carbene and 2,3-dimethyl-2-butene (4S)



Scheme 4 Reaction of allylsulfonecarbene and 2,3-dimethyl-2-butene(4S) (tetrasubstituted alkene)

01.initialcomplex

1\1\GINC-JOKER-C7\Stability\RM06L\Gen\C30H44Cl2N2O2Ru1S1\RISHIRAM\24-S
ep-2017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(rea
d) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
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4381595393,8.3262244809\C,0,-4.6731746034,-2.4096343245,8.1133917815\N
,0,-5.7364494871,-1.0753715249,4.8251628252\C,0,-4.9416445223,-1.22709
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594639888\Ru,0,-3.7633574682,-2.7084909284,3.2328224672\C,0,-4.6090240
437,-3.8824524931,4.3436220166\C,0,-1.4260345944,-4.5960671152,1.15801
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7,-0.7006358691\C,0,-5.2403693984,-0.0128937214,0.5225483427\C,0,-2.38
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.3634283107,1.7699327341,3.8684734203\H,0,-6.7203560223,1.2236564041,2
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,-7.368191303,4.0379797697\H,0,-4.7206106395,-6.6727023801,3.199782298
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\H,0,-0.2743183984,-4.2486535769,3.0008918002\H,0,-2.6894927633,-5.435
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29,-1.0827993281\H,0,-1.295979039,-2.4994238955,-1.3205855971\H,0,-2.7
032526332,-2.0127757014,-0.3671016412\H,0,-6.94691018,-1.0447230459,-0
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1 [X(C30H44Cl2N2O2Ru1S1)]\\@

02.ts

1\1\GINC-JOKER-C3\Stability\RM06L\Gen\C30H44Cl2N2O2Ru1S1\RISHIRAM\02-J
ul-2017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(rea
d) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
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(C30H44Cl2N2O2Ru1S1)]\\@

03.pi

1\1\GINC-JOKER-C7\Stability\RM06L\Gen\C30H44Cl2N2O2Ru1S1\RISHIRAM\07-J
un-2017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(rea
d) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
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1343029,0.4708659119\H,0,-3.7243707788,-5.0802037817,0.2869507362\H,0,
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37,-0.534477176\H,0,-1.8017621725,-2.50990974,-0.9121855131\H,0,-3.025
3163335,-1.7286187001,0.0943592999\H,0,-6.9803286978,-0.7564981499,-0.
3657220163\H,0,-7.2661780531,0.7611771079,0.5083928799\H,0,-6.92699447
15,-0.7453073274,1.4100746103\\Version=ES64L-G09RevE.01\HF=-2841.52917
61\RMSD=2.429e-09\Dipole=0.6216323,2.0357119,-1.1839871\Quadrupole=0.1
86859,6.2070764,-6.3939354,-35.6197736,1.7726604,24.1794682\PG=C01 [X(
C30H44Cl2N2O2Ru1S1)]\\@

04.ts

1\1\GINC-JOKER-C8\Stability\RM06L\Gen\C30H44Cl2N2O2Ru1S1\RISHIRAM\06-J
un-2017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(rea
d) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
\Title\\0,1\C,0,-4.7417412938,-1.5920697187,6.9186920776\C,0,-5.546995
6513,-1.894827541,5.8071005285\C,0,-6.3837251311,-3.0277487588,5.78691
45079\C,0,-6.3684997935,-3.8758533257,6.8977372132\C,0,-5.5631315594,-
3.621338654,8.0157372678\C,0,-4.7588474159,-2.4783122506,8.0026029465\
N,0,-5.5694267382,-0.9795710418,4.7099438425\C,0,-4.8540578305,-1.0579
603094,3.577510849\N,0,-5.0272397038,0.0762365442,2.8744414256\C,0,-5.
8552666566,1.0570292939,3.5861244253\C,0,-6.3530508813,0.2619285401,4.
787226084\Ru,0,-3.7061355492,-2.6284251644,2.9219255282\C,0,-3.9669548
404,-4.3605010646,3.577686714\C,0,-2.4204942562,-4.4732920174,2.061984
3966\C,0,-4.440029466,0.3550193831,1.6018730123\C,0,-3.0826382234,0.72
53897109,1.542511911\C,0,-2.5178501484,0.9539135891,0.2833729209\C,0,-
3.2657918562,0.8482333499,-0.8946190605\C,0,-4.6263452677,0.541163705,
-0.7872025573\C,0,-5.2403815656,0.2990403548,0.445869044\C,0,-2.276972
6079,0.9209565021,2.790004945\C,0,-2.6211682023,1.0339367596,-2.233251
5793\C,0,-6.7111513014,0.0325393215,0.5170612279\C,0,-7.263747356,-3.3
138018689,4.6123616861\C,0,-5.5658794612,-4.5581857515,9.1826850108\C,
0,-3.9234531265,-0.3399025914,6.9849772507\C,0,-2.221221656,-3.1618066
512,1.4412288439\Cl,0,-2.094464791,-2.1461365348,4.7328981202\Cl,0,-5.
5639102452,-3.0617853451,1.3519620485\H,0,-6.169521192,0.7692953302,5.
7494780858\H,0,-7.4326951016,0.0276754139,4.7353808417\H,0,-5.24311943
66,1.9344316716,3.8689043363\H,0,-6.6713823164,1.4167972195,2.93689634
94\H,0,-1.4577904332,1.2348823232,0.2242543664\H,0,-5.2357304515,0.480
5750576,-1.6985642558\H,0,-4.1254851783,-2.2577762726,8.8720628345\H,0
,-7.0040985064,-4.7697861348,6.8859458852\H,0,-1.2703605528,1.30268715
25,2.5520659154\H,0,-2.7574721485,1.6511417495,3.4679332807\H,0,-2.151
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-0.5059782981,7.5463700322\H,0,-7.9022950878,-2.4467676012,4.359583997
8\H,0,-6.6805933483,-3.534245876,3.6990238734\H,0,-7.9190812728,-4.176
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5,-2.620631308\H,0,-5.0083398248,-4.1485776661,10.0412630813\H,0,-6.59
33724491,-4.7833195049,9.5199715342\H,0,-5.1043901993,-5.5222620472,8.
9040438867\C,0,-1.2783101333,-5.0130029796,2.8850400284\C,0,-3.1053636
962,-5.5185554384,1.2110803956\C,0,-3.5334870219,-7.689908711,4.598835
2262\S,0,-4.4145535608,-6.3844992028,5.4305712671\O,0,-4.189748395,-6.
551497018,6.8723285083\O,0,-5.7861054135,-6.3710176083,4.9013437283\C,
0,-3.5845641238,-4.8520332195,4.934182404\H,0,-2.4850829927,-7.7044728
959,4.9323290175\H,0,-3.6099689553,-7.5618831823,3.5085073997\H,0,-4.0
366346639,-8.6231883683,4.896771343\H,0,-4.7156677739,-4.9831374526,3.
0472301202\H,0,-2.5011280563,-4.9891260132,5.0939457655\H,0,-3.8973910
739,-4.1400978136,5.7219622012\C,0,-0.9270871378,-2.4205877577,1.69362
99963\H,0,-0.5522609368,-2.4859366474,2.7219438408\H,0,-1.0402752776,-
1.3507223085,1.4402514934\H,0,-0.1488998132,-2.8232129574,1.011718599\
C,0,-2.6742725667,-2.9348013421,0.0179237983\H,0,-0.3998710276,-5.1575
095885,2.2267057304\H,0,-1.5137473907,-5.9998094212,3.3188516701\H,0,-
0.9734527929,-4.3319418329,3.6957771097\H,0,-2.475154767,-5.7344259484
,0.3267530135\H,0,-4.0926479744,-5.1909304564,0.8502265515\H,0,-3.2337
226367,-6.4693013851,1.7542966792\H,0,-3.599393167,-3.4522850298,-0.25
84656985\H,0,-1.8659564709,-3.2683413814,-0.6665030938\H,0,-2.82506474
36,-1.8560577479,-0.1709783669\H,0,-7.061222258,-0.503903936,-0.380313
7127\H,0,-7.2834273958,0.9795305557,0.5665830559\H,0,-6.9821447571,-0.
5763066521,1.3939731487\\Version=ES64L-G09RevE.01\HF=-2841.5180648\RMS
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6,15.5088905,-8.6394789,-37.0983822,6.8508205,22.3429043\PG=C01 [X(C30
H44Cl2N2O2Ru1S1)]\\@

05.MCB

1\1\GINC-C01\Stability\RM06L\Gen\C30H44Cl2N2O2Ru1S1\RISHIRAMT\23-May-2
017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) g
eom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Tit
le\\0,1\C,0,-4.7745743348,-1.5346449206,6.9191290924\C,0,-5.5617095784
,-1.8498110537,5.7950371704\C,0,-6.3612092516,-3.0085566073,5.75686513
89\C,0,-6.3183572269,-3.872975871,6.8569804221\C,0,-5.5265187022,-3.60
88449503,7.9799064661\C,0,-4.7667375051,-2.4341547261,7.9892751913\N,0
,-5.5840432843,-0.9234986673,4.7052725114\C,0,-4.8623101893,-0.9962829
738,3.5779899951\N,0,-5.0169543575,0.1336211855,2.8720285293\C,0,-5.83
48937316,1.1209055291,3.5888085317\C,0,-6.3796216615,0.3116828962,4.76
0674213\Ru,0,-3.7615314329,-2.5946144583,2.99207794\C,0,-3.8010478651,
-4.5132033258,3.4466432854\C,0,-2.6487159197,-4.5165189784,2.337461465
4\C,0,-4.4309525848,0.3895207339,1.5943974116\C,0,-3.0673462617,0.7356
507369,1.5245749527\C,0,-2.5065253574,0.9407688304,0.2598730185\C,0,-3
.2633435697,0.8355165686,-0.9130028406\C,0,-4.6273122039,0.5496805856,
-0.7951464611\C,0,-5.2383409096,0.3307375967,0.4440401745\C,0,-2.25101
528,0.9269542656,2.7658102882\C,0,-2.6238852257,1.0003010006,-2.256866
7841\C,0,-6.7125962145,0.0864898434,0.5260190809\C,0,-7.2235075557,-3.
3395967099,4.5813350647\C,0,-5.4940778212,-4.5664776096,9.1294150359\C
,0,-3.9908033514,-0.2614956448,7.0004893775\C,0,-2.3794862205,-3.04646
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-5.6363724868,-3.0309404521,1.4580092398\H,0,-6.2437081954,0.811026988
7,5.734285624\H,0,-7.453814306,0.0676475138,4.6570131248\H,0,-5.205123
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459\H,0,-1.4424150671,1.2036903659,0.1915986483\H,0,-5.2427257651,0.48
84870242,-1.7023542965\H,0,-4.1445555827,-2.2050113418,8.8643954029\H,
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3649371\H,0,-4.576653095,0.5381536718,7.4946507853\H,0,-3.0751085118,-

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,0,-6.6851387822,-3.9652812845,3.8468370761\H,0,-8.1135792355,-3.90953
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2.634260323\H,0,-4.9430068729,-4.1568015055,9.9919974431\H,0,-6.512137
2509,-4.8283655305,9.4685824483\H,0,-5.0072999504,-5.5115833015,8.8294
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-5.4922791378,1.2532949301\C,0,-3.450998112,-7.7798697111,4.5343969681
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,4.8887974055\H,0,-3.5063228575,-7.6527536256,3.4426426198\H,0,-3.9528
533388,-8.7165337037,4.8238068411\H,0,-4.712041331,-4.9892841467,3.041
5873703\H,0,-2.482431675,-5.0156414126,5.1645176455\H,0,-4.0015902167,
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.7388687025,-2.9517797972,0.138265523\H,0,-0.5467380401,-5.0434160605,
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22824,-4.3544706511,3.7585268367\H,0,-2.400061755,-5.5389766526,0.4174
363473\H,0,-4.1090117855,-5.2194613016,0.8582043432\H,0,-3.1938262804,
-6.5083950377,1.6779599291\H,0,-3.6984761032,-3.4003764272,-0.13775215
75\H,0,-1.9365335218,-3.4039188538,-0.4798513809\H,0,-2.7827304603,-1.
8823778488,-0.1408291473\H,0,-7.0742879958,-0.4607197884,-0.3601357937
\H,0,-7.2710619525,1.0423179674,0.5603452155\H,0,-6.9902094896,-0.5021
144238,1.4147329506\\Version=ES64L-G09RevE.01\HF=-2841.5274963\RMSD=3.
731e-09\Dipole=0.8800397,1.9268235,-1.2674842\Quadrupole=-4.1574038,11
.8053983,-7.6479945,-38.9141599,5.3775424,24.4584992\PG=C01 [X(C30H44C
l2N2O2Ru1S1)]\\@

06ts

1\1\GINC-JOKER-C8\Stability\RM06L\Gen\C30H44Cl2N2O2Ru1S1\RISHIRAM\06-J
un-2017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(rea
d) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
\Title\\0,1\C,0,-4.7743289867,-1.4639232925,6.940749699\C,0,-5.5684055
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02019\C,0,-6.2900096259,-3.820766896,6.9298975957\C,0,-5.4850715587,-3
.533774624,8.0372790899\C,0,-4.7455954493,-2.3459424456,8.0244723575\N
,0,-5.5861268912,-0.9139939732,4.7109677775\C,0,-4.8722090889,-1.03718
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8433924099,1.0857469197,3.5255964642\C,0,-6.3813451726,0.3213238675,4.
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0232\C,0,-4.4263537907,0.3205748594,1.5715167253\C,0,-3.0631671296,0.6
733862632,1.5311110921\C,0,-2.483131085,0.9186826337,0.2828022129\C,0,
-3.2202718895,0.8409288558,-0.9054351159\C,0,-4.5816382037,0.534081571
6,-0.8176712273\C,0,-5.2114512371,0.2786050369,0.4061389437\C,0,-2.267
2497235,0.8179531933,2.7906984941\C,0,-2.5607659204,1.0511858485,-2.23
32400788\C,0,-6.6842166617,0.0174443813,0.4555953944\C,0,-7.224723021,
-3.3356514795,4.6572058718\C,0,-5.4139067836,-4.4850962614,9.190964998
7\C,0,-3.9882493103,-0.1908100665,6.9840931323\C,0,-2.4685237646,-2.81
4106271,1.6139182385\Cl,0,-2.194607408,-2.2302496387,4.8532512566\Cl,0
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38958,1.9449937916,3.8070494283\H,0,-6.6379253125,1.4642774947,2.86108
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4878050728,-1.7364350499\H,0,-4.1128564546,-2.0991296589,8.8871376051\
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26694,2.5746878747\H,0,-2.7288409524,1.5512357618,3.4784384735\H,0,-2.
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.9798017111\H,0,-4.5712645976,0.6275795064,7.4499528787\H,0,-3.0731678
793,-0.3117160567,7.5869298973\H,0,-7.5335521736,-2.4586583602,4.06532

63858\H,0,-6.7025013962,-4.0121347669,3.956618494\H,0,-8.1288378117,-3
.8686848579,4.9971426082\H,0,-3.2696101541,1.4236599437,-2.9915154026\
H,0,-1.7200125771,1.7622354021,-2.1675292134\H,0,-2.1445898709,0.10311
94774,-2.6245899888\H,0,-4.8364401509,-4.0697172585,10.0332653518\H,0,
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359\C,0,-3.5760074167,-5.0536387825,4.8671113724\H,0,-2.5155419998,-7.
9108573028,4.8014002625\H,0,-3.6516964384,-7.7052306588,3.3944125196\H
,0,-4.0785608939,-8.8116434735,4.7502767864\H,0,-4.7257510277,-5.10632
61899,3.0173420404\H,0,-2.5275232427,-5.1413836377,5.1921316651\H,0,-4
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99944,-1.303661779,1.4418272151\H,0,-0.3597313589,-2.9247682188,1.1649
214366\C,0,-2.836666489,-2.7861831485,0.1583265966\H,0,-0.5365005021,-
4.9218584495,2.1542501871\H,0,-1.2792787233,-6.03474728,3.3127820398\H
,0,-1.0051786168,-4.3317422096,3.7777639447\H,0,-2.2889814122,-5.32412
5067,0.3594201359\H,0,-4.0298079586,-5.2432075312,0.7963755183\H,0,-2.
9970856233,-6.5524543146,1.4247373393\H,0,-3.7576765569,-3.3183140139,
-0.1006012895\H,0,-1.9999111077,-3.145311496,-0.4729839563\H,0,-2.9998
438435,-1.7238606733,-0.1108792668\H,0,-7.0197564788,-0.5355594472,-0.
4374168867\H,0,-7.2544932407,0.9666701866,0.4747186615\H,0,-6.97353617
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93\RMSD=4.304e-09\Dipole=1.0696691,1.9355331,-1.5644635\Quadrupole=-4.
7463599,13.7155325,-8.9691725,-39.4959851,8.3094998,26.438093\PG=C01 [
X(C30H44Cl2N2O2Ru1S1)]\\@

07.pi

1\1\GINC-JOKER-C10\Stability\RM06L\Gen\C30H44Cl2N2O2Ru1S1\RISHIRAM\07-
Jun-2017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(re
ad) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)
\\Title\\0,1\C,0,-4.6861834022,-1.4866856045,6.6983105436\C,0,-5.55166
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722246\C,0,-6.2612696693,-3.785400499,6.9595379723\C,0,-5.3836174656,-
3.443208475,7.9915596703\C,0,-4.6139135745,-2.2824690864,7.8426406915\
N,0,-5.6201018277,-1.0514118312,4.4958241685\C,0,-4.8495525871,-1.1431
34643,3.3786833149\N,0,-5.0328093761,-0.0107450616,2.6613531886\C,0,-5
.8635473951,0.9698729201,3.3731012056\C,0,-6.4670557577,0.1430724329,4
.4931752558\Ru,0,-3.8835600066,-2.8546822191,3.0343902886\C,0,-3.70696
14214,-5.2483615133,3.5557553058\C,0,-2.6691855749,-5.3427827515,2.660
3029847\C,0,-4.348213972,0.4011671838,1.4812472559\C,0,-3.0093183646,0
.8243934001,1.5667979335\C,0,-2.3827681017,1.2653571855,0.395971125\C,
0,-3.0553443841,1.3241284365,-0.8301264415\C,0,-4.3970471556,0.9272968
505,-0.8661714581\C,0,-5.0616184754,0.4589594728,0.2706938766\C,0,-2.2
804878867,0.8206028991,2.8734744462\C,0,-2.3509281282,1.7691795682,-2.
0747847536\C,0,-6.4781013235,-0.0180499476,0.1931829688\C,0,-7.3865608
943,-3.4145461546,4.7599041475\C,0,-5.2697073903,-4.2991781487,9.21410
66475\C,0,-3.8921904112,-0.2216098356,6.602834678\C,0,-2.8756984679,-2
.43640765,1.5220056661\Cl,0,-2.1391651416,-2.4174063746,4.7207292543\C
l,0,-5.8421099748,-3.5749551299,1.7123689952\H,0,-6.4354721671,0.64663
60838,5.4737017645\H,0,-7.5196849536,-0.1417217708,4.297898595\H,0,-5.
2267905535,1.7981081636,3.7428378456\H,0,-6.6184850518,1.407464893,2.7
000640111\H,0,-1.33501739,1.5903178833,0.449849015\H,0,-4.9423191651,0
.9645204266,-1.8185206444\H,0,-3.9315880025,-1.9849260966,8.6496865446
\H,0,-6.8857323672,-4.6831281804,7.0598801316\H,0,-1.2459160986,1.1823
861014,2.7528045152\H,0,-2.7736038193,1.4779224524,3.6144603382\H,0,-2
.2386610182,-0.1866107983,3.3304325685\H,0,-3.5079059978,-0.0491616023
,5.584460036\H,0,-4.5027775645,0.6591290879,6.8835923553\H,0,-3.028085
2558,-0.2426512897,7.2867342186\H,0,-7.4199922566,-2.7211980233,3.9075
925884\H,0,-7.1647862599,-4.4165828579,4.351423894\H,0,-8.3943733429,-

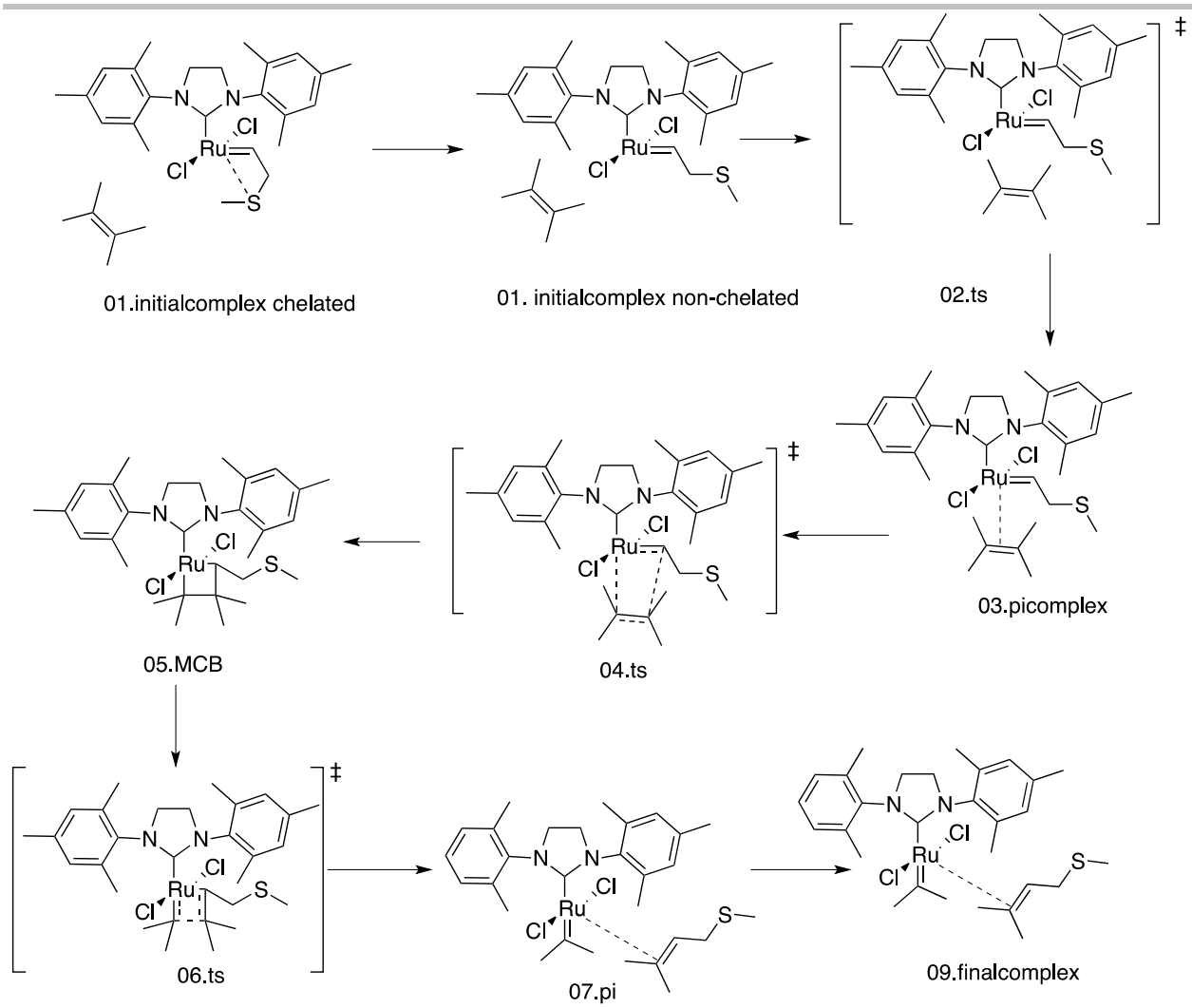
3.4718442218,5.2107863897\H,0,-3.0393723597,2.2578829166,-2.7845871935
\H,0,-1.5286501867,2.4703682864,-1.8541367\H,0,-1.9020718483,0.9104168
296,-2.6093165344\H,0,-4.7001562186,-3.7992967788,10.0150268617\H,0,-6
.2623781359,-4.5680900743,9.6163825703\H,0,-4.7592711936,-5.2494407448
,8.9743485237\C,0,-1.2369271617,-5.3697327514,3.086571033\C,0,-2.93794
07356,-5.6636936,1.2261532096\C,0,-3.499800546,-8.1515453591,4.9896875
764\S,0,-4.3889199469,-6.7835850422,5.7070578512\O,0,-4.1680075942,-6.
8032367656,7.1590496156\O,0,-5.7637202144,-6.814935678,5.1868892466\C,
0,-3.5685395046,-5.3149779984,5.0408081754\H,0,-2.4514405246,-8.123651
5325,5.3237249975\H,0,-3.5728040572,-8.1037623168,3.8917912729\H,0,-3.
9928268839,-9.0630878198,5.3614622045\H,0,-4.7242411945,-5.4181756634,
3.1750400014\H,0,-2.5317290706,-5.3303183128,5.4108196171\H,0,-4.09754
30729,-4.5078294782,5.5816640215\C,0,-1.3795043551,-2.3757145801,1.542
7532459\H,0,-0.922508523,-2.6470163885,2.503101519\H,0,-1.0697889618,-
1.3381978851,1.2965366966\H,0,-0.9558254215,-3.0047307926,0.7320463184
\C,0,-3.4178528942,-2.2804196476,0.1393252383\H,0,-0.5643335419,-5.076
3413615,2.2632460045\H,0,-0.9520074862,-6.4035082196,3.3682781383\H,0,
-1.0372855,-4.7138973079,3.9498313638\H,0,-2.2673694595,-5.110497891,0
.5443747769\H,0,-3.9850254359,-5.4731968119,0.9396202166\H,0,-2.720611
2518,-6.7374862037,1.0541311109\H,0,-4.4976187246,-2.1043275141,0.0843
482264\H,0,-3.2128304236,-3.2248434769,-0.4093107178\H,0,-2.8751577154
,-1.4832363915,-0.4085990309\H,0,-6.8038801605,-0.1287254209,-0.854049
3847\H,0,-7.1852591642,0.6830296863,0.6755359766\H,0,-6.6001525691,-0.
9933745875,0.7001188086\\Version=ES64L-G09RevE.01\HF=-2841.5392213\RMS
D=8.052e-09\Dipole=1.4014246,1.5661002,-1.7515752\Quadrupole=-9.162422
7,19.7879593,-10.6255366,-40.2453551,12.9036825,22.865614\PG=C01 [X(C3
0H44Cl2N2O2Ru1S1)]\\@

09.finalcomplex

1\1\GINC-JOKER-C8\Stability\RM06L\Gen\C30H44Cl2N2O2Ru1S1\RISHIRAM\14-S
ep-2017\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(rea
d) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
\Title\\0,1\C,0,-5.1564168542,-2.2015486926,7.0802603219\C,0,-6.001866
2411,-1.7504383833,6.0528544881\C,0,-7.3752617434,-2.0562009261,6.0413
761533\C,0,-7.8863842292,-2.8518906842,7.0687643538\C,0,-7.0697988434,
-3.3513024359,8.0913239572\C,0,-5.7121233198,-3.0128784221,8.077057049
8\N,0,-5.5068667834,-0.8843662307,5.0351747347\C,0,-4.8398382927,-1.19
07947553,3.8939441353\N,0,-4.6244367352,-0.0215096426,3.2244543095\C,0
,-5.2853523504,1.1178879158,3.8542040502\C,0,-5.6291809229,0.566642514
7,5.2256099713\Ru,0,-4.0237331427,-2.7988743513,3.1503350035\C,0,-4.50
60741937,-4.0690957479,4.4047461472\C,0,-1.852588954,-5.3851520954,0.5
518967103\C,0,-4.1226641292,0.0599339497,1.8896669191\C,0,-2.793507231
4,0.4734517509,1.6726809272\C,0,-2.3274661823,0.5214828089,0.353868135
5\C,0,-3.1403892847,0.1922396517,-0.7339910384\C,0,-4.4779811454,-0.13
82926881,-0.4845596515\C,0,-4.9982522199,-0.1904827081,0.8109986457\C,
0,-1.9128641087,0.9321504693,2.7921239862\C,0,-2.5916667115,0.15895792
63,-2.1262557982\C,0,-6.4643046909,-0.4080744824,1.023532645\C,0,-8.24
89856298,-1.5882455741,4.9188032061\C,0,-7.6320419791,-4.243047044,9.1
552331535\C,0,-3.7112978917,-1.8193231084,7.1166435556\C,0,-2.02450195
64,-4.2918626596,-0.2195280822\C,0,-1.8324400537,-2.8906906975,0.25891
30364\Cl,0,-1.8327623599,-2.2148176198,4.004563112\Cl,0,-5.6218702882,
-3.5809791284,1.5211784579\H,0,-4.9191571159,0.9003381972,6.0070600224
\H,0,-6.6433815085,0.8340555105,5.5657505595\H,0,-4.6117421208,1.99099
47193,3.8912932549\H,0,-6.1839547084,1.4081708536,3.2726498473\H,0,-1.
2861568247,0.8211228666,0.1750759516\H,0,-5.1450712685,-0.3540977821,-
1.3298489391\H,0,-5.0598900406,-3.378743639,8.8811309837\H,0,-8.955400
3168,-3.1021041787,7.0634887397\H,0,-7.0036007804,0.5590602077,0.99151
59574\H,0,-6.894231601,-1.0443736707,0.2339903215\H,0,-6.692129363,-0.
8829773969,1.9904596859\H,0,-0.8827511711,0.5573502263,2.6735475416\H,
0,-1.8536892415,2.0378661822,2.8034476765\H,0,-2.2766093423,0.60040687
44,3.7756362658\H,0,-3.1750123241,-2.1203409636,6.1984643313\H,0,-3.58
09924685,-0.7242109245,7.2011144093\H,0,-3.1995470716,-2.2779081125,7.

9785996027\H,0,-8.2533397791,-0.4880039832,4.8115067214\H,0,-7.9053321
126,-1.9883818745,3.9457133791\H,0,-9.2929357978,-1.9106158796,5.06144
26295\H,0,-3.3406087871,0.4717683547,-2.8737136255\H,0,-1.7030188283,0
.8027439285,-2.2363640354\H,0,-2.2806228282,-0.8677955612,-2.401552213
1\H,0,-7.0356695474,-4.2048550139,10.081965655\H,0,-8.673590637,-3.978
5632488,9.4045141685\H,0,-7.6447414589,-5.2994069906,8.8262669986\C,0,
-2.4816107091,-4.4139041127,-1.6372612312\C,0,-1.4752063098,-5.3814893
778,1.9865230125\C,0,-3.4751734669,-4.9450893384,5.0460090273\C,0,-5.9
061783053,-4.4986321041,4.6699540718\H,0,-2.6217544322,-5.461389292,-1
.951850714\H,0,-1.7651712941,-3.9356500276,-2.3323083574\H,0,-3.443306
9886,-3.8820576339,-1.7787147542\H,0,-2.8010234569,-2.3490155166,0.264
751281\H,0,-1.1805382678,-2.328159565,-0.43685102\H,0,-1.3849968767,-2
.8078614145,1.2617695251\S,0,0.3034731469,-5.485139431,2.3247872642\H,
0,-1.9257695024,-6.2117151632,2.5580490056\H,0,-1.6999855642,-4.437729
9982,2.5182685411\H,0,-6.6667001054,-3.8215911094,4.2606623977\H,0,-6.
0945920446,-4.6619185346,5.7503946917\H,0,-6.0437918606,-5.4827121745,
4.1742680958\H,0,-2.4390800901,-4.7555848514,4.7278263125\H,0,-3.71682
54597,-6.015950388,4.89341185\H,0,-3.517743969,-4.7812140172,6.1435901
274\H,0,-2.026203807,-6.3735280148,0.1022980953\C,0,0.8204281828,-7.02
13512689,1.583994371\O,0,0.9778570803,-4.3936093151,1.6089178554\O,0,0
.4622282303,-5.5986566021,3.7822771904\H,0,1.9016814509,-7.1024082594,
1.7748757722\H,0,0.6290288137,-6.9866288518,0.5006349215\H,0,0.2869211
188,-7.858751248,2.0584641812\\Version=ES64L-G09RevE.01\HF=-2841.52509
58\RMSD=3.247e-09\Dipole=-2.9197779,0.8020828,0.4996115\Quadrupole=3.8
159573,-2.7075613,-1.108396,-0.918792,-40.8295402,4.340891\PG=C01 [X(C
30H44Cl2N2O2Ru1S1)]\\@

Reaction of allylsulfide carbene and 2,3-dimethyl-2-butene (4S)



Scheme 5 Reaction of allylsulfidecarbene and 2,3-dimethyl-2-butene (tetrasubstituted alkene)

01.initialcomplex

1\1\GINC-C01\Stability\RM06L\Gen\C30H44Cl2N2Ru1S1\RISHIRAMT\25-Nov-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
\\0,1\C,0,-4.1823924059,-1.5418835143,6.4621656298\C,0,-5.216222365,-1
.6411779045,5.5156777153\C,0,-6.2282310156,-2.6104403965,5.6250011443\
C,0,-6.1619632257,-3.512273171,6.6916802107\C,0,-5.128424697,-3.469387
2899,7.6346869668\C,0,-4.1578576638,-2.4693203086,7.507973114\N,0,-5.2
434097132,-0.7122034515,4.4370688337\C,0,-4.5440753757,-0.7511440817,3
.2730366855\N,0,-4.8218560838,0.4035980647,2.6032710968\C,0,-5.6171784
967,1.340859205,3.3901243965\C,0,-6.1203595199,0.4611046231,4.52174091
96\Ru,0,-3.3833459442,-2.0814166987,2.4400034566\C,0,-3.6425363273,-3.
4672089777,3.592824637\C,0,-4.1512510662,0.8214920441,1.4156519415\C,0
,-2.8647849692,1.3928072687,1.5180952254\C,0,-2.2009302717,1.734603667
6,0.3361311174\C,0,-2.7918415491,1.5695020293,-0.9212358961\C,0,-4.107
2216297,1.098013281,-0.974737676\C,0,-4.8119562196,0.7268853375,0.1752
482251\C,0,-2.2575226388,1.7422768294,2.8419910547\C,0,-2.0244102399,1
.8662205792,-2.1716344985\C,0,-6.2466649005,0.3144559013,0.0714673343\
C,0,-7.3023443787,-2.7156502117,4.5869783698\C,0,-5.0327868854,-4.4954
616709,8.7207833972\C,0,-3.1315220552,-0.4837359717,6.3350529296\Cl,0,
-1.2324944577,-1.3758061733,3.211459055\Cl,0,-5.0825224066,-2.70960244
07,0.8745386881\H,0,-6.0354137788,0.9323546597,5.515280433\H,0,-7.1762
270943,0.1581697406,4.3840909314\H,0,-4.981956846,2.1766463419,3.74728

74106\H,0,-6.4280743455,1.7740700977,2.7798714645\H,0,-1.188822005,2.1
55747953,0.403420648\H,0,-4.6041795761,1.004019217,-1.9494889266\H,0,-
3.345075288,-2.4133940347,8.2447128452\H,0,-6.9328038969,-4.2896565733
,6.7749166522\H,0,-6.893063473,1.2046149754,-0.0563033548\H,0,-6.41710
47146,-0.3335341566,-0.8041292243\H,0,-6.5929410754,-0.229382974,0.962
7314166\H,0,-1.1590251439,1.6650513698,2.8152298766\H,0,-2.502946007,2
.7904144745,3.1037743581\H,0,-2.6113923742,1.1027242592,3.6652332223\H
,0,-2.5183092896,-0.6227588279,5.4237826863\H,0,-3.5728665331,0.528406
0856,6.2620956233\H,0,-2.4508818016,-0.49046919,7.2024629709\H,0,-8.07
06555227,-1.9277640413,4.6995554457\H,0,-6.891381245,-2.6155822924,3.5
652465105\H,0,-7.826455273,-3.6830311936,4.6510287275\H,0,-2.689649251
3,2.0752274684,-3.0259835134\H,0,-1.3438557174,2.7254420056,-2.0448658
892\H,0,-1.3927990495,1.0032352433,-2.4589079014\H,0,-4.5743439917,-4.
0858488684,9.6367585667\H,0,-6.018946825,-4.9125691516,8.9848248157\H,
0,-4.4000662816,-5.3453682275,8.4003965804\H,0,-1.8250634266,-4.504638
0063,2.9937255717\C,0,-2.7505056686,-4.657962734,3.5790735933\S,0,-2.3
275903451,-5.2334562998,5.260192835\H,0,-3.2942476671,-5.5138789107,3.
1293479729\C,0,-1.2791940379,-3.8726773666,5.8110118433\H,0,-1.8210197
49,-2.9130896228,5.787483071\H,0,-0.370264695,-3.7910504402,5.19108059
58\H,0,-0.9899039333,-4.0959093254,6.8509829593\C,0,-1.0922340055,-3.9
114105862,0.2525888076\C,0,-1.1502545475,-2.6616495902,-0.2754459779\C
,0,-2.0602786783,-5.0092764003,-0.073214297\C,0,0.0459166577,-4.335571
0347,1.1486722578\C,0,-2.2040323181,-2.1809590912,-1.2265546529\C,0,-0
.0861957194,-1.6329826454,-0.0324943701\H,0,0.1921744338,-3.6456389667
,1.9998858211\H,0,1.0112782095,-4.3828571373,0.6075485299\H,0,-0.12655
48511,-5.3433266178,1.5664971015\H,0,0.6534314799,-1.9198763248,0.7297
564043\H,0,-0.5291293793,-0.6689397968,0.2840126981\H,0,0.4644897629,-
1.42444894,-0.9731848094\H,0,-2.9092172842,-4.6942983718,-0.6972089125
\H,0,-2.4791571132,-5.4674046043,0.8431030436\H,0,-1.5431395542,-5.834
8827307,-0.6032227904\H,0,-3.0201235959,-2.8950858433,-1.4065561899\H,
0,-1.7535048989,-1.925299619,-2.2076473913\H,0,-2.6686214064,-1.245264
0739,-0.857315907\H,0,-4.5054207666,-3.5674818486,4.2774397422\\Versio
n=ES64L-G16RevA.03\HF=-2691.2589884\RMSD=4.302e-09\Dipole=-1.1648477,2
.0403376,1.1160786\Quadrupole=7.1923812,-17.2771951,10.0848139,-14.755
9909,-21.0556622,3.3090366\PG=C01 [X(C30H44Cl2N2Ru1S1)]\\@

02.ts

1\1\GINC-C01\Stability\RM06L\Gen\C30H44Cl2N2Ru1S1\RISHIRAMT\26-Nov-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
\\0,1\C,0,-4.1693517146,-1.5837951347,6.4885551204\C,0,-5.1315854104,-
1.7035374101,5.4720661986\C,0,-6.1544812505,-2.6665081537,5.5312994025
\C,0,-6.1676879894,-3.5447605651,6.6187186785\C,0,-5.2052136931,-3.480
9805172,7.6332992206\C,0,-4.2240783407,-2.4870124249,7.5544123622\N,0,
-5.1132060581,-0.7621220664,4.4026765401\C,0,-4.4060071661,-0.79379965
84,3.2444150512\N,0,-4.658368618,0.374710807,2.591772114\C,0,-5.443519
5691,1.3132542828,3.3881841938\C,0,-5.9741207425,0.4231613369,4.497201
29\Ru,0,-3.2223496638,-2.1077600055,2.4115739976\C,0,-3.5853652901,-3.
5276706007,3.4928022598\C,0,-4.0855757995,0.7768102928,1.3491377463\C,
0,-2.7898037132,1.3301892527,1.3227336084\C,0,-2.2578372933,1.70507139
07,0.0824736819\C,0,-2.9873916376,1.5917657817,-1.1034268142\C,0,-4.30
30352679,1.1190198247,-1.0251244258\C,0,-4.8775670334,0.7168842449,0.1
828575405\C,0,-2.0221881617,1.6321529168,2.5731750656\C,0,-2.374494065
5,1.9452425832,-2.4226907344\C,0,-6.3167337724,0.307892961,0.227797572
5\C,0,-7.1689811303,-2.7731696886,4.4344171671\C,0,-5.1952242356,-4.48
04054394,8.7478344176\C,0,-3.1179047555,-0.5205597494,6.4201083085\Cl,
0,-1.1265762931,-1.4956774887,3.4005225334\Cl,0,-4.9295246629,-2.67970
5459,0.8045349075\H,0,-5.8946574814,0.8762053787,5.4994732647\H,0,-7.0
327448438,0.1372244875,4.3425105352\H,0,-4.7941847146,2.1297523699,3.7
646334487\H,0,-6.2393552768,1.773157016,2.7779939121\H,0,-1.2412132787
,2.119765197,0.0513060439\H,0,-4.9060805542,1.0583562116,-1.940870085\
H,0,-3.4678820561,-2.4143283332,8.347722983\H,0,-6.9474254338,-4.31634

63991,6.6656574534\H,0,-6.9728482375,1.2000025552,0.2505482669\H,0,-6.
5969090485,-0.2708875207,-0.6678664122\H,0,-6.5514881669,-0.3074195904
,1.1096694828\H,0,-0.9537716063,1.3844818696,2.4633185517\H,0,-2.08139
6687,2.7150940132,2.7967749603\H,0,-2.3932898698,1.0875023701,3.454322
2362\H,0,-2.4705841378,-0.6402051695,5.5305261242\H,0,-3.5603975524,0.
4915565495,6.3497014754\H,0,-2.4721500337,-0.5395727908,7.3135951757\H
,0,-7.9416570535,-1.9843658712,4.5058689528\H,0,-6.706825629,-2.672868
8285,3.4345703562\H,0,-7.6973141236,-3.7397889596,4.4711224851\H,0,-3.
1240923314,2.3251209892,-3.1373152913\H,0,-1.5804650576,2.7036666723,-
2.3188803573\H,0,-1.9090798397,1.058317443,-2.8936978822\H,0,-4.777242
6431,-4.0585924643,9.6774771754\H,0,-6.204836182,-4.8665401565,8.96715
5607\H,0,-4.5691238149,-5.3542860682,8.4834049184\H,0,-1.6821809519,-4
.5427944625,3.1810383059\C,0,-2.6802257818,-4.6997418779,3.6273892304\
S,0,-2.4943589355,-5.2422119527,5.362563301\H,0,-3.1438089137,-5.57199
46113,3.1228070107\C,0,-1.4199884509,-3.9434736455,6.0032465169\H,0,-1
.8813509135,-2.9488862853,5.8985894663\H,0,-0.4420682812,-3.9458988815
,5.4922025859\H,0,-1.2701133762,-4.1591947409,7.0739579251\C,0,-1.1201
311999,-3.819870817,0.3560064298\C,0,-1.1344344383,-2.5423688423,-0.11
37065341\C,0,-2.1121399804,-4.873930955,-0.0344193718\C,0,0.0166434284
,-4.32061117,1.2128329584\C,0,-2.1391588669,-1.9909314921,-1.078781486
3\C,0,-0.0344919812,-1.567346323,0.1854285576\H,0,0.1946479848,-3.6819
403898,2.0972933618\H,0,0.9706756964,-4.3578052291,0.6512435409\H,0,-0
.1741342182,-5.3460879814,1.5748895092\H,0,0.6240307764,-1.8698648177,
1.0121479555\H,0,-0.4453868331,-0.5699997668,0.4342069282\H,0,0.597207
9592,-1.4237334506,-0.7155419347\H,0,-2.9635673257,-4.4985247039,-0.61
97632241\H,0,-2.5284428256,-5.3837247599,0.855070556\H,0,-1.6144482598
,-5.6704071613,-0.6244305002\H,0,-2.916991101,-2.7024692932,-1.3891510
094\H,0,-1.6239081479,-1.6261596145,-1.9905984764\H,0,-2.6580964018,-1
.109717958,-0.651999603\H,0,-4.5522926783,-3.6614441012,4.0150526159\\
Version=ES64L-G09RevE.01\HF=-2691.2579873\RMSD=9.711e-10\Dipole=-1.072
2786,2.0633023,0.8717289\Quadrupole=6.6342936,-16.0258072,9.3915136,-1
5.3615109,-19.8323743,3.755293\PG=C01 [X(C30H44Cl2N2Ru1S1)]\\@

03.pi

1\1\GINC-C06\Stability\RM06L\Gen\C30H44Cl2N2Ru1S1\RISHIRAMT\19-Nov-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
\\0,1\C,0,-4.1494338602,-1.6149064426,6.4307120445\C,0,-5.0578441984,-
1.8008194044,5.3741928868\C,0,-6.046670982,-2.7994585171,5.417272613\C
,0,-6.0757640784,-3.6467254378,6.5286399938\C,0,-5.1696185003,-3.51237
374,7.5859951249\C,0,-4.2257083552,-2.4820050767,7.5235414936\N,0,-5.0
566563932,-0.8534464395,4.308846556\C,0,-4.3059120512,-0.8228827339,3.
182829355\N,0,-4.5651452979,0.358432389,2.55902442\C,0,-5.4100430359,1
.2457479899,3.3547274884\C,0,-5.9638409599,0.2984566528,4.4022004468\R
u,0,-3.0860019674,-2.1023151039,2.3063360979\C,0,-3.4409692577,-3.5416
476269,3.3713993313\C,0,-4.002541098,0.7986432616,1.3241990114\C,0,-2.
7043691828,1.3442778478,1.3001979284\C,0,-2.1825602599,1.7501745166,0.
0647536447\C,0,-2.9252102112,1.6782906521,-1.1155011042\C,0,-4.2456855
68,1.2179015463,-1.0355258996\C,0,-4.8094939643,0.7823982505,0.1655692
851\C,0,-1.918863371,1.6058740699,2.5483449197\C,0,-2.3236818079,2.062
6933673,-2.4313226005\C,0,-6.2515671192,0.3844103153,0.2142378047\C,0,
-7.0282352163,-2.9557673677,4.2973466209\C,0,-5.1732341351,-4.47656676
07,8.731026178\C,0,-3.1371307016,-0.5132483983,6.3764968484\Cl,0,-1.01
71741363,-1.5072708086,3.4181641316\Cl,0,-5.0126347144,-2.6790291145,0
.8982736777\H,0,-5.951210178,0.7159660737,5.4225692652\H,0,-7.00164140
38,-0.0200149844,4.1823171249\H,0,-4.7991428498,2.0624013671,3.7909717
569\H,0,-6.1904268839,1.7086970945,2.7275413585\H,0,-1.1627682767,2.15
72084549,0.0349878262\H,0,-4.8598467197,1.1913327801,-1.9454669723\H,0
,-3.5146176814,-2.353467316,8.3508337754\H,0,-6.8272277667,-4.44667251
53,6.5633444466\H,0,-6.8992781808,1.2797508162,0.2914444645\H,0,-6.551
2137147,-0.1463974356,-0.7046931272\H,0,-6.4765128773,-0.2742328849,1.
0664614771\H,0,-0.865577455,1.3000723062,2.4387898049\H,0,-1.919382510

7,2.6909196976,2.7687562028\H,0,-2.3175771643,1.0828181702,3.430215512
2\H,0,-2.4662209252,-0.617193405,5.5020608354\H,0,-3.6141997914,0.4819
84122,6.2874112295\H,0,-2.5119549388,-0.5003104459,7.284721104\H,0,-7.
8647757881,-2.2356449501,4.3822083981\H,0,-6.5613845665,-2.7863302594,
3.3090581126\H,0,-7.477784153,-3.9625963604,4.2979140849\H,0,-3.071869
7665,2.496980745,-3.1159123111\H,0,-1.5013067977,2.7879548828,-2.31299
35951\H,0,-1.8996672874,1.1790549059,-2.9458491919\H,0,-4.8581431038,-
3.9998728069,9.6748935835\H,0,-6.1661270992,-4.9305223791,8.888164137\
H,0,-4.4672857835,-5.3091399247,8.5439380772\H,0,-1.4200352944,-4.3297
300706,3.525520183\C,0,-2.4641155482,-4.5958517749,3.7540658215\S,0,-2
.5742319195,-5.0717598523,5.5156825408\H,0,-2.7105113036,-5.5229074376
,3.1968940301\C,0,-1.4644634389,-3.8524313054,6.2445526354\H,0,-1.7739
468171,-2.8250375475,5.9974437865\H,0,-0.4248224434,-4.0088906516,5.90
7977542\H,0,-1.5142425179,-3.9911596154,7.3371964066\C,0,-1.3652313493
,-3.7960219079,0.4803140677\C,0,-1.3699253243,-2.5215523993,-0.0171134
178\C,0,-2.3591783442,-4.8486502922,0.0908061826\C,0,-0.1787230356,-4.
3188615975,1.2488551352\C,0,-2.3617921561,-1.9915266991,-1.0094412328\
C,0,-0.218297358,-1.5818880478,0.1897285386\H,0,0.1410879183,-3.645259
1591,2.062621043\H,0,0.6944134991,-4.4504495825,0.5790910634\H,0,-0.38
8024052,-5.3085207133,1.689742218\H,0,0.4554678788,-1.863630378,1.0097
562817\H,0,-0.5725630393,-0.552314454,0.3850626704\H,0,0.3811088197,-1
.5315369717,-0.7426009896\H,0,-3.2467744198,-4.4610496727,-0.427461932
6\H,0,-2.7161045869,-5.4145410126,0.9708186925\H,0,-1.8705999711,-5.59
64114609,-0.5668774421\H,0,-3.170468052,-2.6875149265,-1.2685002121\H,
0,-1.8291765702,-1.7138048703,-1.9417271541\H,0,-2.8373822317,-1.06022
17658,-0.6457780113\H,0,-4.4820382545,-3.7775024682,3.6753258756\\Vers
ion=ES64L-G09RevE.01\HF=-2691.2584495\RMSD=1.271e-09\Dipole=-0.6845184
,1.9412825,0.4189926\Quadrupole=2.7837528,-12.0857442,9.3019914,-17.25
37478,-16.3623471,4.9108641\PG=C01 [X(C30H44Cl2N2Ru1S1)]\\@

04.ts

1\1\GINC-C05\Stability\RM06L\Gen\C30H44Cl2N2Ru1S1\RISHIRAMT\17-Nov-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
\\0,1\C,0,-4.0938182461,-1.5798244454,6.5466385449\C,0,-4.8572414007,-
1.6811702452,5.3721478465\C,0,-5.8734002624,-2.6469839418,5.2348554074
\C,0,-6.0764056397,-3.5429155929,6.2848067191\C,0,-5.3041474459,-3.504
8390546,7.451475163\C,0,-4.3300605805,-2.5107364782,7.5647709884\N,0,-
4.73527763,-0.6655175715,4.3743581935\C,0,-4.1446928715,-0.7086494002,
3.168242354\N,0,-4.3628128462,0.4744286001,2.5532758549\C,0,-5.1063508
466,1.4272190662,3.383131003\C,0,-5.4471050407,0.5997336067,4.61165637
55\Ru,0,-2.9671580395,-2.1266764315,2.2180888639\C,0,-2.9076480356,-3.
9307348695,2.7251815803\C,0,-3.9992705016,0.8243876205,1.2163680986\C,
0,-2.7205930466,1.3615604983,0.9697245385\C,0,-2.3990023004,1.72392869
67,-0.342159881\C,0,-3.3130718553,1.5888982001,-1.3930173606\C,0,-4.59
39863434,1.1113074216,-1.0964264551\C,0,-4.968069277,0.736909727,0.198
1790847\C,0,-1.7511541065,1.5820557796,2.0883932909\C,0,-2.9200694263,
1.917479007,-2.799691516\C,0,-6.3786224774,0.3238702947,0.4796006062\C
,0,-6.7069782113,-2.7109553704,3.9961104628\C,0,-5.486342789,-4.533863
313,8.524024992\C,0,-3.0877041979,-0.4887263725,6.745378588\Cl,0,-1.21
35809778,-1.5475108109,3.8716948373\Cl,0,-4.9356416909,-2.6814951303,0
.8318961092\H,0,-5.0986161634,1.0572147081,5.5538068594\H,0,-6.5301018
257,0.403345685,4.7210378826\H,0,-4.475399185,2.3059301885,3.611823054
7\H,0,-5.996878002,1.7911672765,2.8406555198\H,0,-1.3994849583,2.13038
98334,-0.5468478958\H,0,-5.3346907696,1.0271826822,-1.9026695424\H,0,-
3.7234698471,-2.4542733406,8.4791666941\H,0,-6.8584911863,-4.307194343
4,6.1831673598\H,0,-7.0311516231,1.2126362171,0.5855383276\H,0,-6.7893
329338,-0.2773910516,-0.3478779463\H,0,-6.4675751453,-0.2762767878,1.3
981316125\H,0,-0.7797371155,1.9388705023,1.7078544987\H,0,-2.126131177
,2.3460170447,2.795938641\H,0,-1.5708133038,0.6669600172,2.6818892262\
H,0,-2.7080810086,-0.0942045434,5.7896917603\H,0,-3.5182290626,0.35490
00065,7.3195001597\H,0,-2.2201736659,-0.8502089069,7.324298612\H,0,-7.

160551244,-1.7327151406,3.7485715393\H,0,-6.106298807,-2.992703365,3.1
103734973\H,0,-7.5253393107,-3.4418991601,4.1028650888\H,0,-3.78309756
69,2.2422560162,-3.4047959113\H,0,-2.152117925,2.7082547446,-2.8394560
113\H,0,-2.4913251679,1.0318160048,-3.3069991091\H,0,-5.1196501792,-4.
1822232197,9.5032126647\H,0,-6.5432143563,-4.8304425314,8.6383329969\H
,0,-4.9258599135,-5.4583822011,8.282744301\H,0,-1.1990734555,-4.127117
412,4.0394734835\C,0,-2.1004503249,-4.6745231088,3.7324566526\S,0,-3.0
808328283,-4.9739229016,5.2549358901\H,0,-1.8050740696,-5.657594658,3.
3159601306\C,0,-1.8624702781,-4.4758369278,6.487384696\H,0,-1.57258947
92,-3.4197117349,6.3500024088\H,0,-0.9647654865,-5.1176795412,6.455201
6177\H,0,-2.3424469865,-4.5892645455,7.4731930529\C,0,-1.5398829814,-3
.6639095241,0.967773068\C,0,-1.6439000553,-2.3072422825,0.4743019195\C
,0,-2.2010386969,-4.7690460029,0.1801614416\C,0,-0.2183208587,-4.05571
10765,1.5775975435\C,0,-2.3518447051,-2.0220458645,-0.8292367947\C,0,-
0.4485150676,-1.3927082607,0.6303214692\H,0,0.0894444965,-3.3944644642
,2.4026859476\H,0,0.5608726189,-3.9860677559,0.7929962492\H,0,-0.21566
53369,-5.0963321642,1.9376001519\H,0,0.0127015324,-1.4087095406,1.6258
144831\H,0,-0.7264687177,-0.350618929,0.3958259419\H,0,0.322303581,-1.
6865765168,-0.1132583221\H,0,-3.2563816664,-4.5546994887,-0.0485138044
\H,0,-2.1494759522,-5.7337780773,0.7138264075\H,0,-1.6629332067,-4.897
7458669,-0.7801654823\H,0,-3.1437262507,-2.7344984288,-1.0860318075\H,
0,-1.5955631297,-2.0279870043,-1.6425472905\H,0,-2.8028193799,-1.01340
06396,-0.8219350612\H,0,-3.7087717847,-4.546459109,2.2631398378\\Versi
on=ES64L-G09RevE.01\HF=-2691.2410935\RMSD=3.922e-09\Dipole=0.0901624,1
.5072919,0.0914793\Quadrupole=-5.255135,-4.0325269,9.2876619,-21.52006
18,-10.9483785,4.0189424\PG=C01 [X(C30H44Cl2N2Ru1S1)]\\@

05.MCB

1\1\GINC-C03\Stability\UM06L\Gen\C30H44Cl2N2Ru1S1\RISHIRAMT\12-Nov-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
\\0,1\C,0,-4.0553113862,-1.5041247431,6.5050796523\C,0,-4.8795935974,-
1.6131808317,5.3740190648\C,0,-5.9036623257,-2.5783679783,5.2960417055
\C,0,-6.0416978775,-3.477233863,6.3528903301\C,0,-5.1979667141,-3.4427
567439,7.4700087772\C,0,-4.2227421471,-2.4459343825,7.5285120405\N,0,-
4.7960355281,-0.6226232181,4.3459025821\C,0,-4.1830101976,-0.678658435
1,3.1531031874\N,0,-4.3937685355,0.4826488398,2.5049138748\C,0,-5.1796
588063,1.4387176595,3.2929225401\C,0,-5.4981543355,0.6521828035,4.5555
807012\Ru,0,-3.0119007552,-2.1379692778,2.3116148044\C,0,-2.6201088338
,-4.0808782317,2.4945460141\C,0,-4.0034046016,0.8120215398,1.170318934
7\C,0,-2.7299068244,1.3713206569,0.952857588\C,0,-2.3886264838,1.74300
99357,-0.3511417128\C,0,-3.2796383321,1.5956058411,-1.4210991584\C,0,-
4.5542560906,1.0864812097,-1.1534934456\C,0,-4.9472482885,0.7000078145
,0.1325426265\C,0,-1.7867598244,1.5967886418,2.0928662179\C,0,-2.86800
70391,1.9459692074,-2.8173358054\C,0,-6.3524936338,0.2486289358,0.3819
415509\C,0,-6.808280663,-2.6467832232,4.1083128443\C,0,-5.3370491759,-
4.4632512142,8.5578294483\C,0,-3.0626268665,-0.3957204564,6.6709830813
\Cl,0,-1.282573674,-1.5395708158,3.96186341\Cl,0,-4.9921524124,-2.8010
220918,1.0030515735\H,0,-5.1236691133,1.1357750567,5.4751860045\H,0,-6
.5786838402,0.4669731076,4.6966237893\H,0,-4.586596718,2.3512008026,3.
4850996342\H,0,-6.0800647562,1.7413982999,2.729238252\H,0,-1.393441623
9,2.1696932184,-0.5346012011\H,0,-5.2757832415,0.9876593204,-1.9753036
141\H,0,-3.5640856478,-2.3898618318,8.4060971639\H,0,-6.8279329502,-4.
2419479731,6.296886127\H,0,-7.0355023015,1.1177281927,0.4509448117\H,0
,-6.7202455274,-0.3804710129,-0.4454103636\H,0,-6.4500854009,-0.338291
4988,1.3080775785\H,0,-0.8224613764,1.9962230296,1.7376764391\H,0,-2.1
981858368,2.326887684,2.8156849216\H,0,-1.5838152437,0.6725607988,2.66
5498489\H,0,-2.8213769062,0.1027109788,5.7200736761\H,0,-3.4424567888,
0.368798691,7.3763581049\H,0,-2.1139434121,-0.7709140599,7.0916730443\
H,0,-7.2498844509,-1.6631777676,3.8617852035\H,0,-6.2661845216,-2.9693
546222,3.1990086728\H,0,-7.6373071309,-3.3527612695,4.2802743872\H,0,-
3.7280428856,2.2512082185,-3.4366350672\H,0,-2.1226183639,2.7587820894

,-2.8357448007\H,0,-2.4041065795,1.0776481894,-3.3232726026\H,0,-4.664
1534323,-4.2562103717,9.4067032029\H,0,-6.369569039,-4.5098614779,8.94
85111743\H,0,-5.1019258236,-5.4788741303,8.1869304393\H,0,-1.128103607
5,-4.134605799,4.0683465505\C,0,-1.975593965,-4.7226635342,3.687628702
6\S,0,-3.1887316636,-4.882033035,5.0367558832\H,0,-1.603997458,-5.7323
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,-4.5257242217,-0.7745383555\H,0,-3.3038351452,-2.6334336495,-0.880285
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2N2Ru1S1)]\\@

06.ts

1\1\GINC-C05\Stability\RM06L\Gen\C30H44Cl2N2Ru1S1\RISHIRAMT\17-Nov-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
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,0,-6.8229862144,-2.7338927703,4.191909133\C,0,-5.2038512167,-4.338094
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2.401155529\H,0,0.3322977611,-3.8483672358,0.6669468808\H,0,-0.0261588
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84,-0.8480283928\H,0,-3.4326755998,-2.48256243,-0.7912887432\H,0,-1.75
7184458,-2.1714637439,-1.3843049569\H,0,-2.7652196958,-0.8415520048,-0
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07.pi

1\1\GINC-C06\Stability\RM06L\Gen\C30H44Cl2N2Ru1S1\RISHIRAMT\19-Nov-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
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,0,-5.7398952582,-3.3786736859,6.7032912039\C,0,-4.8238658451,-3.03248
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2.9225056446\N,0,-4.5891195884,0.2710743101,2.2531540135\C,0,-5.575501
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61,2.7856233717,-2.414101101\C,0,-6.1779225173,0.3074327684,-0.1545142
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09.finalcomplex

1\1\GINC-C11\Stability\RM06L\Gen\C30H44Cl2N2Ru1S1\RISHIRAMT\20-Nov-201
7\0\\#P M06L/chkbasis stable(opt) pop(nbo) scrf(check) guess(read) geo
m(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title
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,3.6154376106\H,0,-7.3909954046,-3.8624724723,4.8621963051\H,0,-3.2988
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\H,0,-2.8663193734,-2.596616908,-1.0880026671\H,0,-2.7826400508,-0.829
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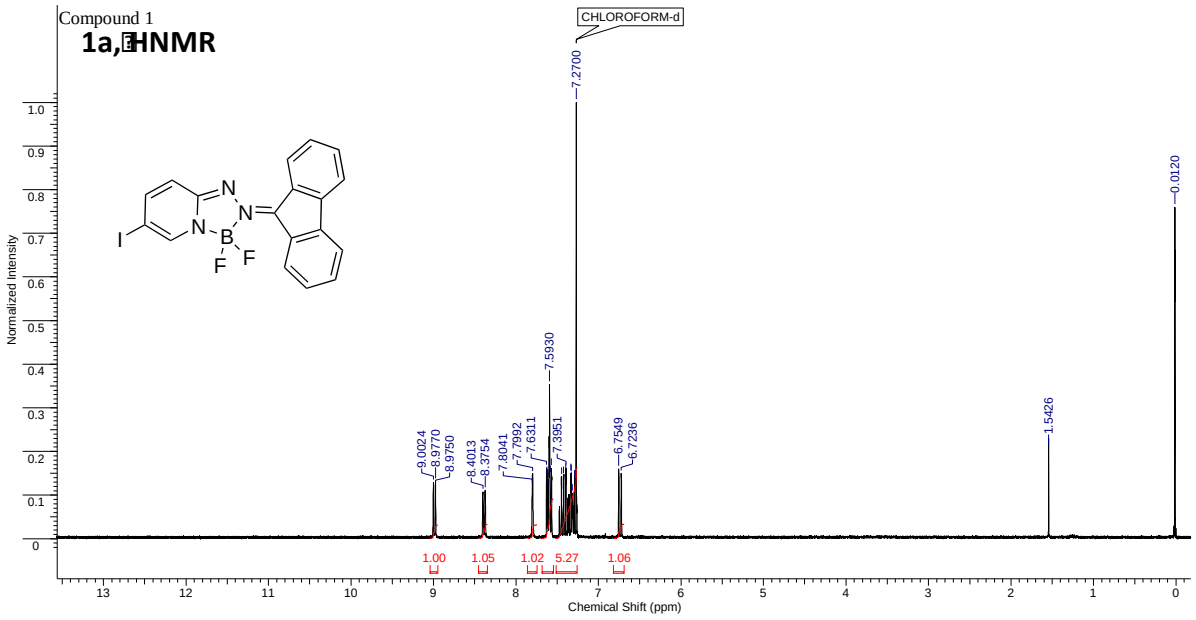
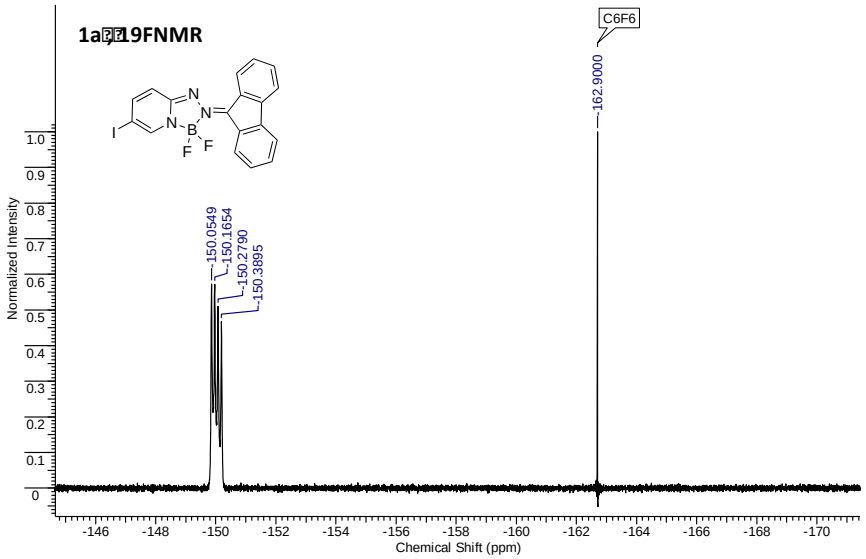
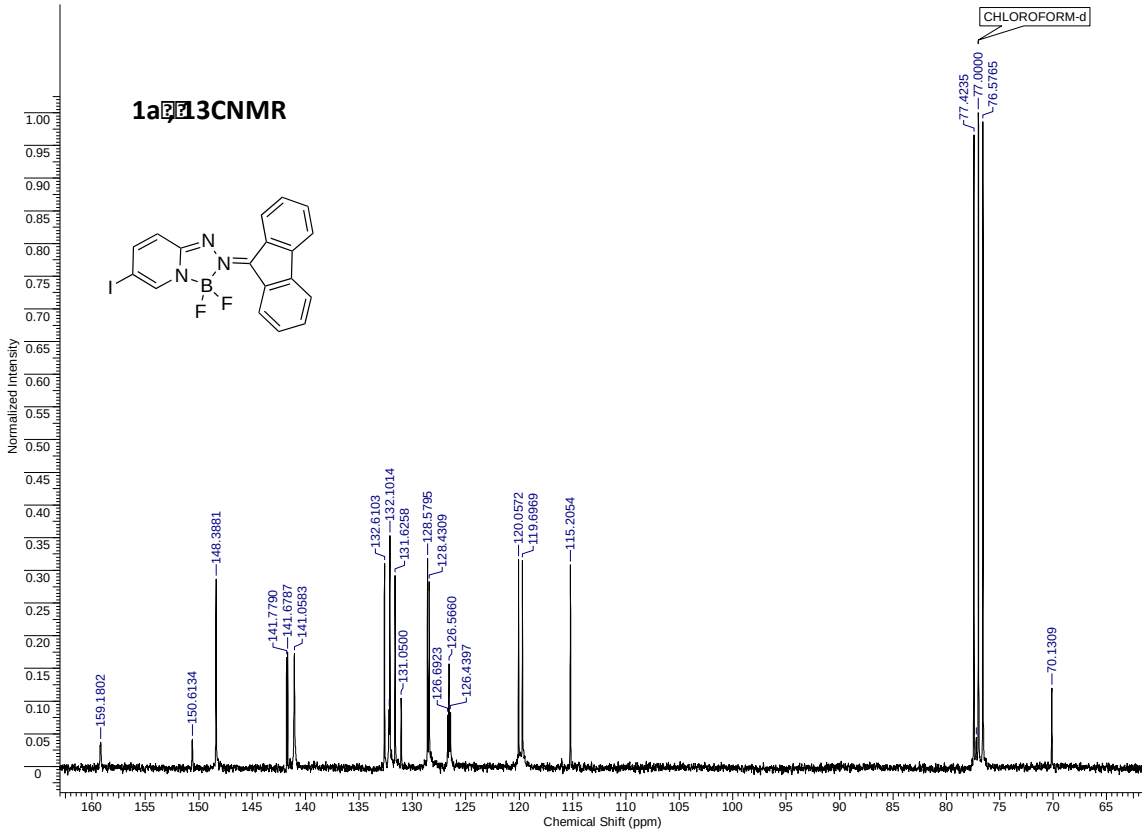
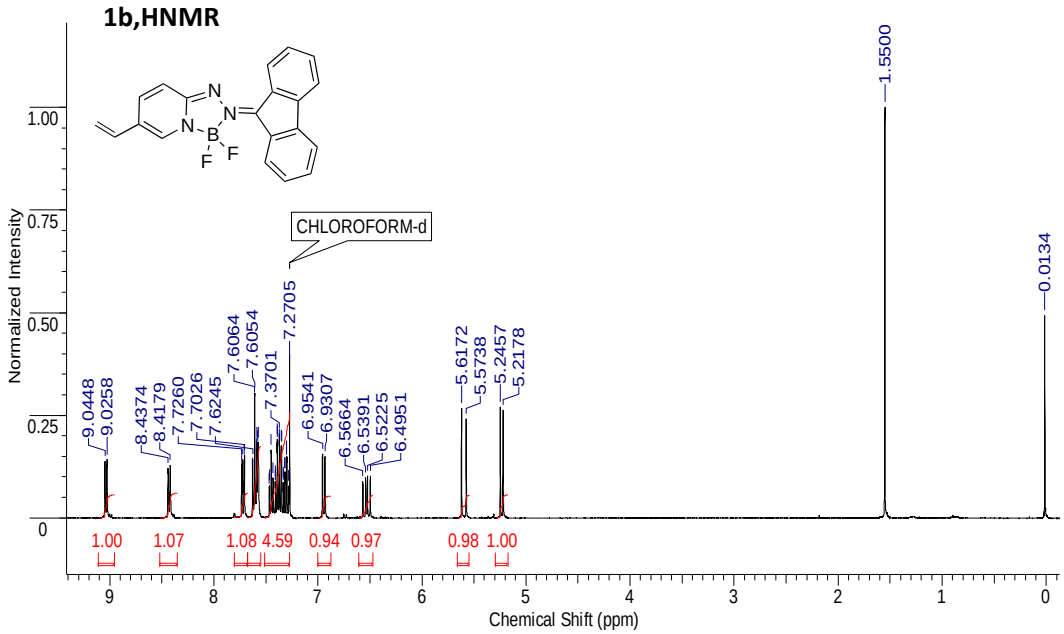
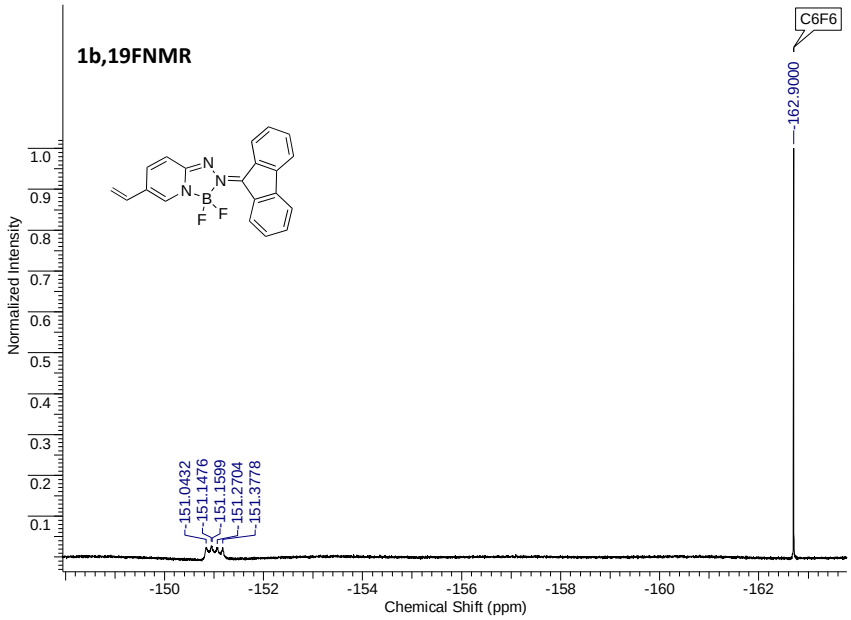
NMR Spectra of the compounds

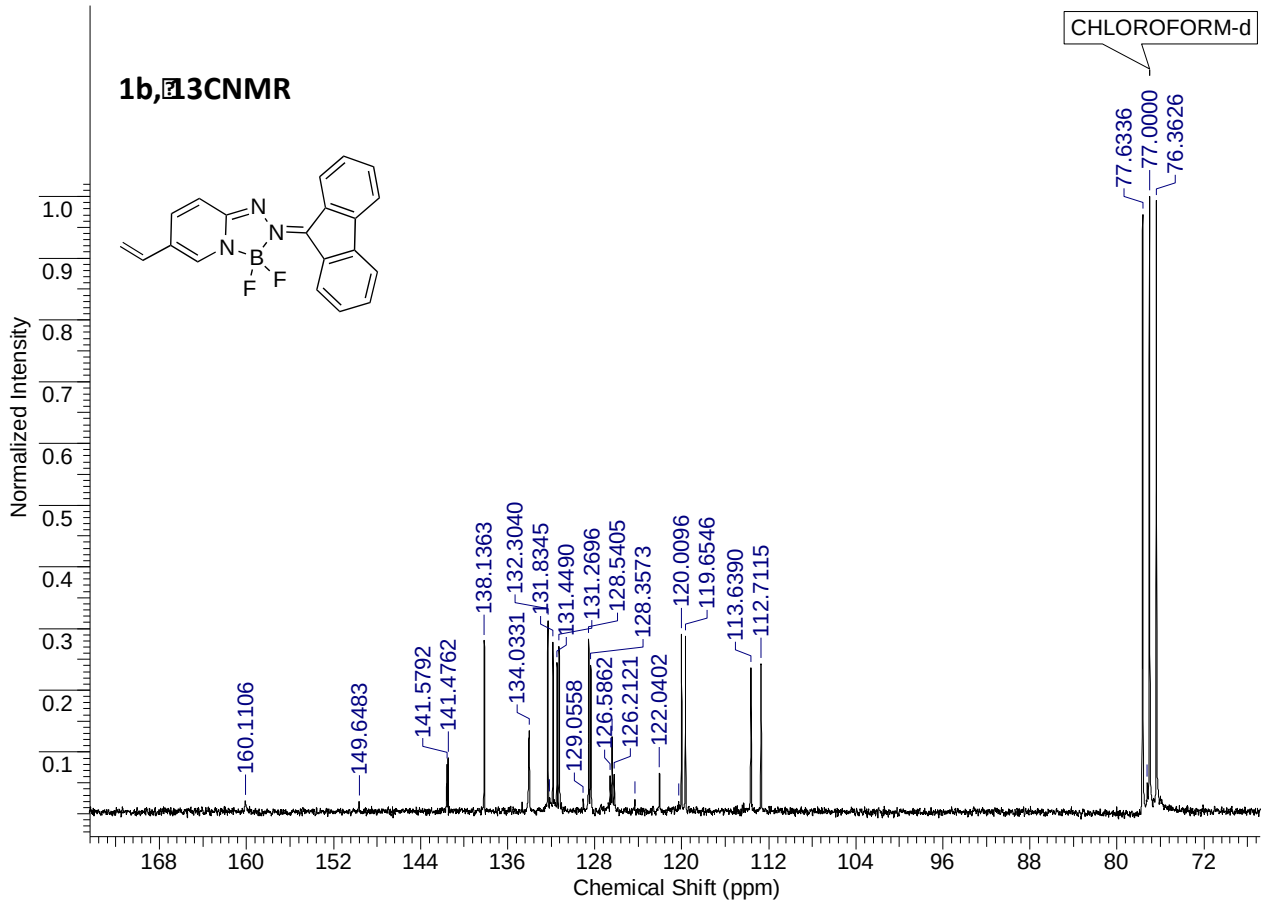


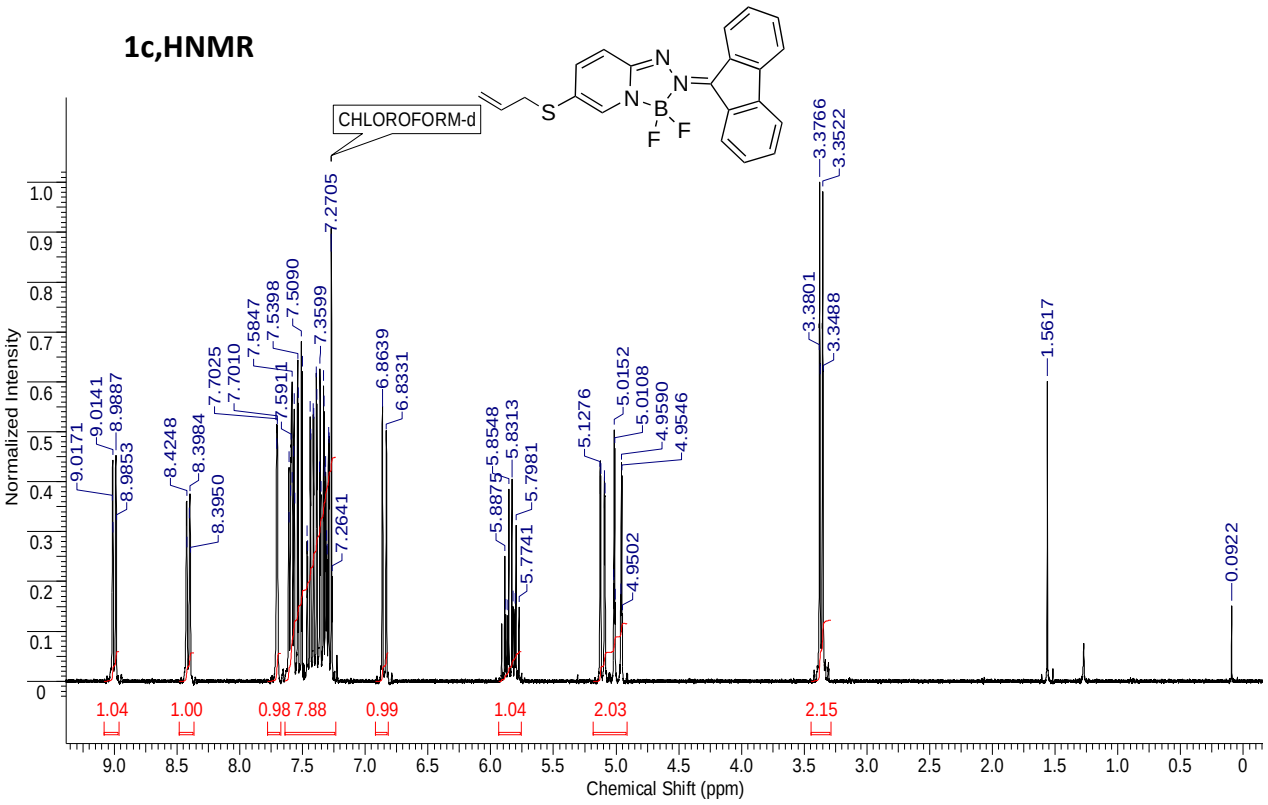

1a19FNMR
C6F6
162.9000
150.0549
150.1654
150.2790
150.3895
Normalized Intensity
Chemical Shift (ppm)

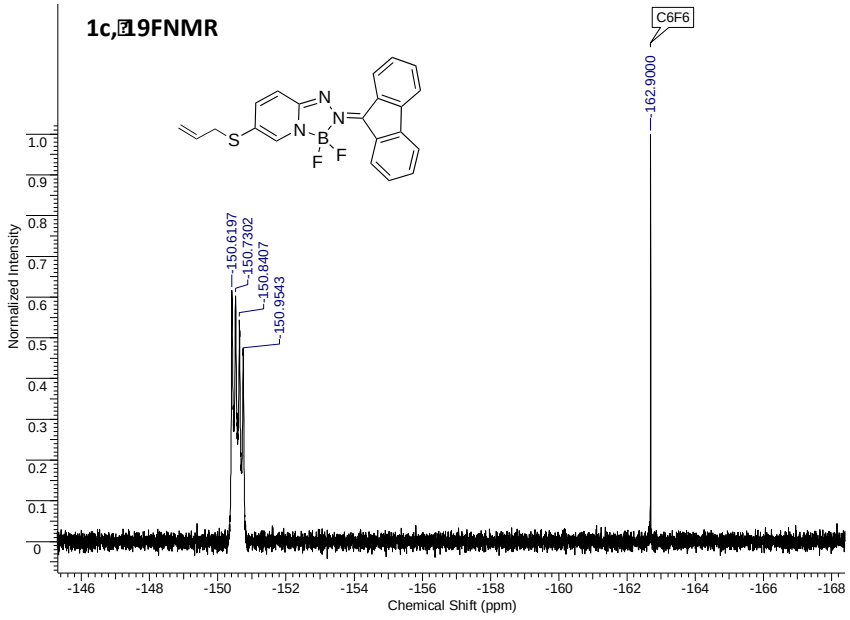

1a13CNMR
CHLOROFORM-d
77.4235
77.0000
76.5765
159.1802
150.6134
148.3881
141.7790
141.6787
141.0583
132.6103
132.1014
131.6258
131.0500
128.5795
128.4309
126.6923
126.5660
126.4397
120.0572
119.6969
115.2054
70.1309
Normalized Intensity
Chemical Shift (ppm)


1b,HNMR
Normalized Intensity
Chemical Shift (ppm)
CHLOROFORM-d
9.0448
9.0258
8.4374
8.4179
7.7260
7.7026
7.6245
7.6064
7.6054
7.3701
7.2705
6.9541
6.9307
6.5664
6.5391
6.5225
6.4951
5.6172
5.5738
5.2457
5.2178
1.5500
0.0134
1.00
1.07
1.08
4.59
0.94
0.97
0.98
1.00

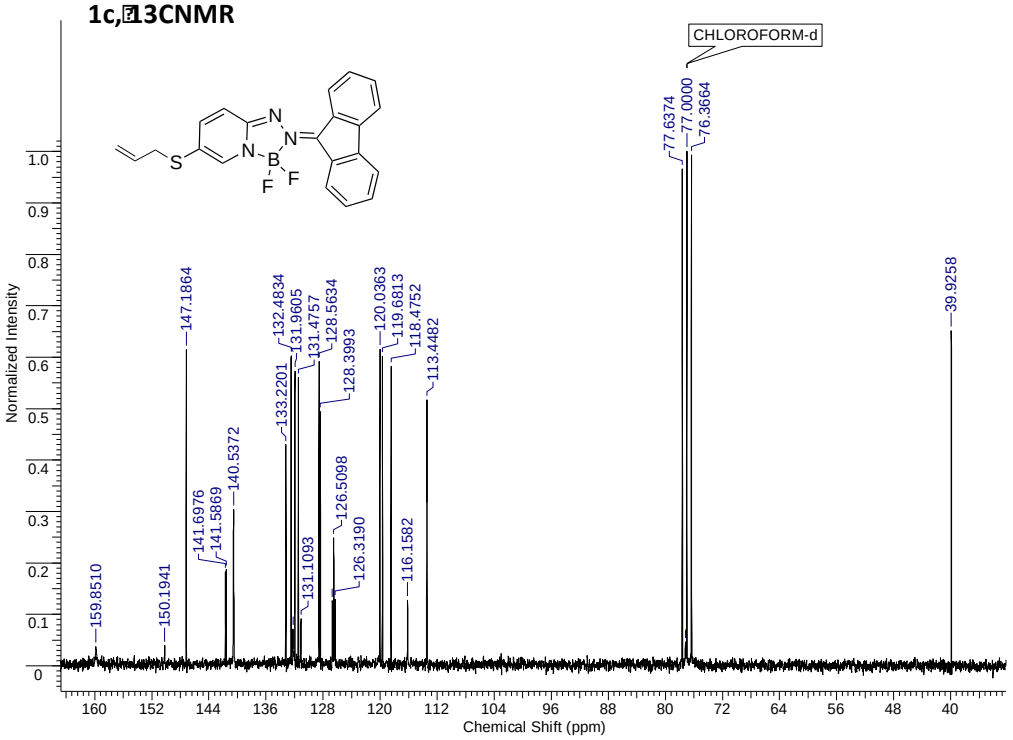

1b,19FNMR
Normalized Intensity
Chemical Shift (ppm)
C6F6
-162.9000
-151.0432
-151.1476
-151.1599
-151.2704
-151.3778


1b,13CNMR
CHLOROFORM-d
77.6336
77.0000
76.3626
160.1106
149.6483
141.5792
141.4762
138.1363
134.0331
132.3040
131.8345
131.4490
131.2696
129.0558
128.5405
126.5862
126.2121
128.3573
122.0402
120.0096
119.6546
113.6390
112.7115
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
168
160
152
144
136
128
120
112
104
96
88
80
72
Chemical Shift (ppm)

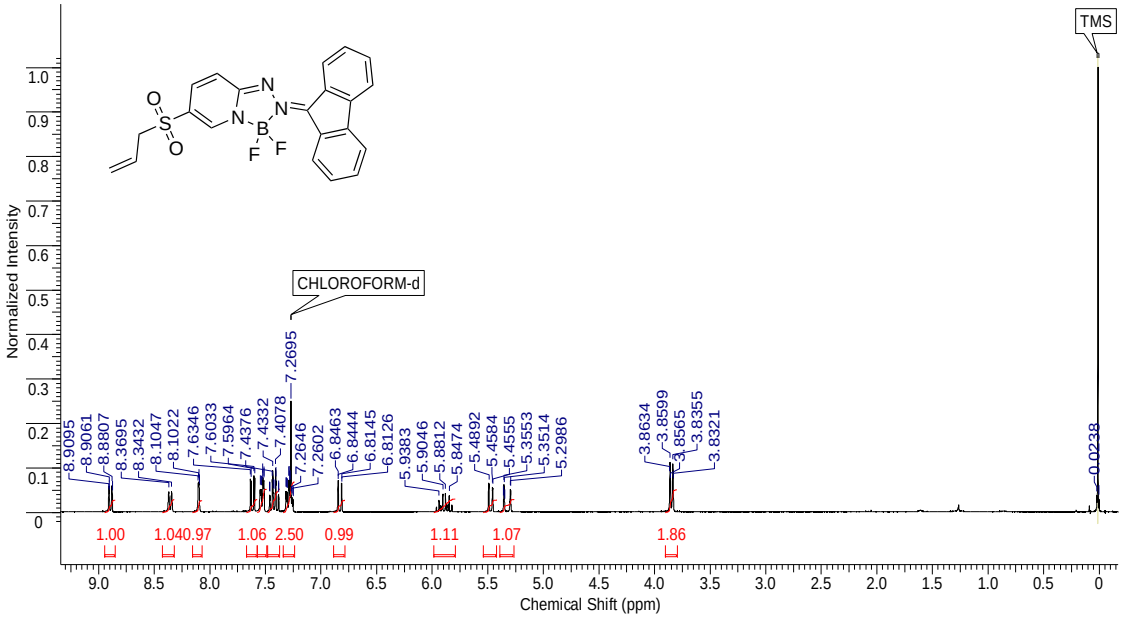

1c,HNMR
CHLOROFORM-d
Normalized Intensity
Chemical Shift (ppm)
9.0171
9.0141
8.9887
8.9853
8.4248
8.3984
8.3950
7.7025
7.7010
7.5911
7.5847
7.5398
7.5090
7.3599
7.2705
7.2641
6.8639
6.8331
5.8875
5.8548
5.8313
5.7981
5.7741
5.1276
5.0152
5.0108
4.9590
4.9546
4.9502
3.3766
3.3522
3.3801
3.3488
1.5617
0.0922
1.04
1.00
0.98
7.88
0.99
1.04
2.03
2.15

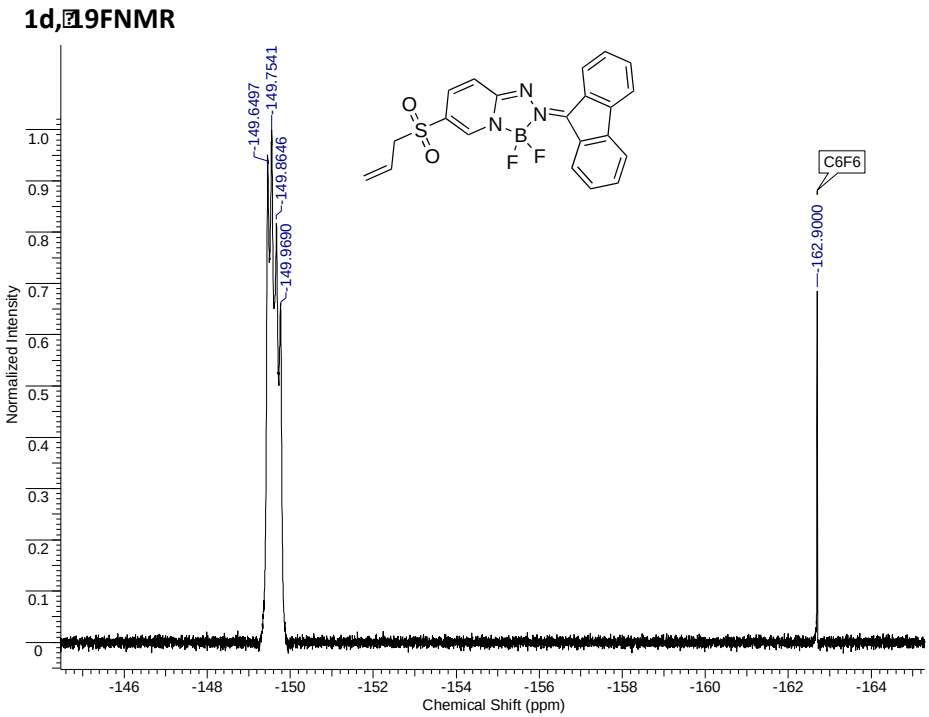

1c,19FNMR
C6F6
Normalized Intensity
Chemical Shift (ppm)
150.6197
150.7302
150.8407
150.9543
162.9000

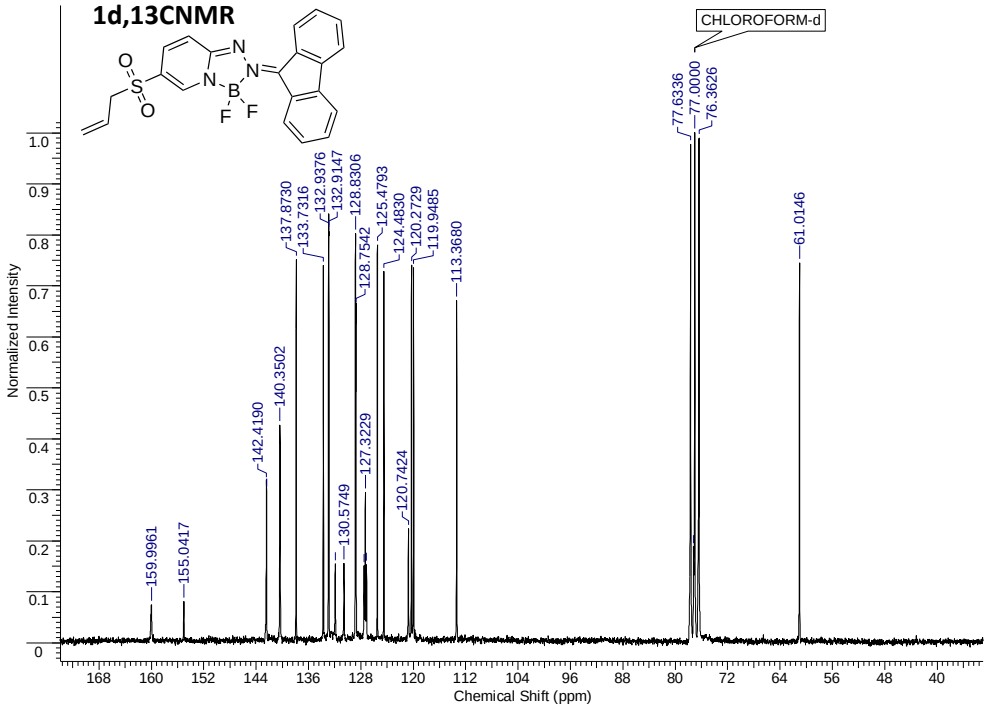
1c,13CNMR



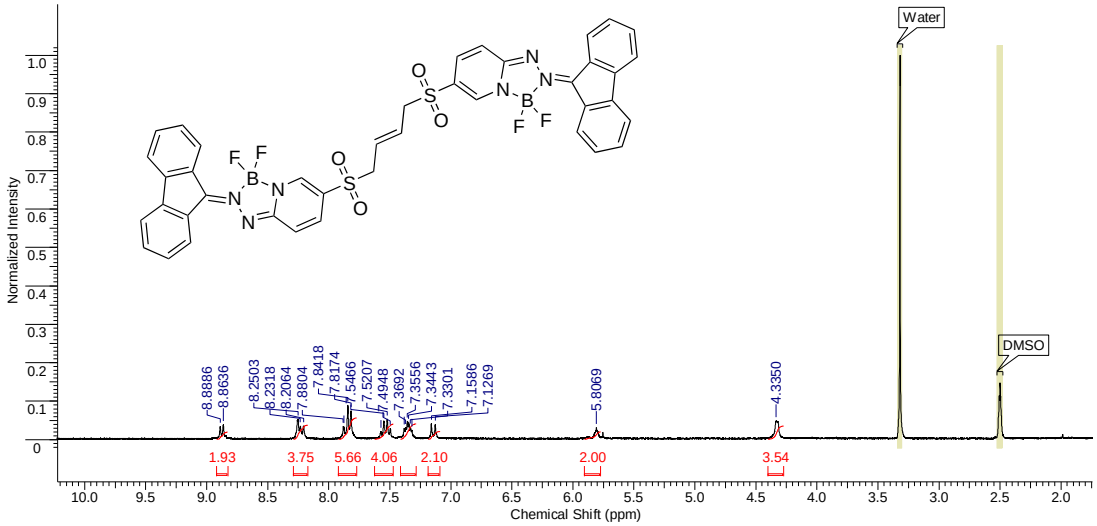
1d,HNMR



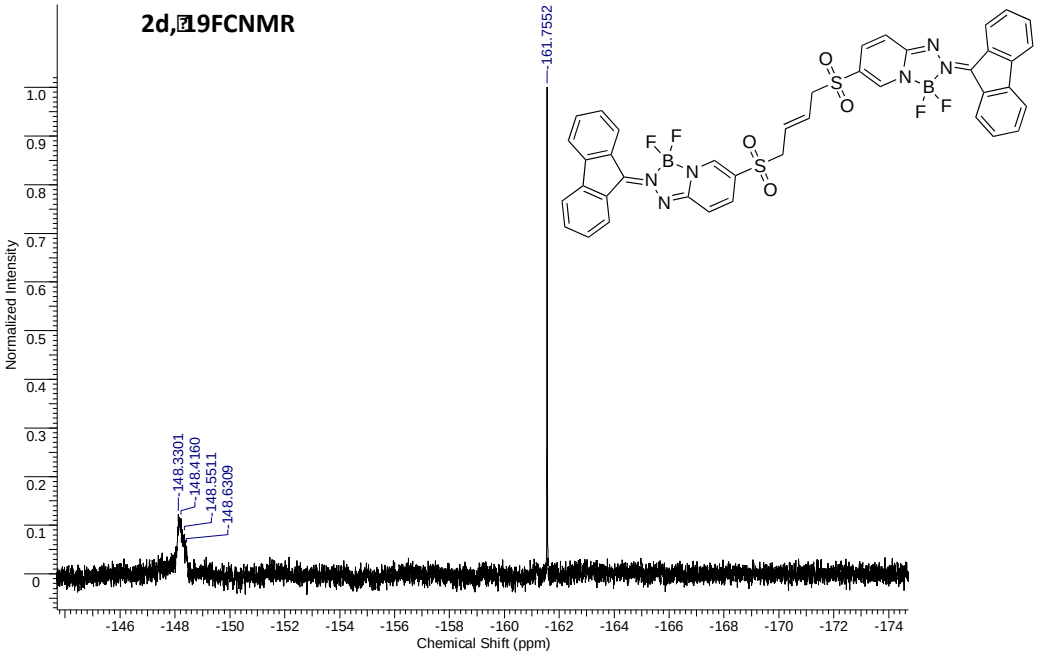

1d,19FNMR
149.6497
149.7541
149.8646
149.9690
162.9000
C6F6
Normalized Intensity
Chemical Shift (ppm)


1d,13CNMR
CHLOROFORM-d
77.6336
77.0000
76.3626
61.0146
137.8730
133.7316
132.9376
132.9147
128.8306
128.7542
125.4793
124.4830
120.2729
119.9485
113.3680
142.4190
140.3502
130.5749
127.3229
120.7424
159.9961
155.0417
Normalized Intensity
Chemical Shift (ppm)

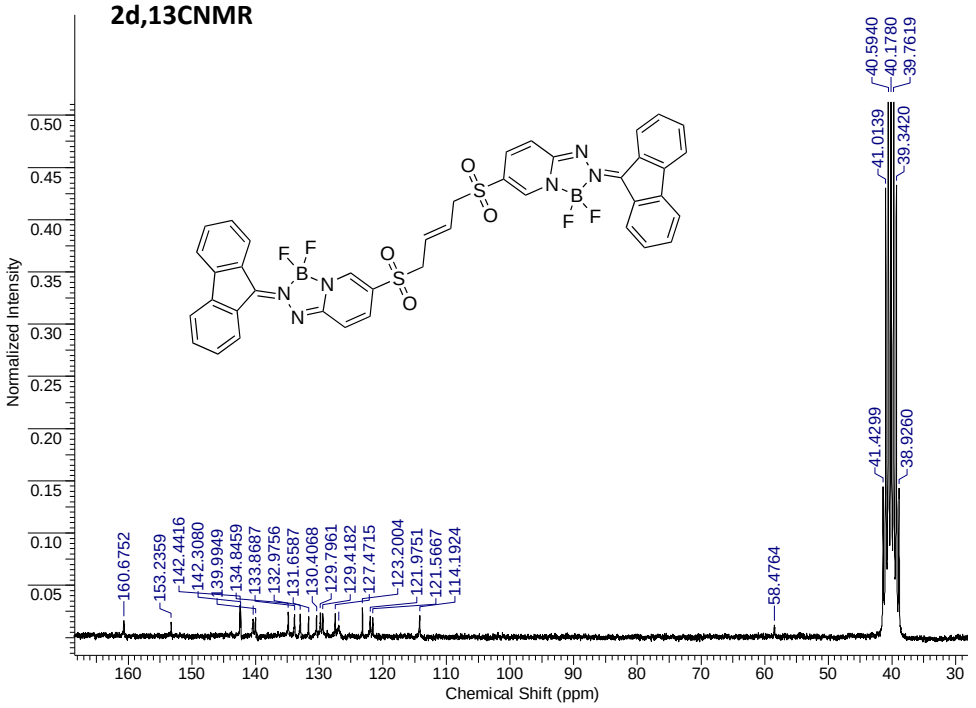
2d,HNMR



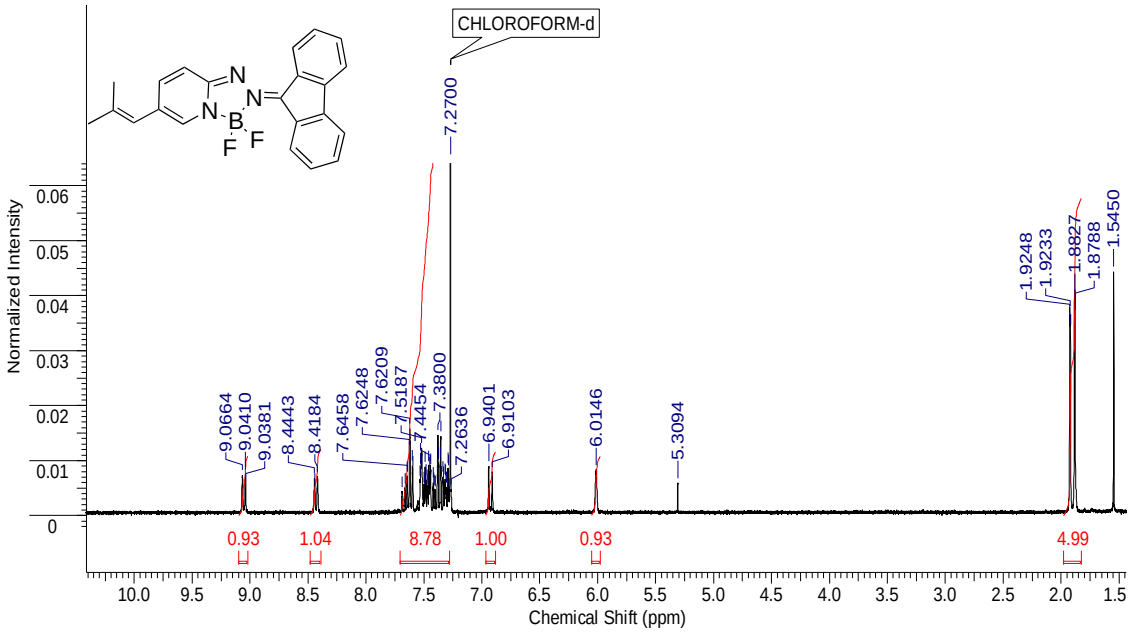
2d,19FCNMR

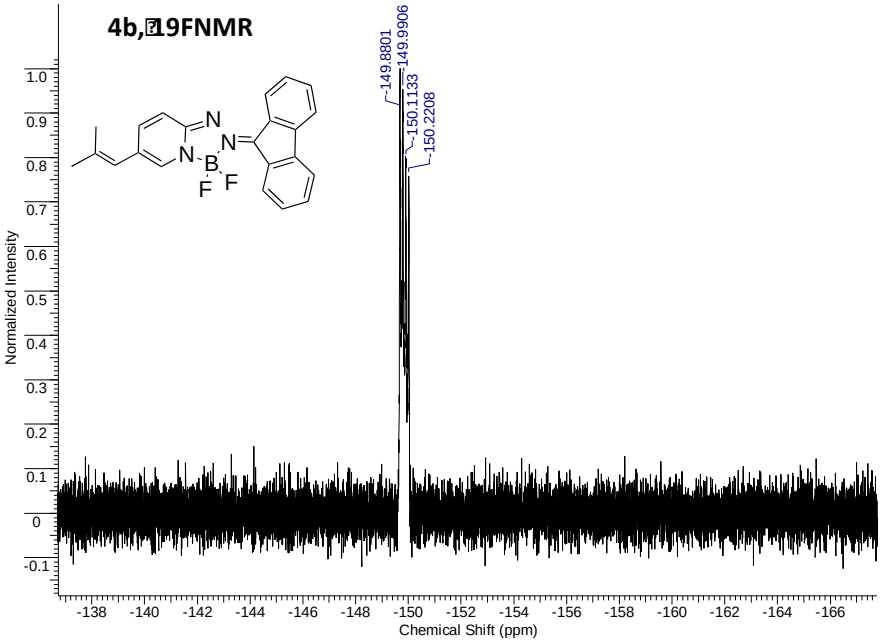


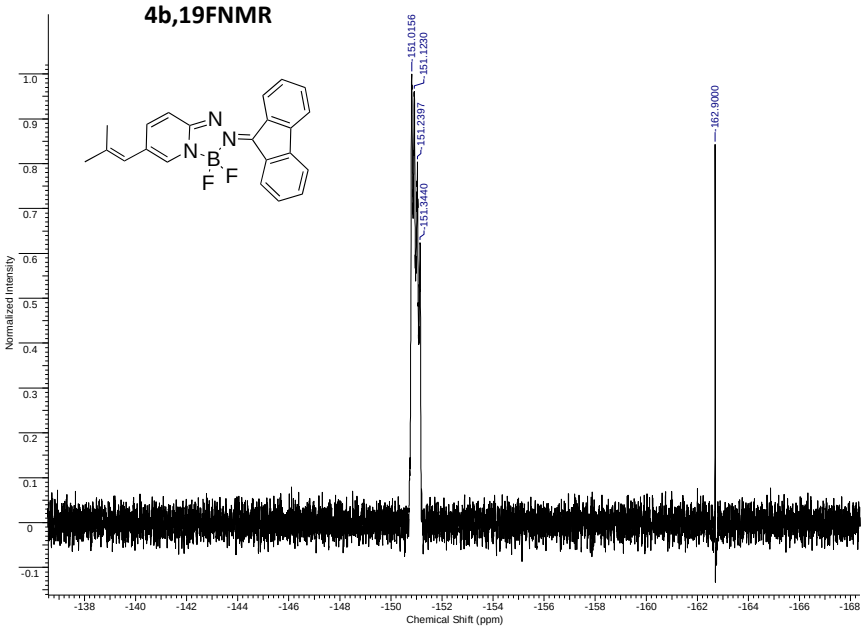
2d,13CNMR

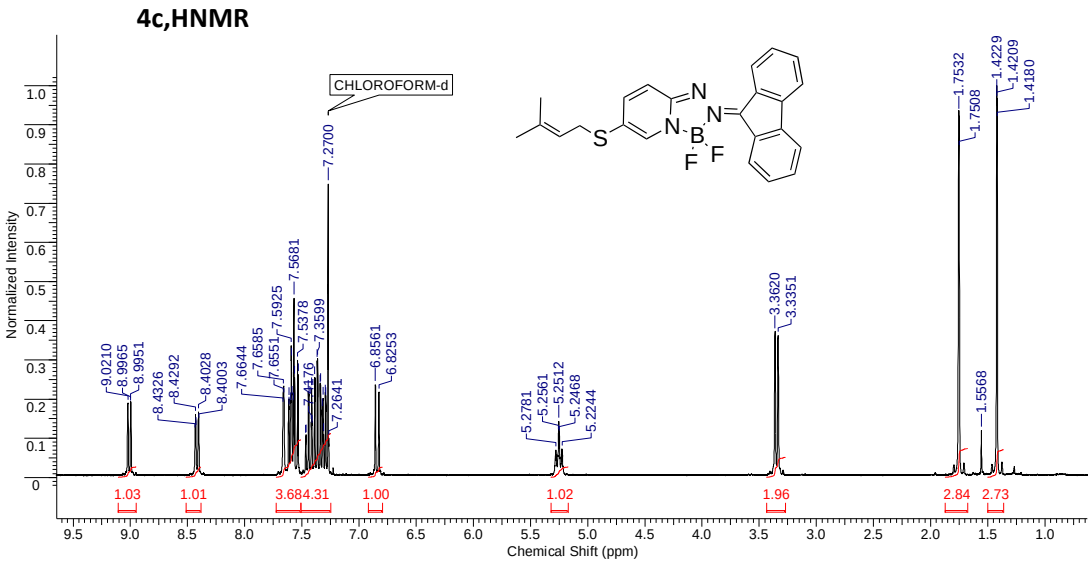


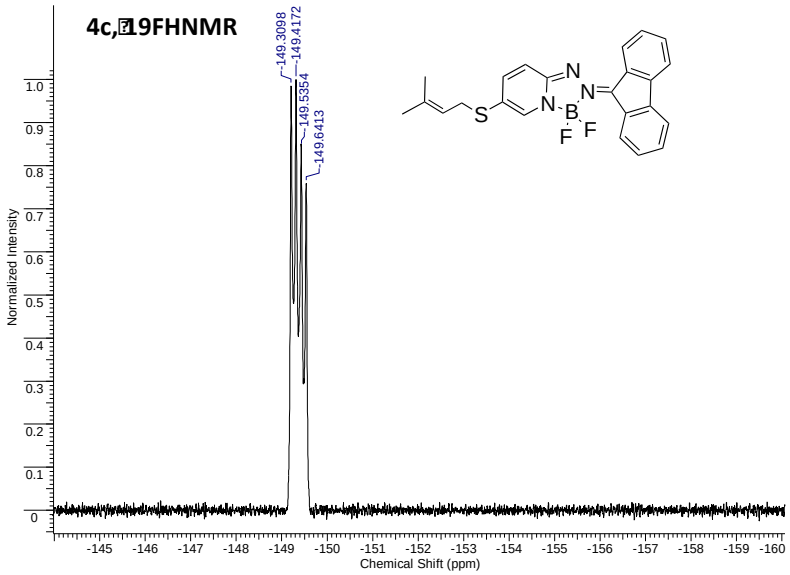
4b,HNMR

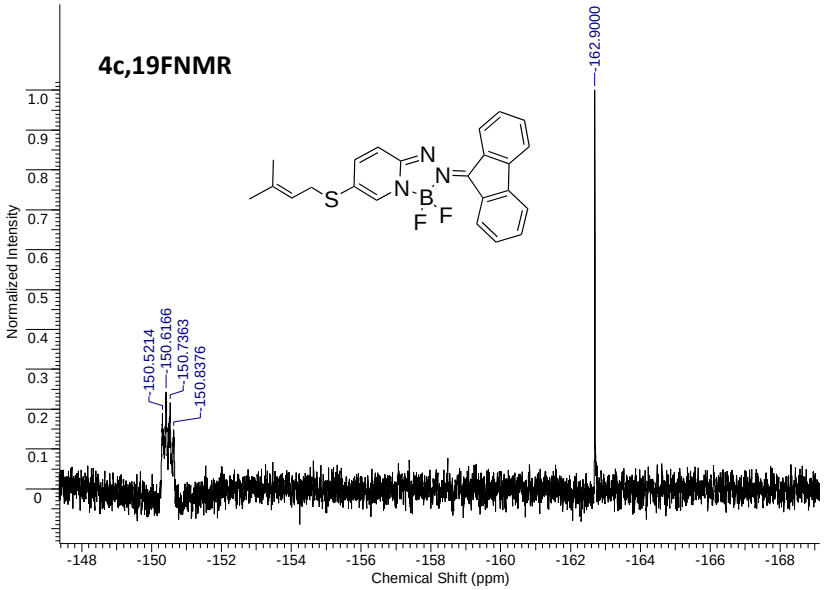


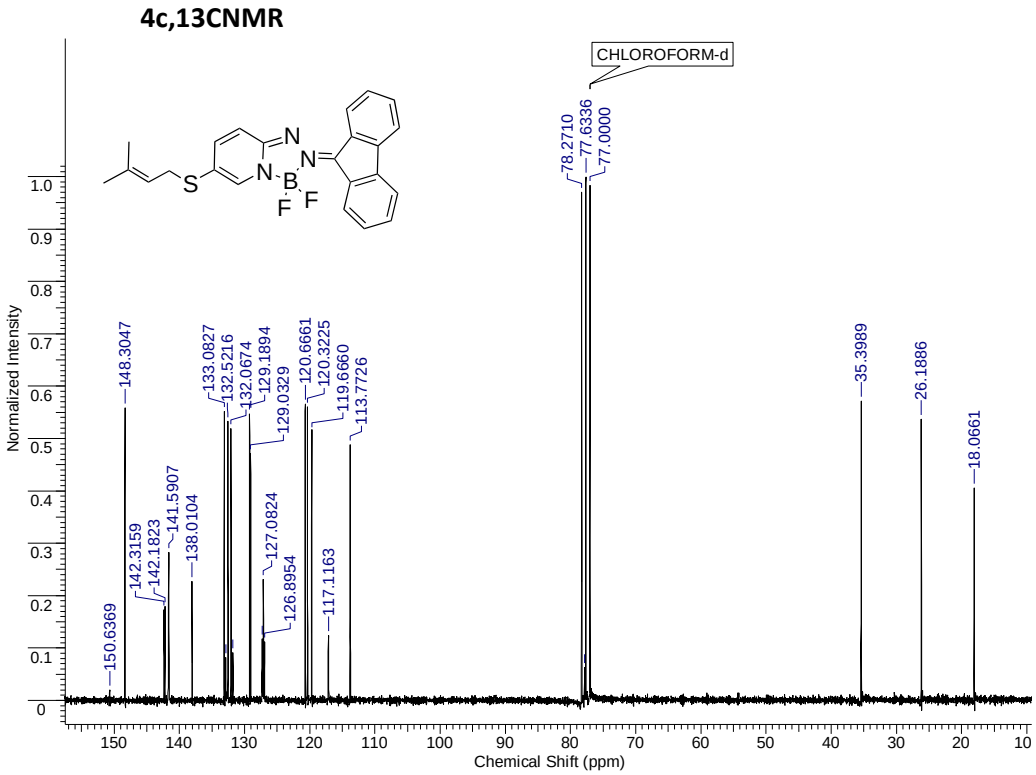

4b,19FNMR
-149.8801
-149.9906
-150.1133
-150.2208
Normalized Intensity
Chemical Shift (ppm)

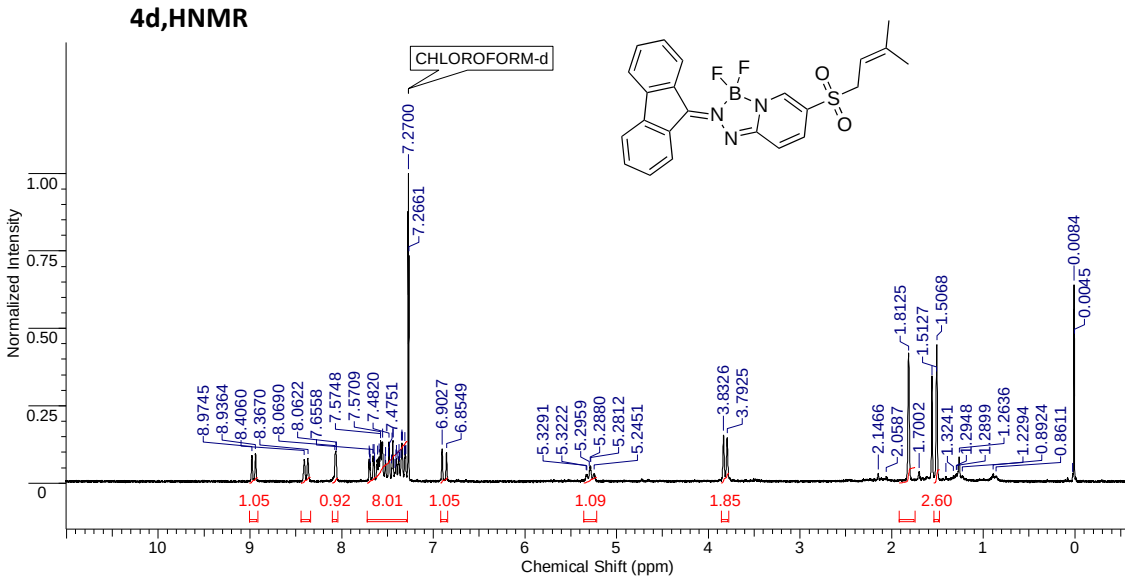

4b,19FNMR
-151.0156
-151.1230
-151.2397
-151.3440
-162.9000
Normalized Intensity
Chemical Shift (ppm)

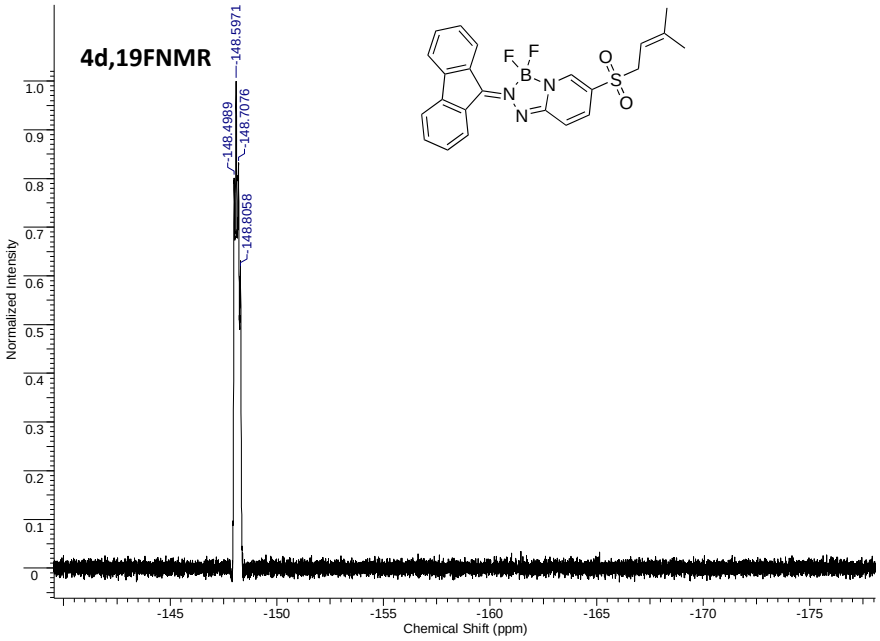

4c,HNMR
CHLOROFORM-d
Normalized Intensity
Chemical Shift (ppm)
9.0210
8.9965
8.9951
8.4326
8.4292
8.4028
8.4003
7.6644
7.6585
7.6551
7.5925
7.5681
7.5378
7.3599
7.2700
7.2641
6.8561
6.8253
5.2781
5.2561
5.2512
5.2468
5.2244
3.3620
3.3351
1.7532
1.7508
1.5568
1.4229
1.4209
1.4180
1.03
1.01
3.68
4.31
1.00
1.02
1.96
2.84
2.73

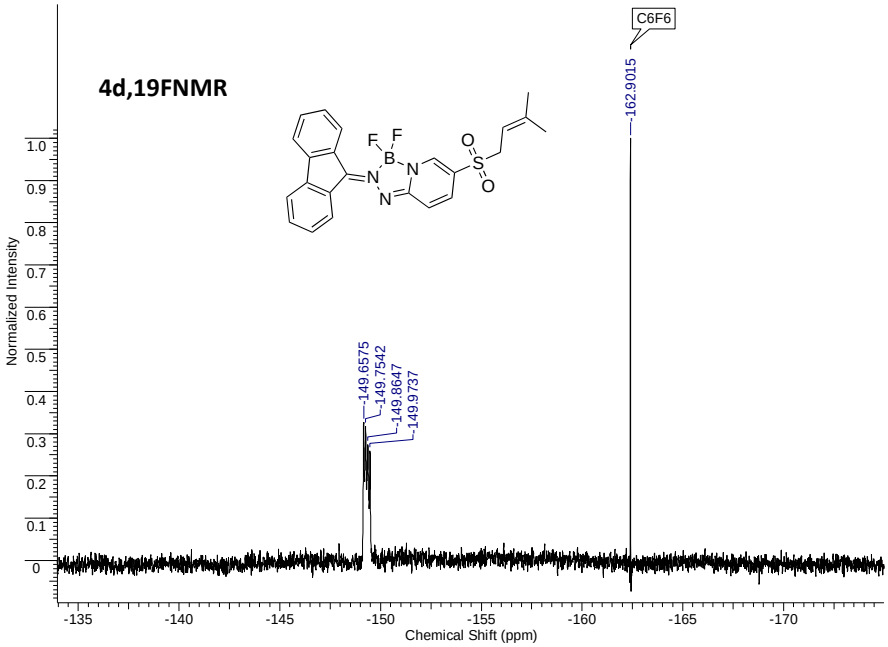

4c,19FHNMR
Normalized Intensity
Chemical Shift (ppm)
-149.3098
-149.4172
-149.5354
-149.6413

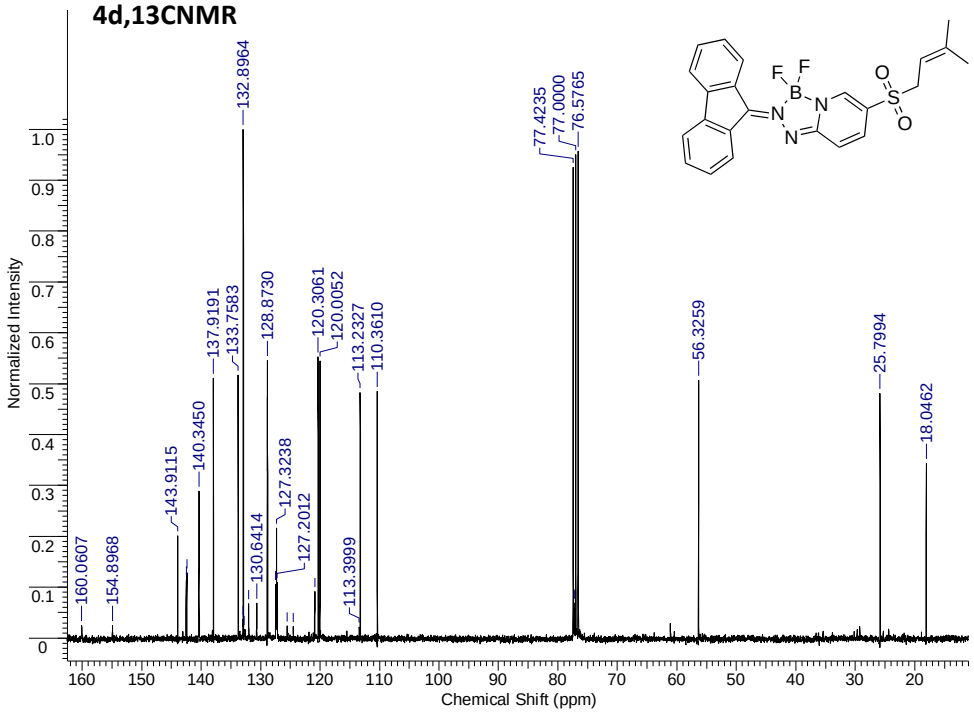

4c,19FNMR
162.9000
150.5214
150.6166
150.7363
150.8376
Normalized Intensity
Chemical Shift (ppm)

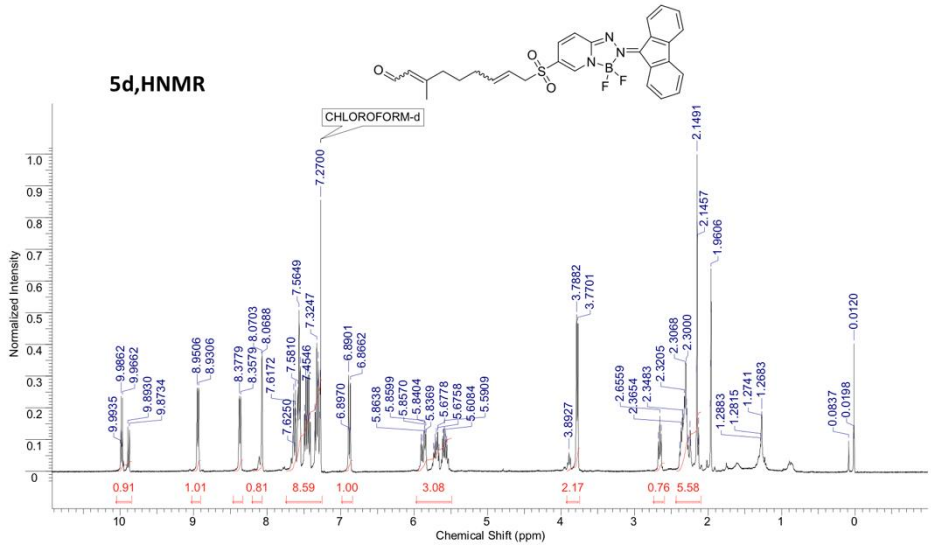

4c,13CNMR
CHLOROFORM-d
78.2710
77.6336
77.0000
148.3047
142.3159
142.1823
141.5907
138.0104
133.0827
132.5216
132.0674
129.1894
129.0329
127.0824
126.8954
120.6661
120.3225
119.6660
117.1163
113.7726
150.6369
35.3989
26.1886
18.0661
Normalized Intensity
Chemical Shift (ppm)

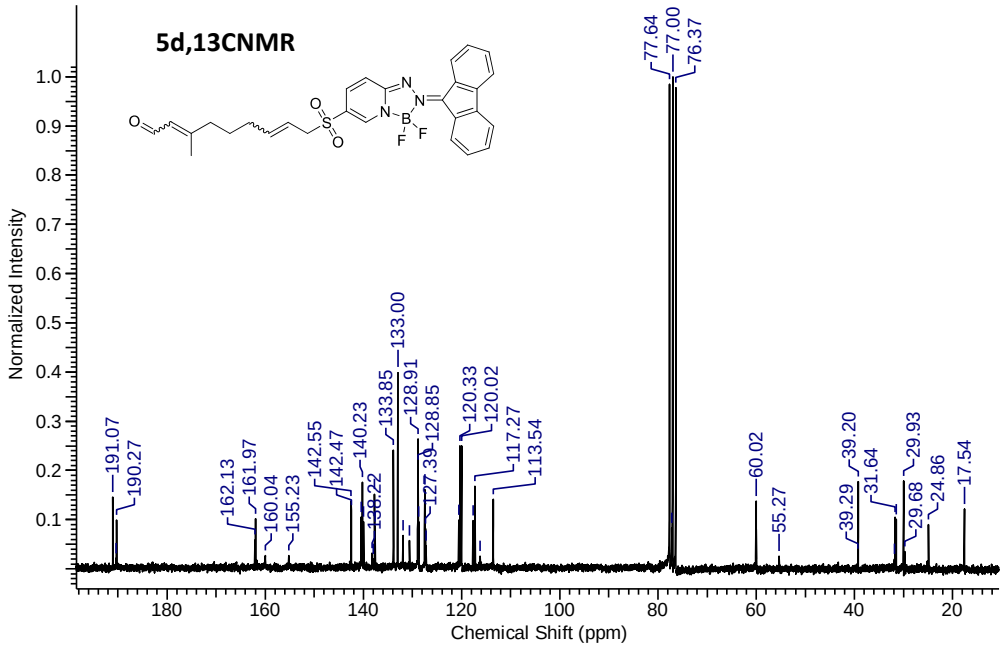

4d,HNMR
CHLOROFORM-d
Normalized Intensity
Chemical Shift (ppm)
7.2700
7.2661
8.9745
8.9364
8.4060
8.3670
8.0690
8.0622
7.6558
7.5748
7.5709
7.4820
7.4751
6.9027
6.8549
5.3291
5.3222
5.2959
5.2880
5.2812
5.2451
3.8326
3.7925
2.1466
2.0587
1.8125
1.7002
1.5127
1.5068
1.3241
1.2948
1.2899
1.2636
1.2294
0.8924
0.8611
0.0084
0.0045
1.05
0.92
8.01
1.05
1.09
1.85
2.60

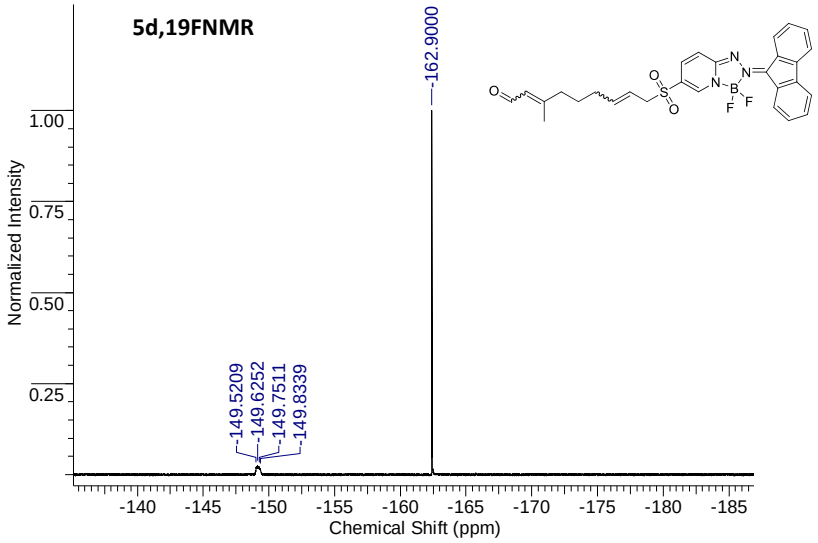

4d,19FNMR
Normalized Intensity
Chemical Shift (ppm)
148.5971
148.4989
148.7076
148.8058

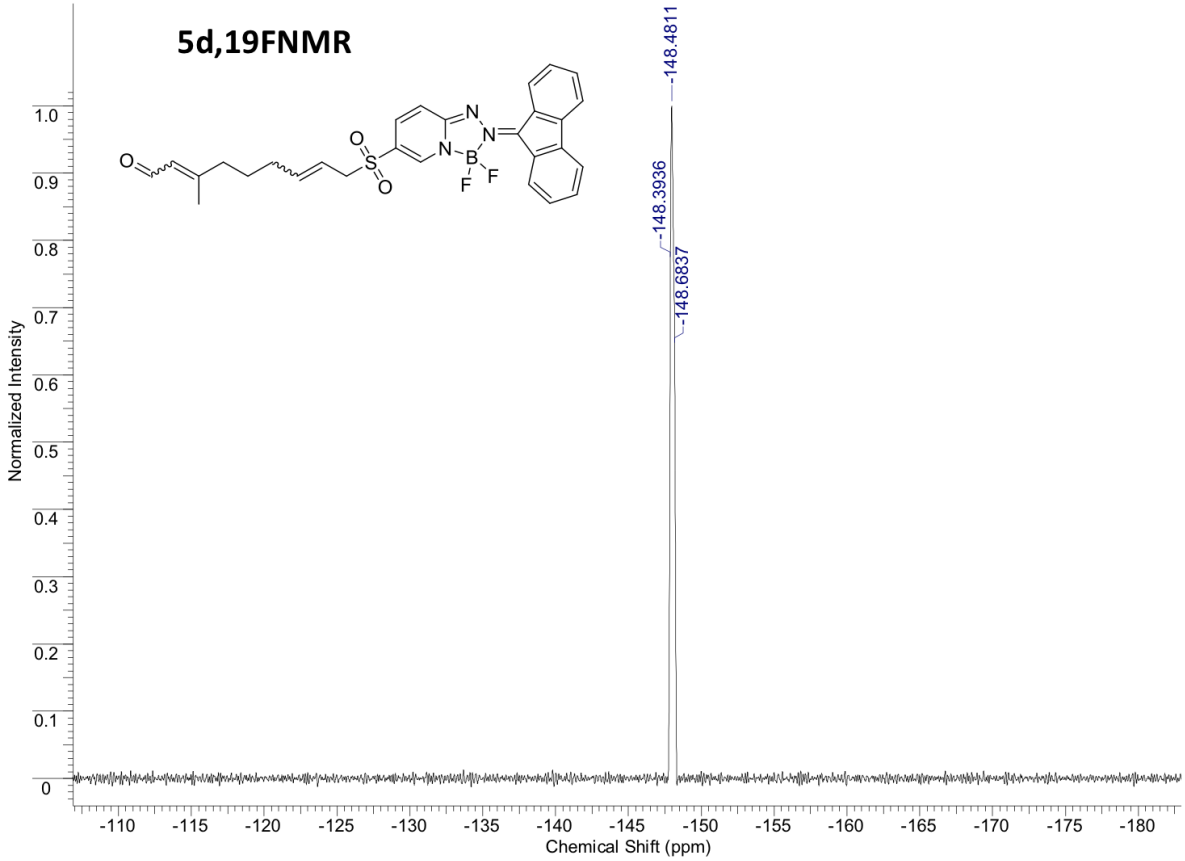

4d,19FNMR
C6F6
162.9015
149.6575
149.7542
149.8647
149.9737
Normalized Intensity
Chemical Shift (ppm)


4d,13CNMR
132.8964
77.4235
77.0000
76.5765
143.9115
140.3450
137.9191
133.7583
130.6414
128.8730
127.3238
127.2012
120.3061
120.0052
113.3999
113.2327
110.3610
160.0607
154.8968
56.3259
25.7994
18.0462
Normalized Intensity
Chemical Shift (ppm)

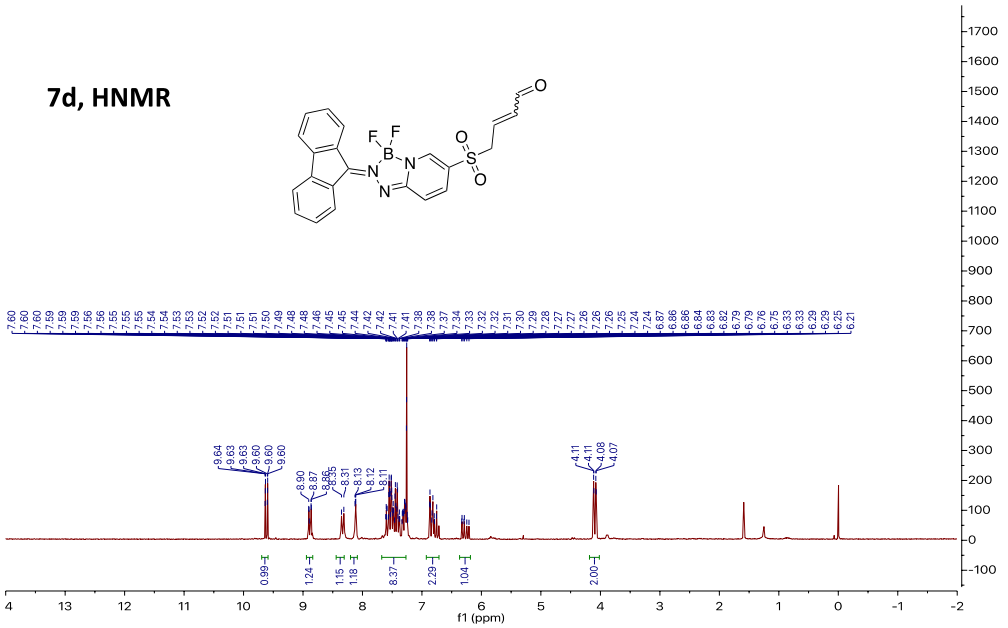

5d,HNMR
CHLOROFORM-d
Normalized Intensity
Chemical Shift (ppm)
0.91
1.01
0.81
8.59
1.00
3.08
2.17
0.76
5.58


5d,13CNMR
Normalized Intensity
Chemical Shift (ppm)
77.64
77.00
76.37
191.07
190.27
162.13
161.97
160.04
155.23
142.55
142.47
140.23
136.22
133.85
133.00
128.91
128.85
127.39
120.33
120.02
117.27
113.54
60.02
55.27
39.29
39.20
31.64
29.93
29.68
24.86
17.54

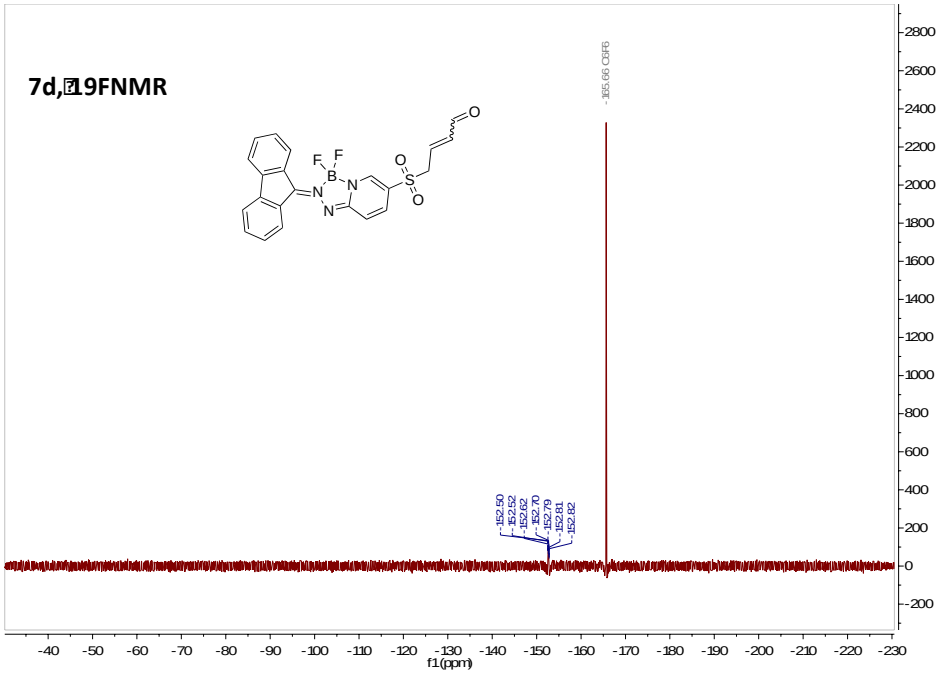

5d,19FNMR
-162.9000
-149.5209
-149.6252
-149.7511
-149.8339
Normalized Intensity
1.00
0.75
0.50
0.25
-140
-145
-150
-155
-160
-165
-170
-175
-180
-185
Chemical Shift (ppm)

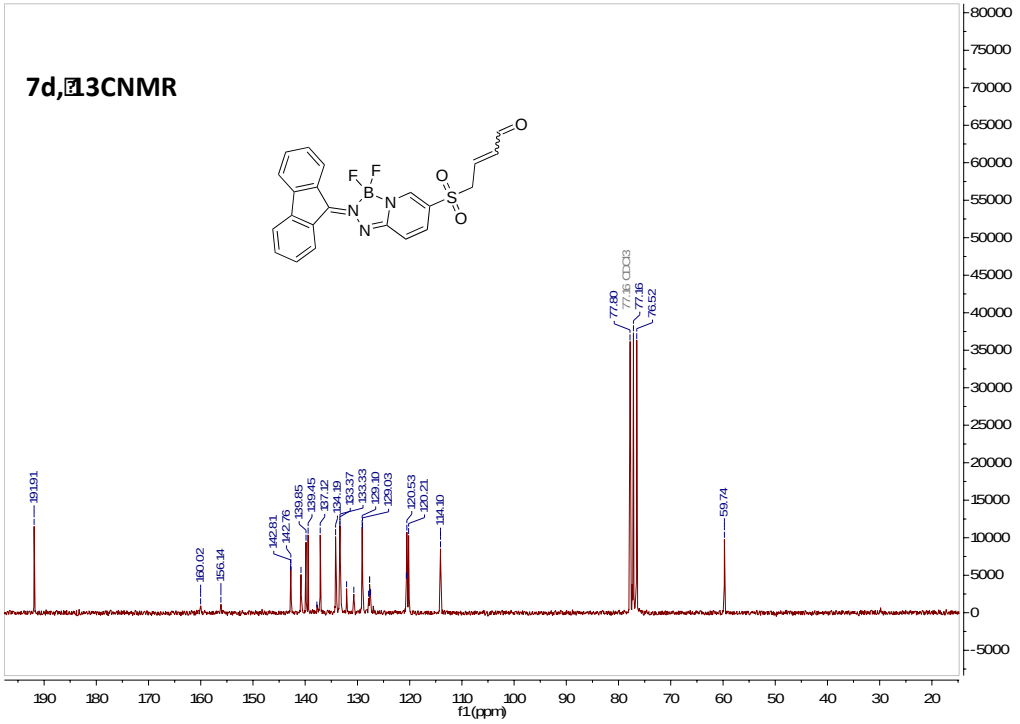

5d,19FNMR
-148.4811
-148.3936
-148.6837
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
-175
-180
Chemical Shift (ppm)

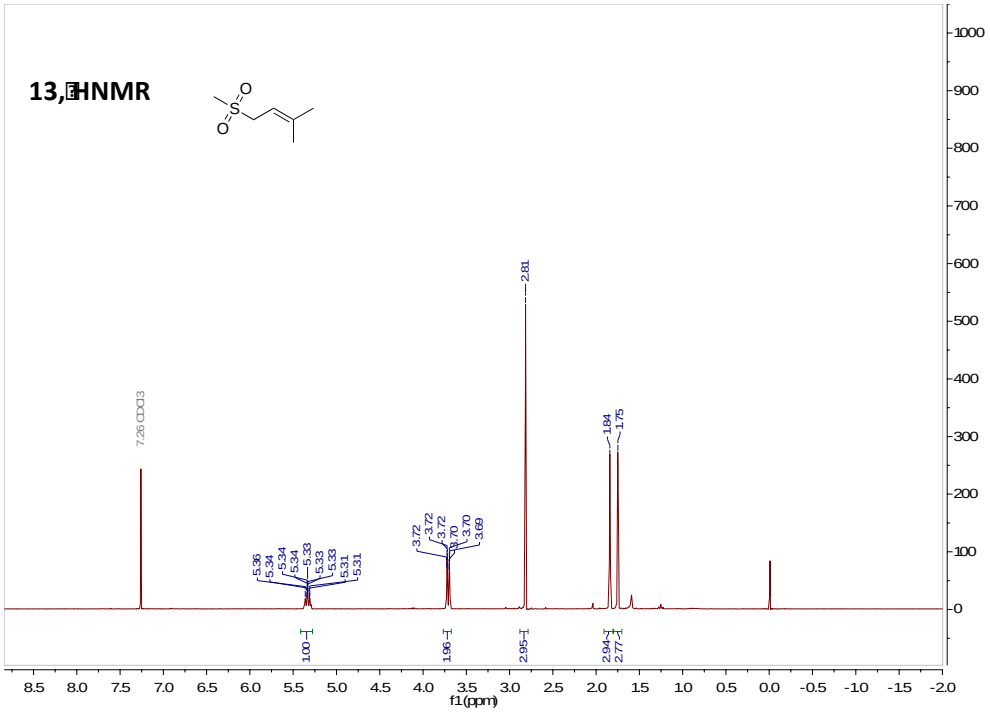
7d, HNMR

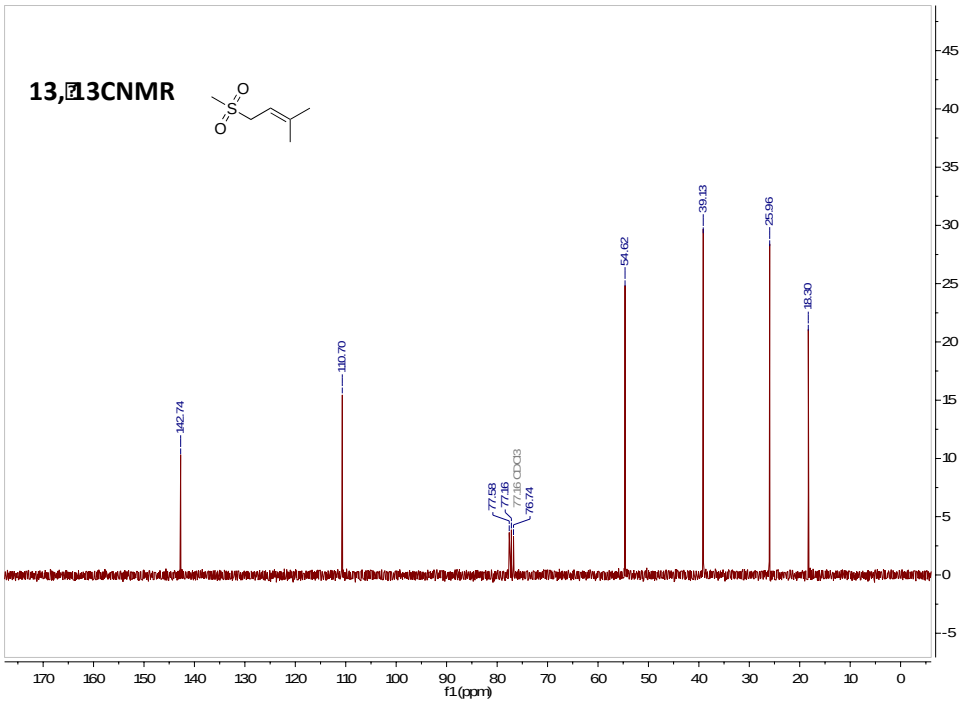


7d, 19FNMR

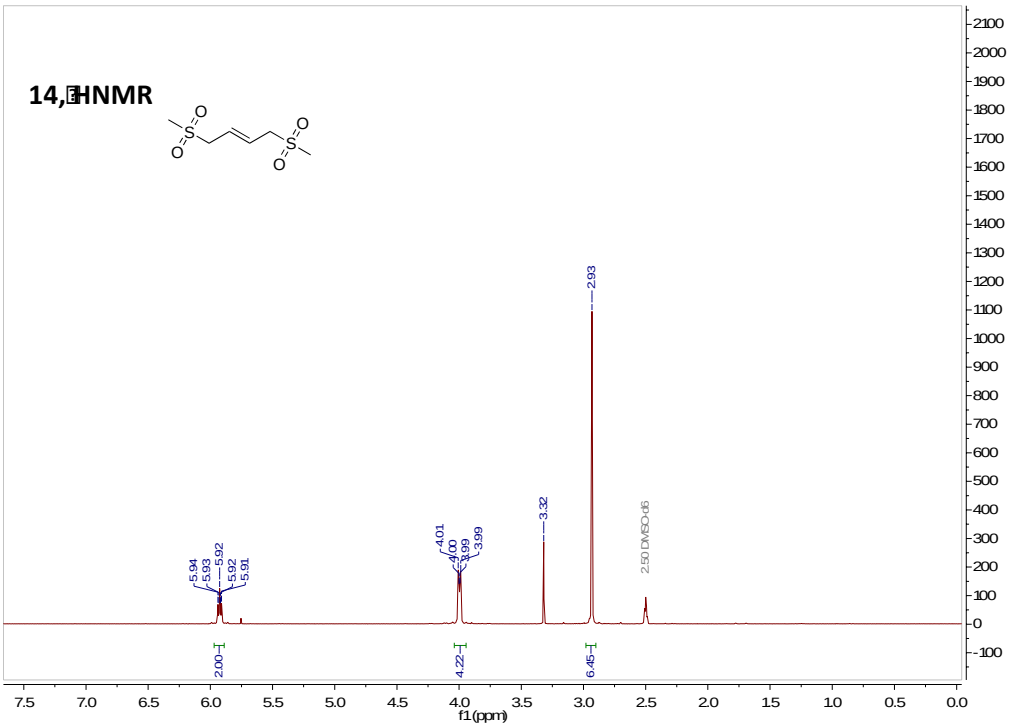



7d,13CNMR
F
F
B
N
N
N
O
S
O
O
77.80
77.16
CDCl3
77.16
76.52
191.91
160.02
156.14
142.81
142.76
139.85
139.45
137.12
134.19
133.37
133.33
129.10
129.03
120.53
120.21
114.10
59.74
f1 (ppm)

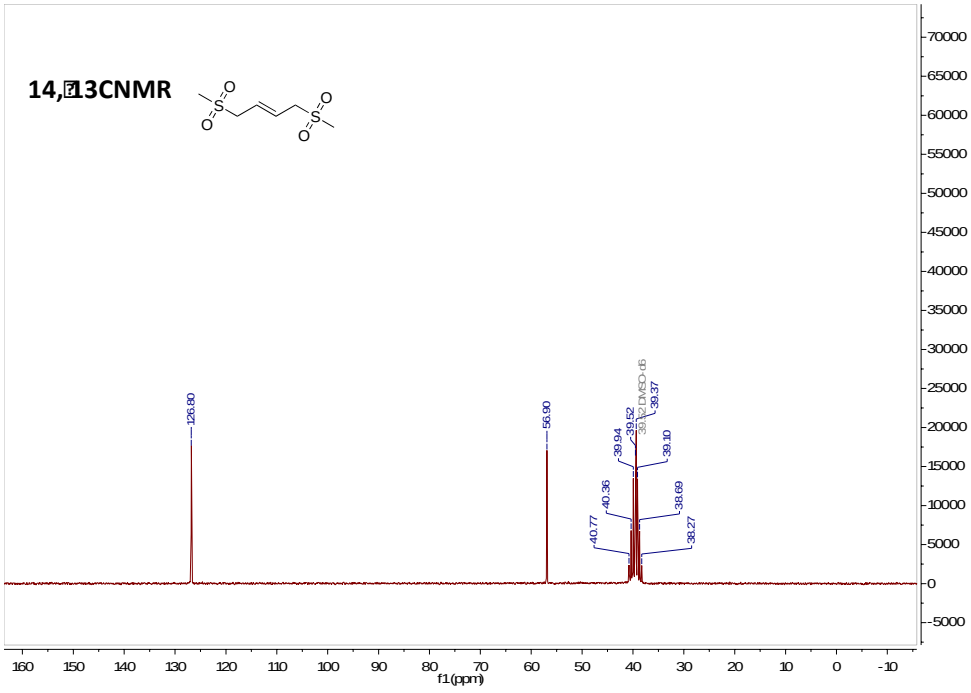

13,HNMR
7.26 CDCl3
5.36
5.34
5.34
5.34
5.33
5.33
5.33
5.31
5.31
3.72
3.72
3.72
3.70
3.70
3.69
2.81
1.84
1.75
1.00
1.96
2.95
2.94
2.77
f1 (ppm)


13,13CNMR
142.74
110.70
77.58
77.36
77.16 CDCl3
76.74
54.62
39.13
25.96
18.30
f1 (ppm)

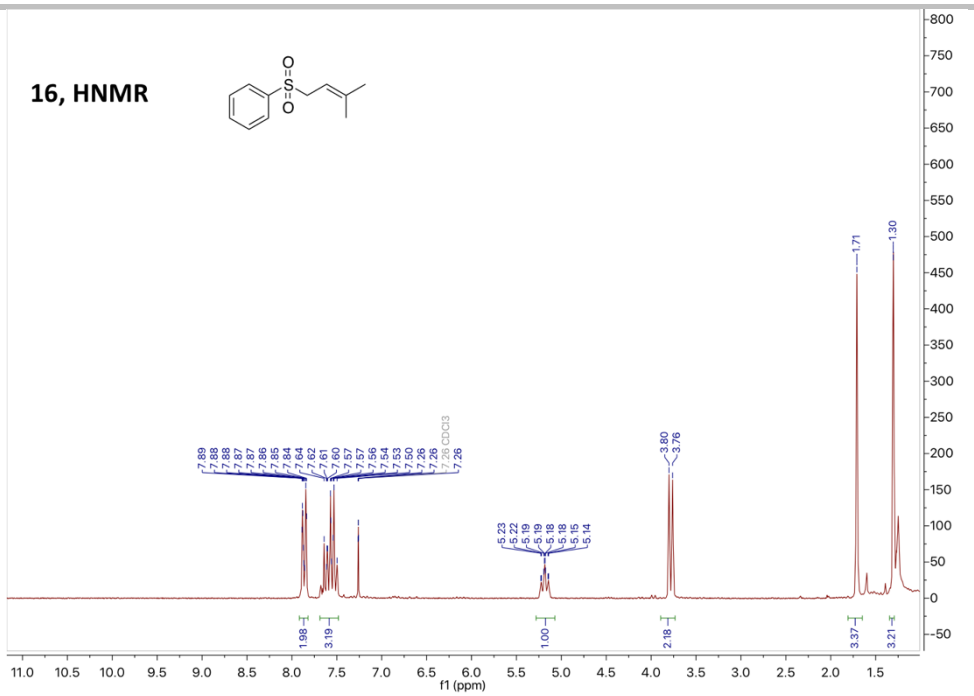
14, HNMR



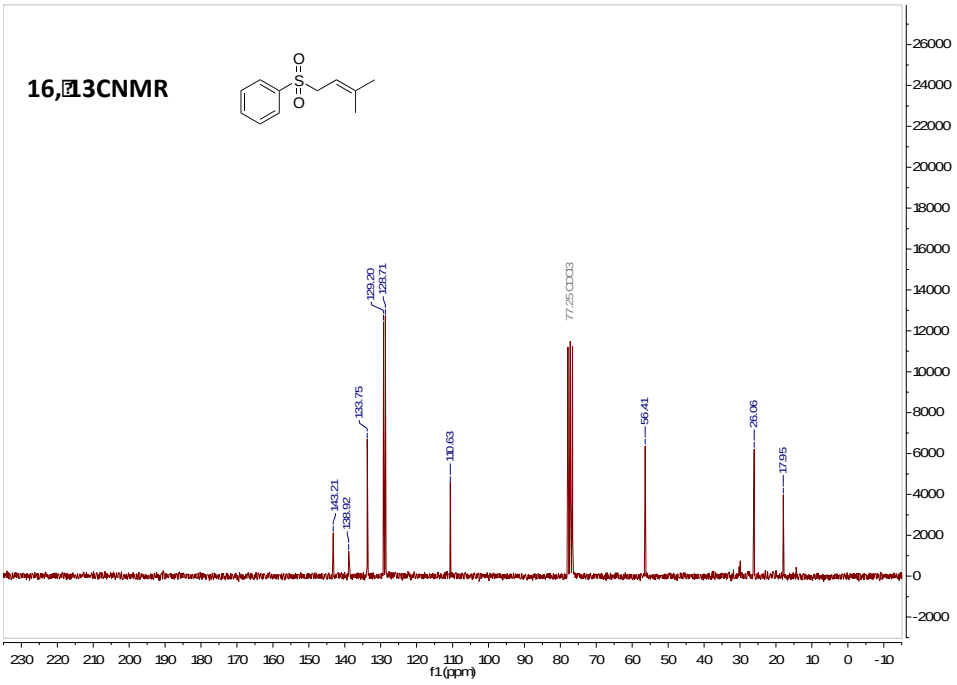
14, 13CNMR

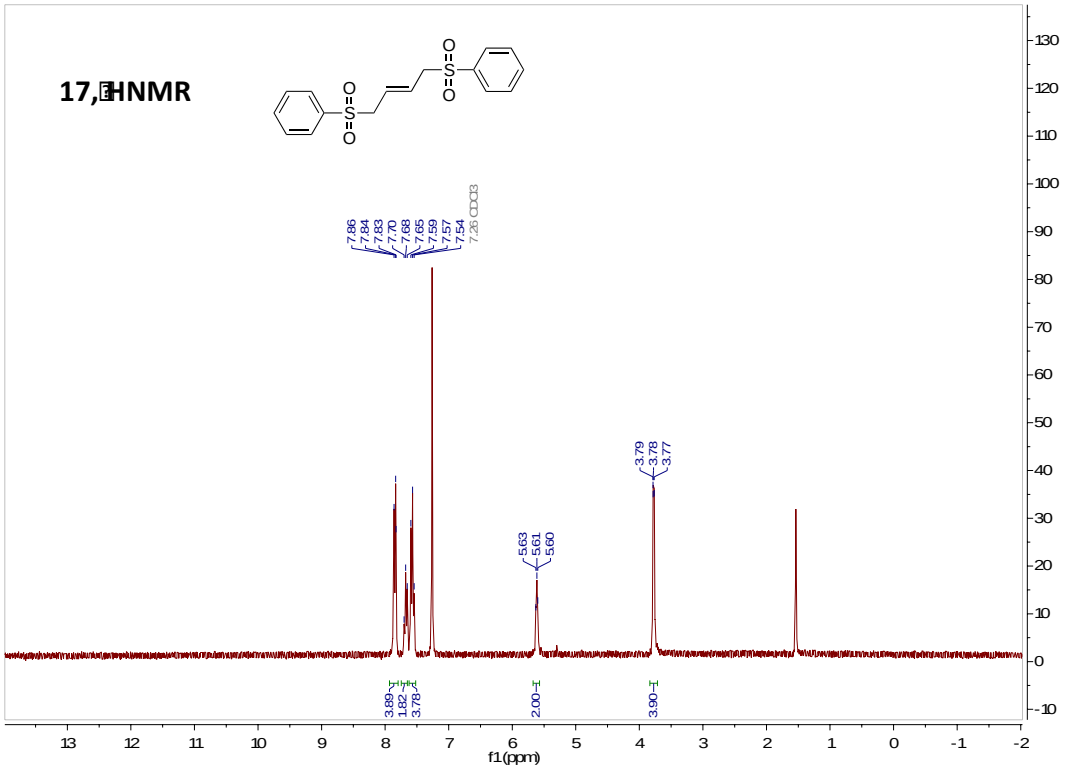


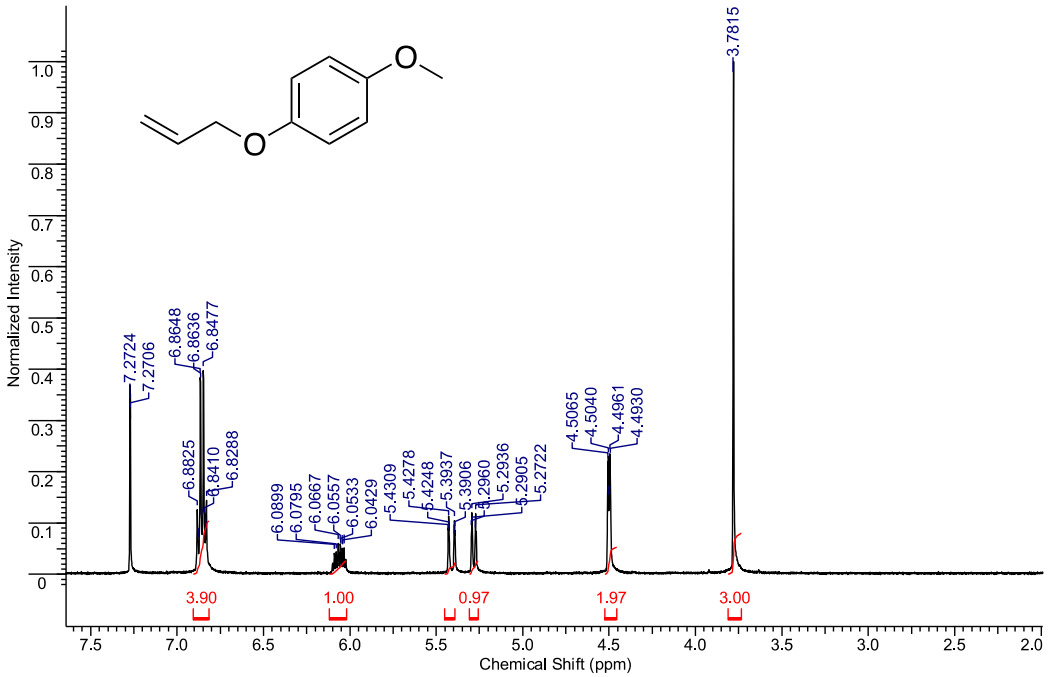
16, HNMR

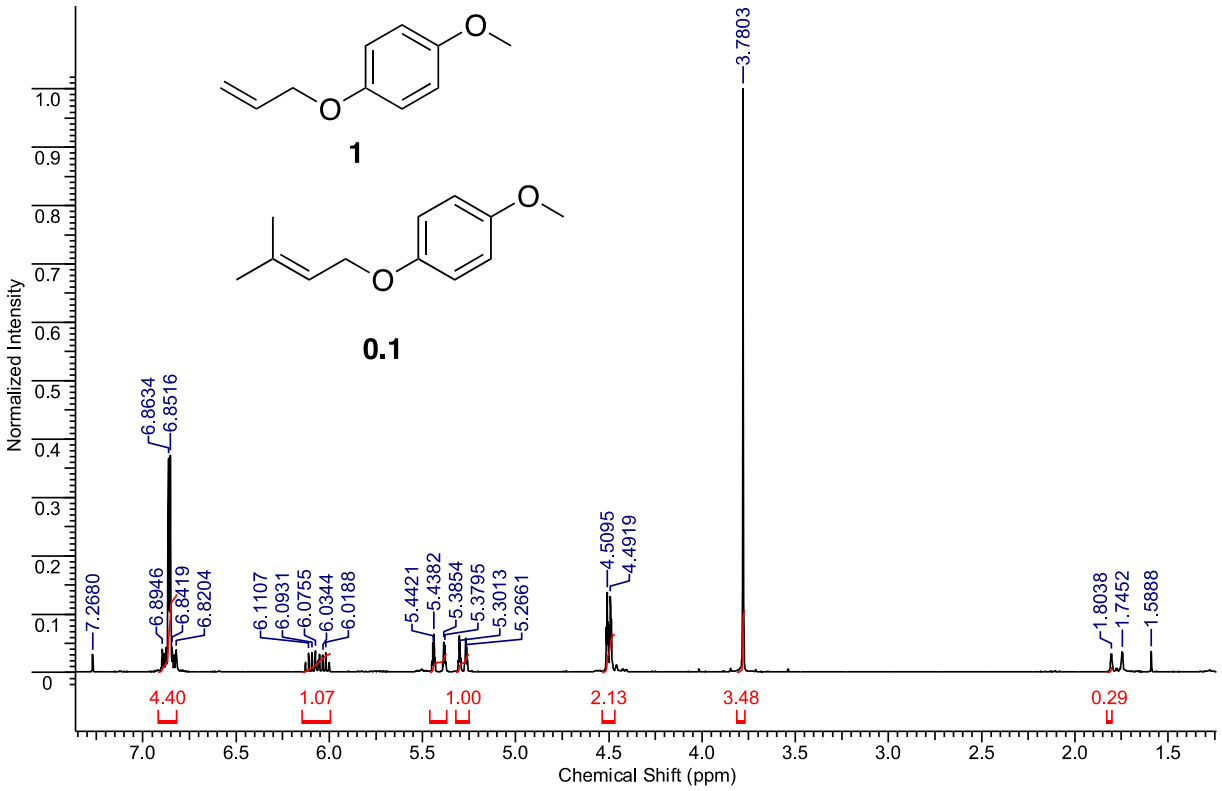


16, 13CNMR




17, HNMR
7.86
7.84
7.83
7.70
7.68
7.65
7.59
7.57
7.54
7.26 CDCl3
5.63
5.61
5.60
3.79
3.78
3.77
3.89
1.82
3.78
2.00
3.90
f1(ppm)


Normalized Intensity
7.2724
7.2706
6.8648
6.8636
6.8477
6.8825
6.8410
6.8288
6.0899
6.0795
6.0667
6.0557
6.0533
6.0429
5.4309
5.4278
5.4248
5.3937
5.3906
5.2960
5.2936
5.2905
5.2722
4.5065
4.5040
4.4961
4.4930
3.7815
3.90
1.00
0.97
1.97
3.00
Chemical Shift (ppm)


1
0.1
Normalized Intensity
Chemical Shift (ppm)
7.2680
6.8946
6.8634
6.8516
6.8419
6.8204
6.1107
6.0931
6.0755
6.0344
6.0188
5.4421
5.4382
5.3854
5.3795
5.3013
5.2661
4.5095
4.4919
3.7803
1.8038
1.7452
1.5888
4.40
1.07
1.00
2.13
3.48
0.29

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