

SUPPLEMENTARY INFORMATION

Atom-Economical Regioselective Ni-Catalyzed Hydroborylative Cyclization of Enynes: Development and Mechanism

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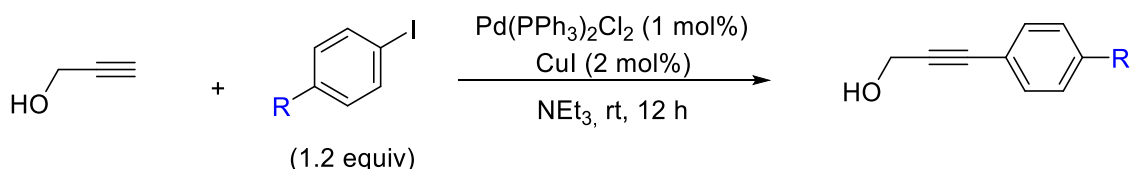
I. Materials and methods

The borylative cyclization reactions were carried out under argon atmosphere in anhydrous toluene stored over activated molecular sieves 4 Å (VWR) and Ar-degassed. Triethylamine, acetone and acetonitrile (VWR) were used as purchased. Pinacolborane (HBpin) was purchased from Sigma-Aldrich Co. The other commercially available chemicals were purchased and used as received without further purifications.

Thin layer chromatography was carried out using pre-coated TLC-aluminum sheets with 0.20 mm of silica gel and fluorescent indicator UV₂₅₄ (ALUGRAM® Xtra SIL G/UV₂₅₄) and visualized under UV light and/or using phosphomolybdic acid or vanillin/conc. H₂SO₄ solutions in ethanol. Column chromatography was carried out using 60 Å pore size silica gel, 40 – 63 µm particle size (230 – 400 mesh particle size), from Sigma-Aldrich Co.

NMR spectra were recorded at 23 °C on a Bruker AV-300. The ¹H and the ¹³C NMR chemical shifts are given in parts per million (ppm) relative to the residual signals of the deuterated solvents.¹ Carbon types were determined from DEPT135-¹³C NMR. The following abbreviations are used to indicate the multiplicity: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; quin, quintuplet; m, multiplet. In some ¹³C NMR spectra, the carbon atoms bonded to the boron atoms were not observed due to line broadening.² Mass spectra were recorded on a Waters VG AutoSpec and GC-MS experiments on a Bruker SCION TQ.

II. General procedure for the synthesis of propargyl alcohols.³



To a solution of iodoarene (1.2 equiv, 9.8 mmol) in trimethylamine (0.34 M, 26 mL) was added Pd(PPh₃)₂Cl₂ (1 mol%, 0.9 mmol) and CuI (2 mol%, 0.18 mmol). The reaction was stirred for 5 min before the addition of propargyl alcohol (1.0 equiv., 8.9 mmol). The resulting mixture was stirred for 12 h. Then, the reaction was treated with a saturated NaHCO₃ solution. The solution was extracted with ethyl acetate (3 × 20 mL), washed with a saturated NaCl solution and dried over anhydrous MgSO₄. The solvent was removed under vacuum and the product was purified by column chromatography (cyclohexane/EtOAc, 9:1 – 7:3).

3-phenylprop-2-yn-1-ol:⁴ The product was obtained as a brown oil in 98% yield (1.15 g). ¹H NMR (300 MHz, CDCl₃) δ 7.39 (m, 2H), 7.26 (m, 3H), 4.45 (d, *J* = 6.2 Hz, 2H), 1.63 (t, *J* = 6.2 Hz, 1H).

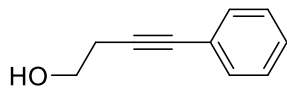
¹ H. E. Gottlieb, V. Kotlyar, A. Nudelman, *J. Org. Chem.* **1997**, 62, 7512 – 7515.

² A. Datta, A. Köllhofer, H. Plenio, *Chem. Commun.*, **2004**, 1508 – 1509.

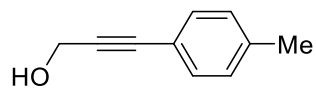
³ G.-Y. Lin, C.-Y. Yang, R.-S. Liu, *J. Org. Chem.*, **2007**, 72, 6753 – 6757.

⁴ S. Bong, H. Alper, *Chem. Commun.*, **2004**, 1306 – 1307.

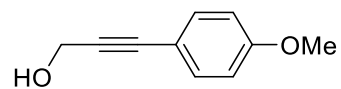
4-phenylbut-3-yn-1-ol:⁵ The product was obtained as a brown oil in 99% yield (1.1 g). ¹H NMR (300 MHz, CDCl₃) δ 7.46 – 7.38 (m, 2H), 7.33 – 7.28 (m, 3H), 3.82 (q, J = 6.3 Hz, 2H), 2.70 (t, J = 6.3 Hz, 2H), 1.81 (t, J = 6.3 Hz, 1H).



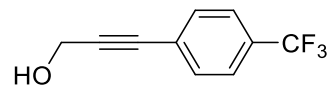
3-(p-tolyl)prop-2-yn-1-ol:⁶ The product was obtained as a yellow oil in 63% yield (820 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.28 (d, J = 7.8 Hz, 2H), 7.06 (d, J = 7.8 Hz, 2H), 4.43 (d, J = 6.1 Hz, 2H), 2.29 (s, 3H), 1.58 (t, J = 6.1 Hz, 1H).



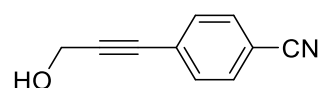
3-(4-methoxyphenyl)prop-2-yn-1-ol:⁷ The product was obtained as a yellow oil in 61% yield (882 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.38 (d, J = 8.9 Hz, 2H), 6.84 (d, J = 8.9 Hz, 2H), 4.48 (d, J = 6.1 Hz, 2H), 3.81 (s, 3H), 1.64 (t, J = 6.1 Hz, 2H).



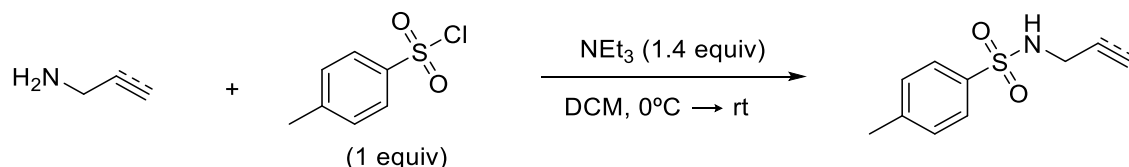
3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-ol:⁶ The product was obtained as a red oil in 99% yield (1.77 g). ¹H NMR (300 MHz, CDCl₃) δ 7.52 (d, J = 8.7 Hz, 2H), 7.48 (d, J = 8.7 Hz, 2H), 4.47 (d, J = 6.2 Hz, 2H), 1.62 (t, J = 6.2 Hz, 1H).



4-(3-hydroxyprop-1-yn-1-yl)benzonitrile:⁸ The product was obtained as a brown oil in 99% yield (698 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.64 (d, J = 8.2 Hz, 2H), 7.54 (d, J = 8.2 Hz, 2H), 4.55 (d, J = 6.2 Hz, 2H), 1.68 (t, J = 6.2 Hz, 1H).



III. General procedures for the synthesis of 4-methylbenzenesulfonamide derivatives



To a solution of allylamine (1.2 equiv, 8.1 mmol) or propargylamine (1.2 equiv, 54.5 mmol) in dichloromethane (1 M) was added triethylamine (1.4 equiv). The reaction was cooled to 0 °C and *p*-toluenesulfonyl chloride was added in portionwise (1 equiv). The mixture was stirred at room temperature for 5 h. Then, water was added to the reaction and the mixture was extracted with dichloromethane. The combined organic phases were washed with brine and dried over anhydrous MgSO₄. Solvent was removed under vacuum and the residue was purified by column chromatography in silica gel using cyclohexane/EtOAc 7:3 as eluent.

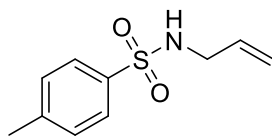
⁵ J. Tummatorn, S. Ruchirawat, P. Ploypradith, *Chem. Eur. J.* **2010**, *16*, 1445 – 1448.

⁶ F. M. Irudayanathan, J. Kim, K. Ho Song, S. Lee, *Asian J. Org. Chem.* **2016**, *5*, 1148 – 1154.

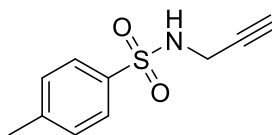
⁷ F. Y. Kwong, H. W. Lee, W. H. Lam, L. Qiu, A. S. C. Chan, *Tetrahedron: Asymmetry*, **2006**, *17*, 1238 – 1252.

⁸ A. Nowak-Król, B. Koszarna, S. Y. Yoo, J. Chromiński, M. K. Węclawski, C.-H. Lee, D. T. Gryko, *Org. Chem.*, **2011**, *76*, 2627–2634.

***N*-allyl-4-methylbenzenesulfonamide:**⁹ The product was obtained as a white solid in 90% yield (1.4 g). ¹H NMR (300 MHz, CDCl₃) δ 7.75 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 5.73 (ddt, *J* = 16.5, 10.3, 5.9 Hz, 1H), 5.17 (dd, *J* = 16.5, 1.0 Hz, 1H), 5.10 (dd, *J* = 10.3, 1.0 Hz, 1H), 4.39 (s, 1H), 3.59 (t, *J* = 5.9 Hz, 2H), 2.43 (s, 3H).

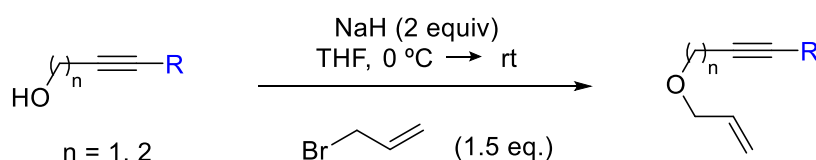


4-methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide:¹⁰ The product was obtained as a white solid in 90% yield (8.6 g). ¹H NMR (300 MHz, CDCl₃) δ 7.82 (d, *J* = 8.1 Hz, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 4.68 (t, *J* = 6.0 Hz, 1H), 3.82 (dd, *J* = 6.0, 2.6 Hz, 2H), 2.48 (s, 3H), 2.15 (t, *J* = 2.6 Hz, 1H).



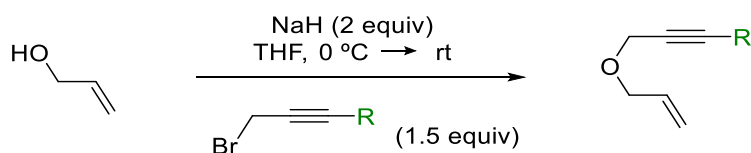
IV. Synthesis of 1,6-enynes (*Z* = O, CH₂)

- General procedure A for the synthesis of 1,6-enynes:¹¹



Under an argon atmosphere, NaH (2 equiv, 60% dispersion mineral oil, previously washed with hexane) and THF (0.4 M) were added to a round bottom flask. The resulting suspension was cooled to 0 °C, and the corresponding propargyl alcohol was added dropwise. The mixture was stirred for 1 h at rt. Then, the mixture was cooled to 0 °C and was kept at this temperature during the addition of the allyl bromide derivative (1.5 equiv). Next, it was stirred for 2 additional hours at rt. When the starting propargyl alcohol was consumed, water was added dropwise at 0 °C. The mixture was extracted with EtOAc, the combined organic layers were washed with brine and dried over anhydrous MgSO₄. The solvent was removed under vacuum and the product was purified by column chromatography (cyclohexane/EtOAc, 95:5).

- General procedure B for the synthesis of 1,6-enynes:¹⁵



Under an argon atmosphere, NaH (2 equiv, 60% dispersion mineral oil, previously washed with hexane) and THF (0.4 M) were added to a round bottom flask. The reaction was cooled to 0 °C, and the corresponding allyl alcohol was added dropwise. The mixture was stirred for 1 h at rt. Then, the mixture was cooled to 0 °C and was kept at this temperature during the addition of

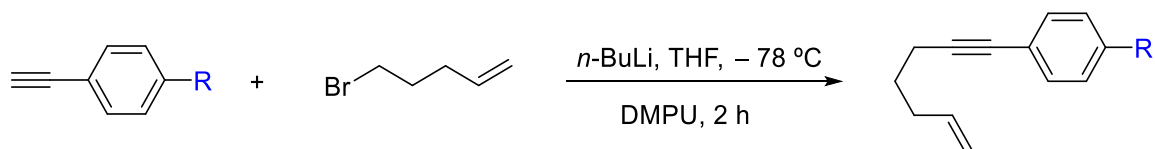
⁹ S. E. Gibson, K. A. C. Kaufmann, P. R. Haycock, A. J. P. White, D. J. Hardick, M. J. Tozer, *Organometallics*, **2007**, 26, 1578 – 1580.

¹⁰ N. Dieltiens, K. Moonen, C. V. Stevens, *Chem. Eur. J.*, **2007**, 13, 203 – 214.

¹¹ Y. Xie, M. Yu, Y. Zhang, *Synthesis*, **2011**, 2803 – 2809.

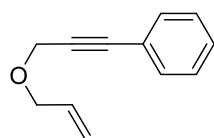
the allyl bromide derivative (1.5 equiv). Next, it was stirred for 2 additional hours at rt. When the starting propargyl alcohol was consumed, water was added dropwise at 0 °C. The mixture was extracted with EtOAc, the combined organic layers were washed with brine and dried over anhydrous MgSO₄. The solvent was removed under vacuum and the product was purified by column chromatography (cyclohexane/EtOAc, 95:5).

- *General procedure C for the synthesis of 1,6-enynes:*¹²



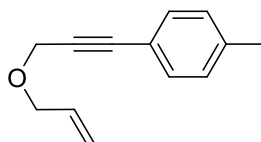
To a solution of the corresponding alkyne (9.8 mmol) in dry THF (0.5 M) at – 78 °C, *n*-BuLi (1.6 M in hexanes, 9.8 mmol) was added dropwise within 10 min, and the mixture was stirred for 30 min. Then, 5-bromopent-1-ene (11.8 mmol) and DMPU (19.6 mmol) were added and the reaction mixture was stirred for 2 h at rt. Then, it was quenched with saturated solution of NH₄Cl and extracted with EtOAc, washed with brine and dried over anhydrous MgSO₄. The solvent was removed under vacuum and the enyne was purified by column chromatography (cyclohexane).

(3-(allyloxy)prop-1-yn-1-yl)benzene (1a):¹³ The product was obtained following the *general*



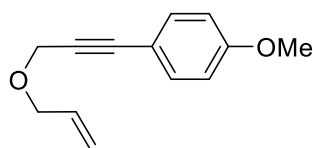
procedure A as a yellow oil in 94% yield (2.3 g). ¹H NMR (300 MHz, CDCl₃) δ 7.47 – 7.44 (m, 2H), 7.33 – 7.30 (m, 3H), 5.96 (ddt, *J* = 16.6, 10.4, 5.8 Hz, 1H), 5.35 (ddd, *J* = 16.6, 3.2, 1.6 Hz, 1H), 5.24 (dd, *J* = 10.4, 1.6 Hz, 1H), 4.39 (s, 2H), 4.14 (dt, *J* = 5.8, 1.6 Hz, 2H).

1-(3-(allyloxy)prop-1-yn-1-yl)-4-methylbenzene (1b):¹³ The product was obtained following the



general procedure A as a yellow oil in 77% yield (805 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.29 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 5.90 (ddt, *J* = 16.1, 10.4, 5.8 Hz, 1H), 5.29 (dq, *J* = 16.1, 1.4 Hz, 1H), 5.18 (dd, *J* = 10.4, 1.4 Hz, 1H), 4.32 (s, 2H), 4.08 (dt, *J* = 5.8, 1.4 Hz, 2H), 2.29 (s, 3H).

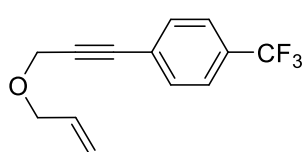
1-(3-(allyloxy)prop-1-yn-1-yl)-4-methoxybenzene (1c):¹³ The product was obtained following



the *general procedure A* as a colorless oil in 93% yield (1.0 g). ¹H NMR (300 MHz, CDCl₃) δ 7.39 (d, *J* = 8.9 Hz, 2H), 6.84 (d, *J* = 8.9 Hz, 2H), 5.95 (ddt, *J* = 17.2, 10.4, 5.8 Hz, 1H), 5.34 (ddd, *J* = 17.2, 3.0, 1.4 Hz, 1H), 5.23 (ddd, *J* = 10.3, 3.0, 1.4 Hz, 1H), 4.37 (s, 2H), 4.13

(dt, *J* = 5.8, 1.4 Hz, 2H), 3.81 (s, 3H).

1-(3-(allyloxy)prop-1-yn-1-yl)-4-(trifluoromethyl)benzene (1d):⁷ The product was obtained



following the *general procedure A* as a yellow liquid in 91% yield (1.9 g). ¹H NMR (300 MHz, CDCl₃) δ 7.58 (d, *J* = 9.0 Hz, 2H), 7.54 (d, *J* = 9.0 Hz, 2H), 5.95 (ddd, *J* = 17.2, 10.4, 5.7 Hz, 1H), 5.35 (dd, *J* = 17.2, 1.3

¹² N. Topolovčan, I. Panov, M. Kotora, *Synlett*, **2016**, 27, 432 – 436.

¹³ F. Y. Kwong, Y. M. Li, W. H. Lam, L. Qiu, H. W. Lee, C. H. Yeung, K. S. Chan, A. S. C. Chan, *Chem. Eur. J.*, **2005**, 11, 3872 – 3880.

Hz, 1H), 5.26 (dd, $J = 10.4, 1.3$ Hz, 1H), 4.39 (s, 2H), 4.14 (dt, $J = 5.7, 1.3$ Hz, 2H).

4-(3-(allyloxy)prop-1-yn-1-yl)benzonitrile (1e):¹⁴ The product was obtained following the *general procedure A* as an orange oil in 47% yield (405 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.55 (d, $J = 8.4$ Hz, 2H), 7.47 (d, $J = 8.4$ Hz, 2H), 5.89 (ddd, $J = 17.3, 10.5, 5.8$ Hz, 1H), 5.29 (dd, $J = 17.3, 1.5$ Hz, 1H), 5.20 (d, $J = 10.5$ Hz, 1H), 4.34 (s, 2H), 4.07 (d, $J = 5.8$ Hz, 2H). ¹³C NMR (75 MHz, CDCl₃) δ 133.9 (CH), 132.3 (2 $\times$ CH), 132.1 (2 $\times$ CH), 127.6 (C), 118.4 (C), 118.2 (CH₂), 111.9 (C), 89.8 (C), 84.6 (C), 71.1 (CH₂), 57.8 (CH₂). HRMS (ESI, MeOH) calcd. for C₁₃H₁₁NO [M + Na]⁺: 220.2370; Found: 220.0739.

Hept-6-en-1-yn-1-ylbenzene (1q):¹² The product was obtained following the *general procedure C*, using phenylacetylene, as a pale yellow oil in 74% yield (1.3 g). ¹H NMR (300 MHz, CDCl₃) δ 7.40 (dd, $J = 6.5, 3.2$ Hz, 2H), 7.28 (dd, $J = 5.0, 2.0$ Hz, 3H), 5.84 (ddt, $J = 17.0, 10.2, 6.7$ Hz, 1H), 5.07 (ddd, $J = 17.0, 3.5, 1.6$ Hz, 1H), 5.01 (ddt, $J = 10.2, 3.5, 1.6$ Hz, 1H), 2.43 (t, $J = 7.1$ Hz, 2H), 2.23 (dt, $J = 7.1, 1.3$ Hz, 2H), 1.70 (quin, $J = 7.1$ Hz, 2H).

1-(hept-6-en-1-yn-1-yl)-4-methylbenzene (1r):¹⁵ The product was obtained following the *general procedure C*, using 4-ethynyltoluene, as a pale yellow oil in 76% yield (1.2 g). ¹H NMR (300 MHz, CDCl₃) δ 7.29 (d, $J = 8.1$ Hz, 2H), 7.09 (d, $J = 8.1$ Hz, 2H), 5.84 (ddt, $J = 17.0, 10.2, 6.7$ Hz, 1H), 5.07 (ddd, $J = 17.0, 3.5, 1.6$ Hz, 1H), 5.03–4.97 (ddt, $J = 10.2, 3.5, 1.1$ Hz, 1H), 2.41 (t, $J = 7.1$ Hz, 2H), 2.33 (s, 3H), 2.27–2.17 (qt, $J = 7.1, 1.1$ Hz, 2H), 1.70 (p, $J = 7.1$ Hz, 2H).

Allyl 3-phenylpropiolate (1u):¹⁶ To a solution of 3-phenylpropionic acid (6.8 mmol) and allyl alcohol (9.5 mmol) in CH₂Cl₂ (22 mL), was added dropwise a solution of DCC (8.2 mmol) and DMAP (0.7 mmol) in CH₂Cl₂ (5 mL) at 0 °C. The mixture was stirred for 1 h at rt. The solvent was removed under vacuum and the enyne was purified by column chromatography using cyclohexane/EtOAc 98:2. The product was obtained as a pale yellow oil in 92% yield (1.1 g). ¹H NMR (300 MHz, CDCl₃) δ 7.62–7.57 (m, 2H), 7.49–7.42 (m, 1H), 7.41–7.34 (m, 2H), 5.98 (ddt, $J = 17.1, 10.4, 5.9$ Hz, 1H), 5.41 (ddd, $J = 17.1, 2.8, 1.2$ Hz, 1H), 5.32 (ddd, $J = 10.4, 2.4, 1.2$ Hz, 1H), 4.73 (dt, $J = 5.9, 1.2$ Hz, 2H).

(4-(allyloxy)but-1-yn-1-yl)benzene (1w):¹⁷ The product was obtained following the *general procedure A* as a yellow oil in 95% yield (1.3 g). ¹H NMR (300 MHz, CDCl₃) δ 7.46–7.33 (m, 2H), 7.30–7.27 (m, 3H), 5.94 (ddt, $J = 17.2, 10.4, 5.6$ Hz, 1H), 5.32 (ddd, $J = 17.2, 3.2, 1.4$ Hz, 1H), 5.21 (ddd, $J = 10.4, 2.9, 1.4$ Hz, 1H), 4.06 (dt, $J = 5.6, 1.4$ Hz, 2H), 3.66 (t, $J = 7.1$ Hz, 2H), 2.71 (t, $J = 7.1$ Hz, 2H).

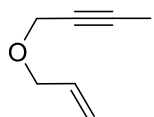
¹⁴ S. Yu, C. Wu, S. Ge, *J. Am. Chem. Soc.* **2017**, *139*, 6526–6529.

¹⁵ N. Topolovčan, I. Panov, M. Kotora, *Eur. J. Org. Chem.*, **2015**, 2868–2878.

¹⁶ T. Tsujihara, K. Takenaka, K. Onitsuka, M. Hatanaka, H. Sasai, *J. Am. Chem. Soc.*, **2009**, *131*, 3452–3453.

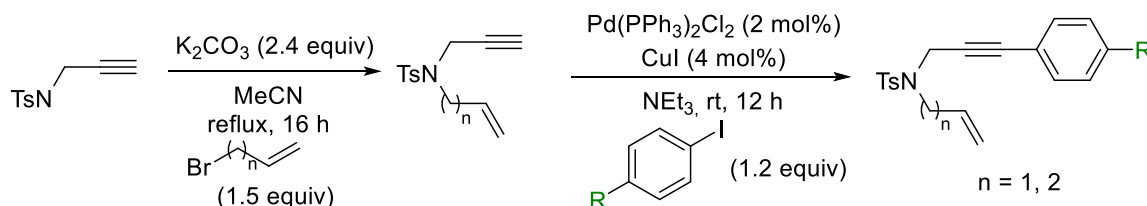
¹⁷ Z. Zhao, Y. Ding, G. Zhao, *J. Org. Chem.*, **1998**, *63*, 9285–9291.

1-(allyloxy)but-2-yne (3g):¹³ The product was obtained following the *general procedure B* as a yellow oil in 16% yield (130 mg). ¹H NMR (300 MHz, CDCl₃) δ 5.91 (ddd, J = 17.0, 10.4, 5.8 Hz, 1H), 5.30 (dd, J = 17.0, 1.4 Hz, 1H), 5.20 (dd, J = 10.4, 1.4 Hz, 1H), 4.11 (q, J = 2.3 Hz, 2H), 4.04 (d, J = 5.7 Hz, 2H), 1.86 (t, J = 2.3 Hz, 3H).



V. Synthesis of 1,6-enynes (Z = NTs)

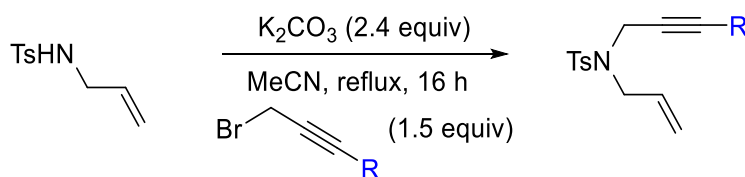
- *General procedure D for the synthesis of 1,6-enynes:*



Step 1:¹⁸ 4-Methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide (1 equiv, 28.7 mmol), K₂CO₃ (2.4 equiv, 60.1 mmol) and acetonitrile (0.4 M) were added to a sealed tube. The corresponding allyl bromide (1.5 equiv, 43.1 mmol) was added and the reaction mixture was heated under reflux overnight. Then, the mixture was cooled to rt, the salts were filtered and the solvent was evaporated. The enyne was purified by column chromatography using cyclohexane/EtOAc 95:5.

Step 2:¹⁹ Under an argon atmosphere, the enyne resulting from the previous step (1 equiv), the iodoarene (1.2 equiv) and trimethylamine (0.4 M) were added to a round bottom flask. Then, Pd(PPh₃)₂Cl₂ (2 mol %) and CuI (4 mol %) were added, and the mixture was stirred overnight at rt. The mixture was treated with a saturated NaHCO₃ solution and then was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were washed with brine and dried over anhydrous MgSO₄. The solvent was removed under vacuum and the product was purified by column chromatography (cyclohexane/EtOAc, 95:5).

- *General procedure E for the synthesis of 1,6-enynes:*¹⁸



N-Allyl-4-methylbenzenesulfonamide (1 equiv, 3.3 mmol), K₂CO₃ (2.4 equiv, 8.0 mmol) and acetonitrile (0.4 M) were added to a sealed tube. The corresponding propargyl bromide (1.5 equiv, 5.0 mmol) was added and the reaction mixture was heated under reflux overnight. Then, the mixture was cooled to rt, the salts were filtered and the solvent was evaporated. The product was purified by column chromatography using cyclohexane/EtOAc 95:5.

¹⁸ S.-K. Kang, T.G. Baik, A. N. Kulak, Y.-H. Ha, Y. Lim, J. Park, *J. Am. Chem. Soc.*, **2000**, 122, 11529 – 11530.

¹⁹ G.-Y. Lin, C.-Y. Yang, R.-S. Liu, *J. Org. Chem.*, **2007**, 72, 6753 – 6757.

N-allyl-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide:²⁰ The product was obtained following the *general procedure D* as a white solid in 96% yield (1.7 g). ¹H NMR (300 MHz, CDCl₃) δ 7.73 (d, J = 8.3 Hz, 2H), 7.30 (d, J = 8.3 Hz, 2H), 5.73 (ddt, J = 16.5, 10.0, 6.5 Hz, 1H), 5.32 – 5.25 (m, 1H), 5.26 – 5.16 (m, 1H), 4.09 (d, J = 2.5 Hz, 2H), 3.82 (dd, J = 6.5, 1.4 Hz, 2H), 2.42 (s, 3H), 2.00 (t, J = 2.5 Hz, 1H).

N-(but-3-en-1-yl)-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide:²¹ The product was obtained following the *general procedure D* as a white solid in 88% yield (3.4 g). ¹H NMR (300 MHz, CDCl₃) δ 7.72 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.2 Hz, 2H), 5.77 (ddt, J = 17.0, 10.1, 6.7 Hz, 1H), 5.16 – 4.99 (m, 2H), 4.14 (d, J = 2.4 Hz, 1H), 3.26 (t, J = 7.0 Hz, 2H), 2.42 (s, 3H), 2.34 (q, J = 7.0 Hz, 2H), 2.03 (t, J = 2.4 Hz, 1H).

N-allyl-4-methyl-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1f):²² The product was obtained following the *general procedure D* as a pale orange solid in 77% yield (997 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.77 (d, J = 8.3 Hz, 2H), 7.27 – 7.21 (m, 4H), 7.06 (d, J = 7.2 Hz, 2H), 5.80 (dd, J = 17.1, 10.0 Hz, 1H), 5.33 (d, J = 17.1, 1H), 5.27 (d, J = 10.0 Hz, 1H), 4.31 (s, 2H), 3.89 (d, J = 6.5 Hz, 2H), 2.34 (s, 3H).

N-allyl-N-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1g):²² The product was obtained following the *general procedure D* as an orange oil in 80% yield (1.2 g). ¹H NMR (300 MHz, CDCl₃) δ 7.77 (d, J = 8.2 Hz, 2H), 7.25 (d, J = 8.2 Hz, 2H), 7.01 (d, J = 8.8 Hz, 2H), 6.76 (d, J = 8.8 Hz, 2H), 5.80 (ddt, J = 17.1, 10.1, 6.5 Hz, 1H), 5.32 (dd, J = 17.1, 1.3 Hz, 1H), 5.26 (dd, J = 10.1, 1.3 Hz, 1H), 4.29 (s, 2H), 3.88 (d, J = 6.5 Hz, 2H), 3.79 (s, 3H), 2.36 (s, 3H).

N-allyl-4-methyl-N-(3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-yl)benzenesulfonamide (1h):²² The product was obtained following the *general procedure D* as an orange solid in 89% yield (1.4 g). ¹H NMR (300 MHz, CDCl₃) δ 7.77 (d, J = 8.3 Hz, 2H), 7.50 (d, J = 8.1 Hz, 2H), 7.26 (d, J = 8.3 Hz, 2H), 7.16 (d, J = 8.1 Hz, 2H), 5.80 (ddt, J = 17.0, 10.0, 6.4 Hz, 1H), 5.35 (dd, J = 17.0, 1.4 Hz, 1H), 5.25 (d, J = 10.0, 1.4 Hz, 1H), 4.32 (s, 2H), 3.89 (dt, J = 6.5, 1.4 Hz, 2H), 2.34 (s, 3H).

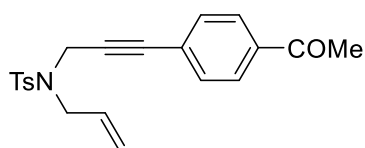
N-allyl-N-(3-(4-cyanophenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1i):²⁰ The product was obtained following the *general procedure D* as an orange oil in 87% yield (612 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.81 (d, J = 8.3 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 8.3 Hz, 2H), 7.15 (d, J = 8.4 Hz, 2H), 5.79 (ddt, J = 16.5, 9.9, 6.4 Hz, 1H), 5.32 (d, J = 16.5 Hz, 1H), 5.27 (d, J = 6.4 Hz, 1H), 4.32 (s, 2H), 3.88 (d, J = 6.4 Hz, 2H), 2.35 (s, 3H).

²⁰ K. T. Sylvester, P. J. Chirik, *J. Am. Chem. Soc.*, **2009**, *131*, 8772 – 8774.

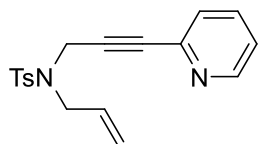
²¹ J. H. Park, S. Min Kim, Y. K. Chung, *Chem. Eur. J.*, **2011**, *17*, 10852 – 10856.

²² A. Lin, Z.-W. Zhang, J. Yang, *Org. Lett.*, **2014**, *16*, 386 – 389.

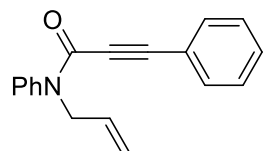
***N*-(3-(4-acetylphenyl)prop-2-yn-1-yl)-*N*-allyl-4-methylbenzenesulfonamide (1j):**²³ The product was obtained following the *general procedure D* as an orange solid in 89% yield (1.4 g). ¹H NMR (300 MHz, CDCl₃) δ 7.84 – 7.75 (m, 4H), 7.25 (d, *J* = 8.3 Hz, 2H), 7.14 (d, *J* = 8.3 Hz, 2H), 5.79 (ddt, *J* = 16.4, 9.9, 6.4 Hz, 1H), 5.37 – 5.23 (m, 1H), 4.32 (s, 2H), 3.88 (d, *J* = 6.4 Hz, 2H), 2.58 (d, *J* = 1.8 Hz, 3H), 2.34 (s, 3H).



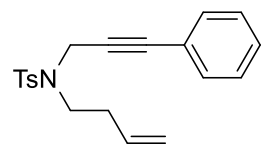
***N*-allyl-4-methyl-*N*-(3-(pyridin-2-yl)prop-2-yn-1-yl)benzenesulfonamide (1k):** The product was obtained following the *general procedure D* as a yellow solid in 56% yield (340 mg). ¹H NMR (300 MHz, CDCl₃) δ 8.52 (d, *J* = 4.5 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.58 (tq, *J* = 7.8, 0.9 Hz, 1H), 7.25 – 7.19 (m, 3H), 7.00 (d, *J* = 7.8 Hz, 1H), 5.78 (ddt, *J* = 16.6, 10.0, 6.4 Hz, 1H), 5.30 (ddd, *J* = 13.6, 10.0, 0.9 Hz, 2H), 4.33 (s, 2H), 3.91 (d, *J* = 6.3 Hz, 2H), 2.31 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 149.7 (CH), 143.4 (C), 142.1 (C), 135.8 (CH), 135.7 (C), 131.7 (CH), 129.4 (2 × CH), 127.6 (2 × CH), 126.8 (CH), 122.9 (CH), 119.9 (CH₂), 84.9 (C), 81.7 (C), 49.2 (CH₂), 36.4 (CH₂), 21.2 (CH₃). HRMS (ESI, MeOH) calcd. for C₁₈H₂₈N₂O₂S [M + H]⁺: 327.2980; Found: 327.1154.



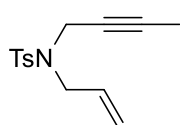
***N*-allyl-*N*,3-diphenylpropiolamide (1v):**²⁴ To a solution of 3-phenylpropionic acid (6.8 mmol) in CH₂Cl₂ (15 mL), was added dropwise a solution of DCC (7.5 mmol) and DMAP (0.7 mmol) in CH₂Cl₂ (10 mL) at – 10 °C. *N*-phenylbut-3-en-1-amine (6.8 mmol) was then added and the mixture was stirred for 20 h at rt. The solid was filtered off and the filtrate was washed with 0.1 N HCl (10 mL) and dried over anhydrous MgSO₄. The solvent was removed under vacuum and the enyne was purified by column chromatography using cyclohexane/EtOAc 9:1. The product was obtained as a pale yellow solid in 69% yield (1.2 g). ¹H NMR (300 MHz, CDCl₃) δ 7.41 (t, *J* = 7.5 Hz, 3H), 7.33 (m, 3H), 7.23 (t, *J* = 7.5 Hz, 2H), 7.14 – 7.07 (m, 2H), 5.90 (ddt, *J* = 16.1, 9.9, 6.2 Hz, 1H), 5.22 – 5.13 (m, 2H), 4.42 (d, *J* = 6.2 Hz, 2H).



***N*-(but-3-en-1-yl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1x):**²¹ The product was obtained following the *general procedure D* as a pale brown solid in 90% yield (1.1 g). ¹H NMR (300 MHz, CDCl₃) δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.26 – 7.19 (m, 5H), 7.10 – 7.02 (m, 2H), 5.81 (ddt, *J* = 16.9, 10.1, 6.8 Hz, 1H), 5.17 – 5.05 (m, 2H), 4.35 (s, 2H), 3.33 (t, *J* = 7.2 Hz, 2H), 2.40 (q, *J* = 7.2 Hz, 2H), 2.34 (s, 3H).



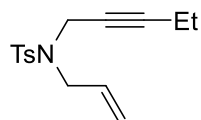
***N*-allyl-*N*-(but-2-yn-1-yl)-4-methylbenzenesulfonamide (3a):**²⁰ The product was obtained following the *general procedure E* as a white solid in 90% yield (785 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.74 (d, *J* = 8.1 Hz, 2H), 7.32 – 7.27 (d, *J* = 8.1 Hz, 2H), 5.73 (ddt, *J* = 16.4, 10.0, 6.4 Hz, 1H), 5.30 – 5.25 (m, 1H), 5.24 – 5.23 (m, 1H), 4.02 (d, *J* = 2.4 Hz, 2H), 3.79 (d, *J* = 6.4 Hz, 2H), 2.42 (s, 3H), 1.54 (t, *J* = 2.4 Hz, 3H).



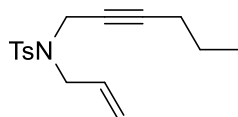
²³ Y. Tang, L. Deng, Y. Zhang, G. Dong, J. Chen, Z. Yang, *Org. Lett.*, **2005**, 7, 1657 – 1659.

²⁴ M.-B. Zhou, W.-T. Wei, Y.-X. Xie, Y. Lei, J.-H. Li, *J. Org. Chem.*, **2010**, 75, 5635 – 5642.

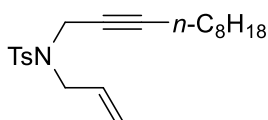
N-allyl-4-methyl-N-(pent-2-yn-1-yl)benzenesulfonamide (3b):²⁵ The product was obtained following the *general procedure E* as a colorless oil in 94% yield (622 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 5.74 (ddt, *J* = 16.4, 9.9, 6.4 Hz, 1H), 5.37 – 5.12 (m, 2H), 4.05 (t, *J* = 2.1 Hz, 2H), 3.80 (d, *J* = 6.4 Hz, 2H), 2.42 (s, 3H), 1.91 (qt, *J* = 7.5, 2.1 Hz, 2H), 0.90 (t, *J* = 7.5 Hz, 3H).



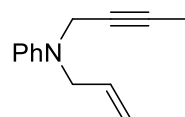
N-allyl-N-(hex-2-yn-1-yl)-4-methylbenzenesulfonamide (3c):²⁶ The product was obtained following the *general procedure E* as a yellow oil in 72% yield (873 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.74 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.3 Hz, 2H), 5.75 (ddt, *J* = 16.5, 10.0, 6.4 Hz, 1H), 5.32 – 5.19 (m, 2H), 4.06 (t, *J* = 2.2 Hz, 2H), 3.81 (d, *J* = 6.4 Hz, 2H), 2.42 (s, 3H), 1.88 (tt, *J* = 7.0, 2.2 Hz, 2H), 1.28 (quin, *J* = 7.3 Hz, 1H), 0.81 (t, *J* = 7.3 Hz, 3H).



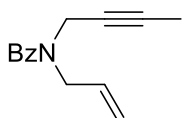
N-allyl-4-methyl-N-(undec-2-yn-1-yl)benzenesulfonamide (3d): The product was obtained following the *general procedure E* as a yellow oil in 84% yield (433 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.74 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 5.75 (ddt, *J* = 16.5, 10.0, 6.5 Hz, 1H), 5.34 – 5.14 (m, 2H), 4.05 (s, 2H), 3.80 (d, *J* = 6.5 Hz, 2H), 2.42 (s, 3H), 1.94 – 1.85 (m, 2H), 1.34 – 1.15 (m, 12H), 0.89 (t, *J* = 6.8 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 143.2 (C), 136.3 (C), 132.2 (CH), 129.3 (2 $\times$ CH), 127.8 (2 $\times$ CH), 119.5 (CH₂), 86.3 (C), 72.3 (C), 48.9 (CH₂), 36.4 (CH₂), 31.8 (CH₂), 29.2 (CH₂), 29.0 (CH₂), 28.8 (CH₂), 28.4 (CH₂), 22.6 (CH₂), 21.5 (CH₃), 18.4 (CH₂), 14.1 (CH₃). HRMS (ESI, MeOH) calcd. for C₂₁H₃₁NO₂S [M + H]⁺: 362.5440; Found: 362.2142.



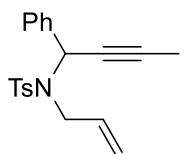
N-allyl-N-(but-2-yn-1-yl)aniline (3e):²⁷ The product was obtained following the *general procedure E* as a colorless oil in 84% yield (265 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.25 (t, *J* = 8.1 Hz, 2H), 6.84 (d, *J* = 8.1 Hz, 2H), 6.76 (t, *J* = 7.3 Hz, 1H), 5.89 (ddd, *J* = 15.4, 10.2, 5.1 Hz, 1H), 5.31 – 5.10 (m, 2H), 3.97 (s, 3H), 1.80 (s, 3H).



N-allyl-N-(but-2-yn-1-yl)benzamide (3f):²⁸ The product was obtained following the *general procedure E* as a colorless oil in 52% yield (612 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.60 – 7.35 (m, 5H), 5.99 – 5.66 (m, 1H), 5.29 – 5.16 (m, 2H), 4.25 (br s, 2H), 4.03 – 3.89 (m, 2H), 1.85 (s, 3H).



N-allyl-4-methyl-N-(1-phenylbut-2-yn-1-yl)benzenesulfonamide (3i): To a solution of *N*-allyl-4-methylbenzenesulfonamide (1.8 mmol), 1-phenylbut-2-yn-1-ol (1.5 mmol) and triphenylphosphine (1.8 mmol) in THF (4 mL) was added DIAD (1.8 mmol) at 0 °C. Then, the mixture was stirred at rt for 5 h until the complete consumption of the sulfonamide. The solvent was removed under vacuum and the product was purified by column chromatography on silica gel using cyclohexane/EtOAc 95:5. The product was obtained as a colorless oil in 43% yield (221 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.57 (dd, *J* = 7.0, 1.3 Hz, 2H), 7.32 (dd, *J* = 8.3, 2.9 Hz, 5H), 6.03 (d, *J* = 2.0 Hz, 1H), 5.41 (ddt, *J* = 16.2, 10.1, 6.5 Hz, 1H), 4.82 (dd, *J* = 16.2, 1.4 Hz, 1H), 4.75 (dd, *J* = 10.1,



²⁵ D. A. Candito, M. Lautens, *Synlett*, **2011**, 1987 – 1992.

²⁶ M. E. Krafft, L. V. R. Boñaga, J. A. Wright, C. Hirose, *J. Org. Chem.*, **2002**, 67, 1233 – 1246.

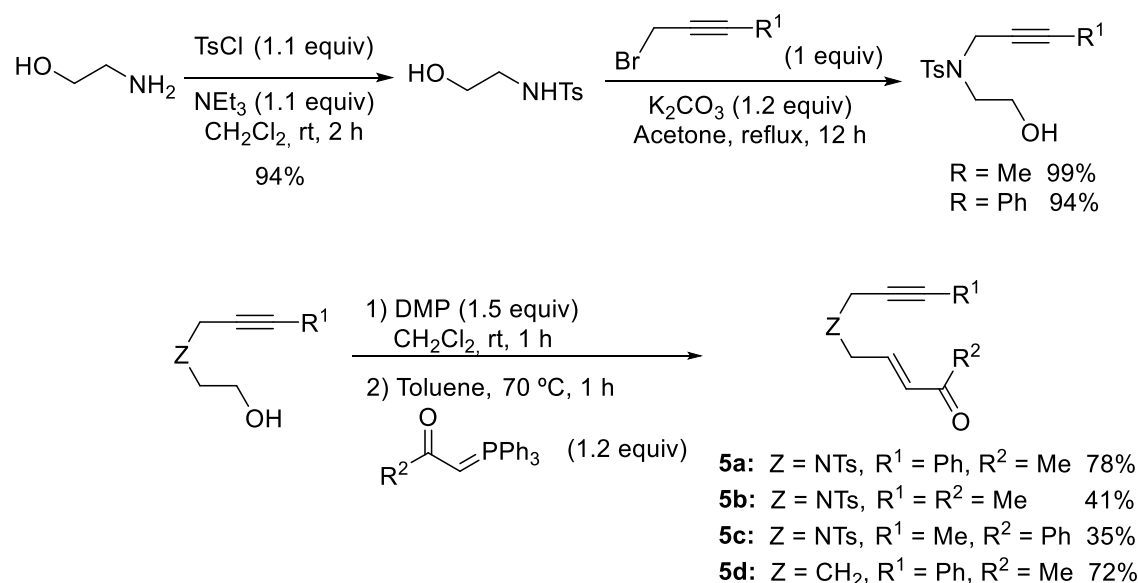
²⁷ S. J. Sturla, S. L. Buchwald, *J. Org. Chem.*, **1999**, 64, 5547 – 5550.

²⁸ J. B. Diccianni, T. Heitmann, T. Diao, *J. Org. Chem.*, **2017**, 82, 6895 – 6903.

1.4 Hz, 1H), 3.64 (qd, $J = 16.2, 6.5$ Hz, 2H), 2.45 (s, 3H), 1.69 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 143.3 (C), 137.1 (C), 136.5 (C), 134.7 (CH), 129.3 (2 $\times$ CH), 128.4 (2 $\times$ CH), 128.3 (2 $\times$ CH), 128.2 (CH), 128.1 (2 $\times$ CH), 116.7 (CH_2), 84.6 (C), 73.7 (C), 54.0 (CH), 48.0 (CH_2), 21.6 (CH_3), 3.4 (CH_3). HRMS (ESI, MeOH) calcd. for $\text{C}_{20}\text{H}_{21}\text{NO}_2\text{S}$ [$\text{M} + \text{Na}$] $^+$: 362.4530; Found: 362.1182.

***N*-(but-2-yn-1-yl)-*N*-(but-3-en-2-yl)-4-methylbenzenesulfonamide (3j):**²⁹ To a solution of *N*-(but-2-yn-1-yl)-4-methylbenzenesulfonamide (1.9 mmol), but-3-en-2-ol (2.3 mmol) and triphenylphosphine (2.3 mmol) in THF (4 mL) was added DIAD (2.3 mmol) at 0 °C. Then, the mixture was stirred at rt for 5 h until the complete consumption of the sulfonamide. The solvent was removed under vacuum and the product was purified by column chromatography on silica gel using cyclohexane/EtOAc 95:5. The product was obtained as a colorless oil in 82% yield (438 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.80 (d, $J = 8.3$ Hz, 2H), 7.27 (d, $J = 8.3$ Hz, 2H), 5.83 – 5.70 (m, 1H), 5.15 (d, $J = 1.7$ Hz, 1H), 5.11 (ddd, $J = 7.1, 1.7, 1.0$ Hz, 1H), 4.61 – 4.49 (m, 1H), 4.07 (dq, $J = 18.2, 2.4$ Hz, 1H), 3.82 (dq, $J = 18.2, 2.4$ Hz, 1H), 2.42 (s, 3H), 1.67 (t, $J = 2.4$ Hz, 3H), 1.25 (d, $J = 7.0$ Hz, 3H).

VI. Synthesis of enones



Step 1:³⁰ To a solution of ethanolamine (1 equiv, 16.4 mmol) and *p*-toluenesulfonyl chloride (1.1 equiv, 18.0 equiv) in CH_2Cl_2 (0.45 M) at 0 °C, was added triethylamine dropwise. The mixture was allowed to warm to room temperature and was stirred for 2 h. The reaction was quenched with H_2O and extracted with CH_2Cl_2 . The combined organic layers were washed with brine and dried over anhydrous MgSO_4 . Solvent was removed under vacuum and the residue was purified by column chromatography in silica gel using cyclohexane/AcOEt 1:1 as eluent.

²⁹ D. E. Kim, S. H. Park, Y. H. Choi, S.-G. Lee, D. Moon, J. Seo, N. Jeong, *Chem. Asian J.*, **2011**, 6, 2009 – 2014.

³⁰ A. R. O. Venning, M. R. Kwiatkowski, J. E. Roque Peña, B. C. Lainhart, A. A. Guruparan, E. J. Alexanian, *J. Am. Chem. Soc.* **2017**, 139, 11595 – 11600.

Step 2: the reaction was performed using ethanolamine (1 equiv, 10.7 mmol), K₂CO₃ (1.2 equiv, 12.8 mmol) in acetone (0.5 M) and following the *General Procedure E*. The residue was purified by column chromatography in silica gel using cyclohexane/EtOAc 7:3 as eluent.

Step 3:³¹ To a solution of the corresponding alcohol (1 equiv) in CH₂Cl₂ at 0 °C, DMP (1.5 equiv) was added. The resulting mixture was stirred at that temperature for 5 min and for another 30 min at rt. Then, the reaction was quenched with Na₂S₂O₃ and NaHCO₃ solution and extracted with EtOAc. The combined organic layer was washed with brine, dried over anhydrous MgSO₄ and filtered. The filtrate was concentrated under reduced pressure. The residue was dissolved in toluene (0.2 M) and the corresponding phosphorus ylide (1.2 equiv) was added. Then, the mixture was heated to 70 °C for 1 h. The solvent was evaporated under vacuum and the residue was purified by column chromatography in silica gel using cyclohexane/EtOAc 9:1 as eluent.

***N*-(2-hydroxyethyl)-4-methylbenzenesulfonamide:**³⁰ The product was obtained following the *Step 1* as a white solid in 94% yield (3.33 g). ¹H NMR (300 MHz, CDCl₃) δ 7.75 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.3 Hz, 2H), 5.40 (br s, 1H), 3.68 (d, *J* = 4.7 Hz, 2H), 3.07 (d, *J* = 4.7 Hz, 2H), 2.57 (br s, 1H), 2.42 (s, 3H).

***N*-(2-hydroxyethyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide:**³¹ The product was obtained following the *Step 2* as a yellow solid in 94% yield (1.29 g). ¹H NMR (300 MHz, CDCl₃) δ 7.79 (d, *J* = 8.3 Hz, 2H), 7.39 – 7.18 (m, 5H), 7.09 (d, *J* = 8.3 Hz, 2H), 4.42 (s, 2H), 3.84 (dd, *J* = 10.8, 5.5 Hz, 2H), 3.42 (t, *J* = 5.2 Hz, 2H), 2.35 (s, 3H), 2.22 (t, *J* = 5.9 Hz, 1H).

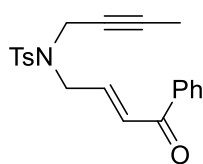
***N*-(but-2-yn-1-yl)-*N*-(2-hydroxyethyl)-4-methylbenzenesulfonamide:**³¹ The product was obtained following the *Step 2* as a yellow solid in 99% yield (2.89 g). ¹H NMR (300 MHz, CDCl₃) δ 7.75 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.3 Hz, 2H), 4.16 – 4.06 (m, 2H), 3.77 (t, *J* = 5.2 Hz, 2H), 3.32 (t, *J* = 5.2 Hz, 2H), 2.43 (s, 3H), 1.88 (t, *J* = 2.5 Hz, 1H), 1.59 (t, *J* = 2.4 Hz, 3H).

(*E*)-4-methyl-*N*-(4-oxopent-2-en-1-yl)-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (5a):³¹ The product was obtained following the *general procedure D* as a yellow oil in 69% yield (434 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.78 (d, *J* = 8.3 Hz, 2H), 7.34 – 7.19 (m, 5H), 7.08 (dd, *J* = 8.3, 1.6 Hz, 2H), 6.71 (dt, *J* = 16.0, 5.8 Hz, 1H), 6.31 – 6.24 (dt, *J* = 16.0, 1.4 Hz, 1H), 4.31 (s, 2H), 4.07 (d, *J* = 5.8 Hz, 2H), 2.36 (s, 3H), 2.25 (s, 3H).

(*E*)-*N*-(but-2-yn-1-yl)-4-methyl-*N*-(4-oxopent-2-en-1-yl)benzenesulfonamide (5b): The product was obtained following the *general procedure D* as a yellow oil in 41% yield (675 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 5.80 (ddt, *J* = 17.1, 10.1, 6.5 Hz, 1H), 5.32 (dd, *J* = 17.1, 1.3 Hz, 1H), 5.26 (dd, *J* = 10.1, 1.3 Hz, 1H), 4.29 (s, 2H), 3.88 (d, *J* = 6.5 Hz, 2H), 3.79 (s, 3H), 2.36 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 197.9 (C), 143.7 (C), 140.9 (CH), 135.6 (C), 132.8 (CH), 129.4 (2 × CH), 127.7 (2 × CH), 82.3 (C), 71.2 (C), 47.5 (CH₃), 37.4 (CH₃), 27.0 (CH₂), 21.4 (CH₂), 3.1 (CH₃). HRMS (ESI, MeOH) calcd. for C₁₆H₁₉NO₃S [M + H]⁺: 306.1086; Found: 306.1162.

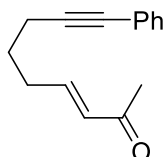
³¹ Z. Yu, L. Liu, J. Zhang, *Chem. Eur. J.* **2016**, 22, 8488 – 8492.

(E)-N-(but-2-yn-1-yl)-4-methyl-N-(4-oxo-4-phenylbut-2-en-1-yl)benzenesulfonamide (5c):³¹



The product was obtained following the *general procedure D* as a yellow oil in 34% yield (683 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.91 (dd, J = 8.3, 1.3 Hz, 2H), 7.76 (d, J = 8.3 Hz, 2H), 7.61 – 7.55 (m, 1H), 7.47 (dd, J = 8.0, 6.7 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.08 (dt, J = 15.4, 1.4 Hz, 1H), 6.87 (dt, J = 15.4, 5.4 Hz, 1H), 4.08 (d, J = 4.8 Hz, 4H), 2.42 (s, 3H), 1.58 (t, J = 2.3 Hz, 3H).

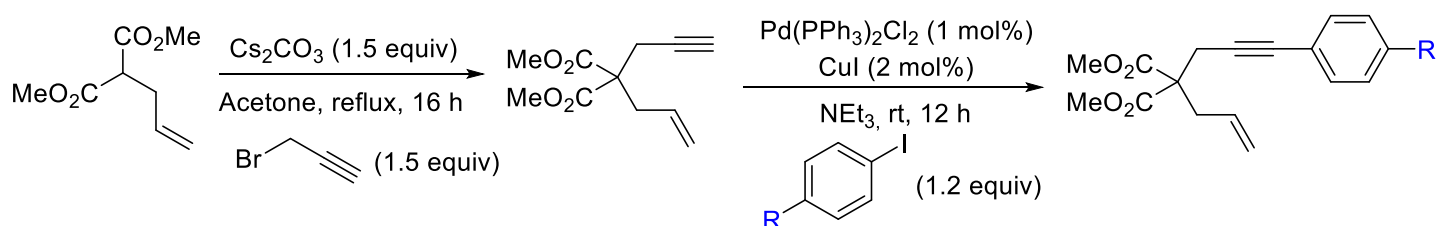
(E)-9-phenylnon-3-en-8-yn-2-one (5d):³² The product was obtained following the *general*



procedure D as a light brown oil in 71% yield (259 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.39 (dd, J = 6.6, 3.0 Hz, 2H), 7.31 – 7.27 (m, 3H), 6.84 (dt, J = 15.9, 6.9 Hz, 1H), 6.14 (d, J = 15.9 Hz, 1H), 2.47 (t, J = 7.0 Hz, 2H), 2.44 – 2.38 (m, 2H), 2.25 (s, 3H), 1.79 (p, J = 7.0 Hz, 2H).

VII. Synthesis of 1,6-enynes (Z = C(CO₂Me)₂, C(CH₂OR)₂)

- *General procedure F for synthesis of 1,6 enynes:*



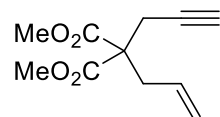
Step 1:³³ Dimethyl 2-allylmalonate (1 equiv, 29.0 mmol), Cs₂CO₃ (1.5 equiv, 43.5 mmol) and acetone (0.4 M) were added to a sealed tube. The corresponding propargyl bromide (1.5 equiv, 43.5 mmol) was added and the reaction mixture was heated under reflux overnight. Then, the mixture was cooled to rt, the salts were filtered and the solvent was evaporated. The compound was purified by column chromatography using cyclohexane/EtOAc 95:5.

Step 2:¹⁹ The iodoarene (1.2 equiv.) and trimethylamine (0.4 M) were added to a round bottom flask. Then, Pd(PPh₃)₂Cl₂ (1 mol%) and CuI (2 mol%) were added, and the mixture was stirred for 5 min. Finally, the enyne resulting from the previous step (1 equiv.) was added and the mixture was stirred overnight at rt. The reaction mixture was treated with a saturated NaHCO₃ solution and then it was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were washed with brine and dried over anhydrous MgSO₄. The solvent was removed under vacuum and the product was purified by column chromatography (cyclohexane/EtOAc, 95:5).

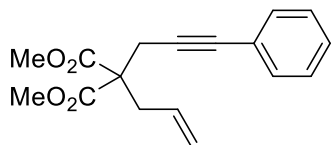
³² J.-C. Hsieh, Y.-C. Hong, C.-M. Yang, S. Mannathan, C.-H. Cheng, *Org. Chem. Front.* **2017**, 4, 1615–1619.

³³ J. W. Faller, P. P. Fontaine, *J. Organomet. Chem.*, **2006**, 691, 1912 – 1918.

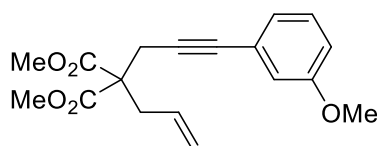
Dimethyl 2-allyl-2-(prop-2-yn-1-yl)malonate.³⁴ The product was obtained following the *general procedure F* as a colorless oil in 94% yield (5.7 g). ¹H NMR (300 MHz, CDCl₃) δ 5.62 (ddt, J = 17.5, 10.0, 7.5 Hz, 1H), 5.24 – 5.15 (m, 1H), 5.14 (d, J = 10.0 Hz, 1H), 3.74 (s, 6H), 2.86 – 2.78 (m, 4H), 2.02 (t, J = 2.7 Hz, 1H).



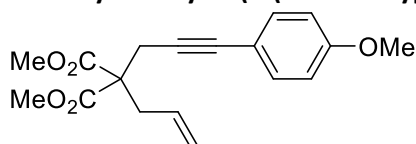
Dimethyl 2-allyl-2-(3-phenylprop-2-yn-1-yl)malonate (1l).³⁵ The product was obtained following the *general procedure F* as a brown oil in 87% yield (1.2 g). ¹H NMR (300 MHz, CDCl₃) δ 7.37 (dd, J = 6.7, 3.0 Hz, 2H), 7.30 – 7.27 (dd, J = 6.7, 3.0 Hz, 3H), 5.68 (ddt, J = 17.1, 10.1 7.6 Hz, 1H), 5.21 (d, J = 17.1 Hz, 1H), 5.15 (d, J = 10.1 Hz, 1H), 3.76 (s, 6H), 3.02 (s, 2H), 2.87 (d, J = 7.6 Hz, 2H).



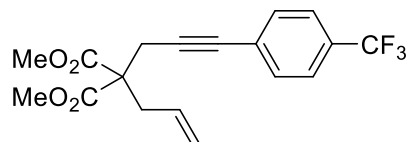
Dimethyl 2-allyl-2-(3-(3-methoxyphenyl)prop-2-yn-1-yl)malonate (1m).³⁶ The product was obtained following the *general procedure F* as a brown oil in 62% yield (468 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.19 (t, J = 7.9 Hz, 1H), 6.97 (d, J = 7.9 Hz, 1H), 6.92 – 6.81 (m, 2H), 5.68 (dd, J = 17.1, 9.8 Hz, 1H), 5.30 – 5.14 (m, 2H), 3.79 (s, 3H), 3.76 (s, 6H), 3.02 (s, 2H), 2.87 (d, J = 7.5 Hz, 2H).



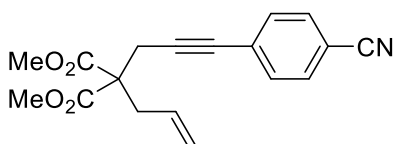
Dimethyl 2-allyl-2-(3-(4-methoxyphenyl)prop-2-yn-1-yl)malonate (1n).³⁶ The product was obtained following the *general procedure F* as a brown solid in 67% yield (1.0 g). ¹H NMR (300 MHz, CDCl₃) δ 7.30 (d, J = 8.2 Hz, 2H), 6.81 (d, J = 8.2 Hz, 2H), 5.69 (ddt, J = 17.0, 10.0, 7.6 Hz, 1H), 5.20 (d, J = 17.0 Hz, 1H), 5.14 (d, J = 10.0 Hz, 1H), 3.80 (s, 3H), 3.76 (s, 6H), 3.00 (s, 2H), 2.87 (d, J = 7.6 Hz, 2H).



Dimethyl 2-allyl-2-(3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-yl)malonate (1o).³⁴ The product was obtained following the *general procedure F* as an orange oil in 98% yield (330 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.48 (d, J = 8.3 Hz, 2H), 7.41 (d, J = 8.3 Hz, 2H), 5.62 (ddt, J = 17.0, 10.0, 7.5 Hz, 1H), 5.15 (dd, J = 17.0, 1.3 Hz, 1H), 5.10 (dd, J = 10.0, 1.3 Hz, 1H), 3.71 (s, 6H), 2.98 (s, 2H), 2.80 (d, J = 7.5 Hz, 2H).



Dimethyl 2-allyl-2-(3-(4-cyanophenyl)prop-2-yn-1-yl)malonate (1p).³⁶ The product was obtained following the *general procedure F* as a pale yellow solid in 84% yield (1.25 g). ¹H NMR (300 MHz, CDCl₃) δ 7.57 (d, J = 8.3 Hz, 2H), 7.44 (d, J = 8.3 Hz, 2H), 5.75 – 5.57 (m, 1H), 5.28 – 5.11 (m, 2H), 3.76 (s, 6H), 3.04 (s, 2H), 2.84 (d, J = 7.4 Hz, 2H).



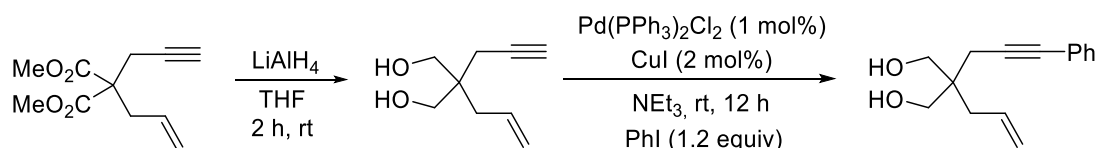
³⁴ Z. Chai, H.-F. Wang, G. Zhao, *Synlett*, **2009**, 1785 – 1790.

³⁵ Z.-L. Lu, E. Neumann, A. Pfaltz, *Eur. J. Org. Chem.*, **2007**, 4189 – 4192.

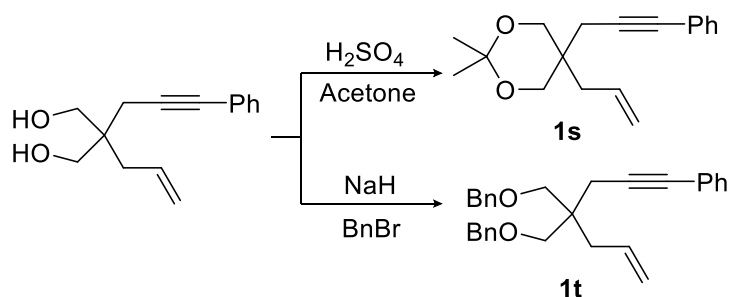
³⁶ A. Escribano-Cuesta, P. Pérez-Galán, E. Herrero-Gómez, M. Sekine, A. A. C. Braga, F. Maseras, A. M. Echavarren, *Org. Biomol. Chem.*, **2012**, 10, 6105 – 6111.

Dimethyl 2-allyl-2-(but-2-yn-1-yl)malonate (3h):³⁷ The product was obtained following the *step 1 of general procedure F*, using 1-bromobut-2-yne as starting material, as a pale yellow oil in 92% yield (1.2 g). ¹H NMR (300 MHz, CDCl₃) δ 5.63 (ddt, J = 17.4, 10.0, 7.5 Hz, 1H), 5.16 (dd, J = 17.4, 1.6 Hz, 1H), 5.11 (dd, J = 10.0, 1.6 Hz, 1H), 3.73 (s, 6H), 2.78 (d, J = 7.5 Hz, 2H), 2.74 (q, J = 2.5 Hz, 2H), 1.76 (t, J = 2.5 Hz, 3H).

- *General procedure G for synthesis of 1,6-enynes:*³⁸



Step 1: To a solution of dimethyl 2-allyl-2-(prop-2-yn-1-yl)malonate (5.5 mmol) in anhydrous THF (0.13 M), LiAlH₄ (11 mmol, 1 M in THF) was added dropwise. The resulting mixture was stirred during 2 h. Then, the mixture was cooled to 0 °C and water was added dropwise. The mixture was extracted with EtOAc, the combined organic layers were washed with brine and dried over anhydrous MgSO₄. The solvent was removed under vacuum and the product was used without further purification. The resulting 2-allyl-2-(prop-2-yn-1-yl)propane-1,3-diol was transformed in the desired product following the *general procedure for the synthesis of propargyl alcohols*.



Step 2: To a solution of 2-allyl-2-(3-phenylprop-2-yn-1-yl)propane-1,3-diol (1.1 mmol) in acetone (0.5 M), H₂SO₄ (0.2 mL) was added dropwise until the solution was acid. The resulting mixture was stirred during 2 h. Then, the mixture was cooled to 0 °C and NaOH solution was added dropwise. The mixture was extracted with EtOAc, the combined organic layers were washed with brine and dried over anhydrous MgSO₄. The solvent was removed under vacuum and the product was purified by column chromatography (cyclohexane/EtOAc, 95:5).

2-allyl-2-(3-phenylprop-2-yn-1-yl)propane-1,3-diol:³⁸ The product was obtained following the *step 1 of the general procedure G* as a colorless oil in 91% yield (821 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.44 – 7.36 (m, 2H), 7.32 – 7.27 (m, 3H), 5.89 (ddt, J = 17.6, 10.0, 7.6 Hz, 1H), 5.16 (dd, J = 12.5, 10.0 Hz, 2H), 3.73 (t, J = 5.7 Hz, 4H), 2.48 (s, 2H), 2.23 (d, J = 7.6 Hz, 2H), 2.15 (t, J = 5.7 Hz, 2H).

³⁷ C. Gryparis, C. Efe, C. Raptis, I. N. Lykakis, M. Stratakis, *Org. Lett.*, **2012**, 14, 2956 – 2959.

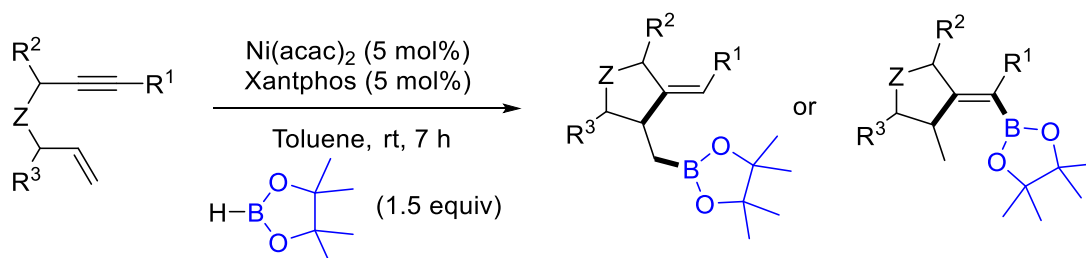
³⁸ J. H. Park, Y. Cho, Y. K. Chung, *Angew. Chem. Int. Ed.*, **2010**, 49, 5138 – 5141.

5-allyl-2,2-dimethyl-5-(3-phenylprop-2-yn-1-yl)-1,3-dioxane (1s):³⁸ The product was obtained following the step 2 of the *general procedure G* as yellow oil in 51% yield (153 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.41 – 7.38 (m, 2H), 7.32 – 7.26 (m, 3H), 5.81 (dq, J = 10.0, 7.6 Hz, 1H), 5.22 – 5.10 (m, 2H), 3.80 – 3.66 (m, 4H), 2.60 (s, 2H), 2.23 (d, J = 7.6 Hz, 2H), 1.44 (s, 6H).

((2-allyl-2-(3-phenylprop-2-yn-1-yl)propane-1,3-diyl)bis(oxy))bis(methylene)dibenzene (1t):³⁸

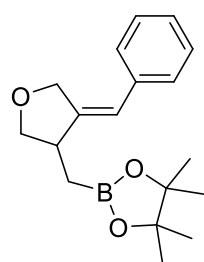
The product was obtained following the *general procedure A*, using 2-allyl-2-(3-phenylprop-2-yn-1-yl)propane-1,3-diol and (bromomethyl)benzene as starting materials, as a yellow oil in 73% yield (324 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.37 – 7.30 (m, 9H), 7.28 (d, J = 3.6 Hz, 6H), 5.84 (ddt, J = 17.6, 10.0, 7.6 Hz, 1H), 5.11 (dd, J = 10.0, 6.1 Hz, 2H), 4.53 (s, 4H), 3.52 – 3.40 (m, 4H), 2.50 (s, 2H), 2.31 (d, J = 7.6 Hz, 2H).

VIII. General procedure for borylative cyclization of 1,6-enynes



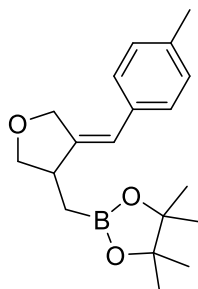
A vial was charged with Ni(acac)₂ (5.1 mg, 0.02 mmol), Xantphos (11.6 mg, 0.02 mmol), the corresponding enyne (0.4 mmol) and a stir bar in air. The vial was sealed by a septum, dried under vacuum and backfilled with Ar. Then, anhydrous and Ar-degassed toluene (2 mL) and HBpin (87 μ L, 0.6 mmol) were added. The resulting mixture was stirred for 7 h at room temperature. When the complete consumption of the enyne was verified by TLC, the solvent was evaporated under vacuum and the product was purified by column chromatography in silica gel.

(Z)-2-((4-benzylidenetetrahydrofuran-3-yl)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2a):



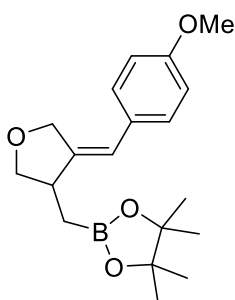
The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a yellow oil in 38% yield (46 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.33 (t, J = 7.3 Hz, 2H), 7.20 (t, J = 7.3 Hz, 1H), 7.12 (d, J = 7.3 Hz, 2H), 6.33 (d, J = 2.3 Hz, 1H), 4.63 (dd, J = 14.1, 1.8 Hz, 1H), 4.55 (dt, J = 14.1, 1.8 Hz, 1H), 4.11 (t, J = 7.8 Hz, 1H), 3.44 (t, J = 7.8 Hz, 1H), 3.10 – 2.94 (m, 1H), 1.25 (d, J = 2.6 Hz, 12H), 1.19 (d, J = 5.9 Hz, 1H), 1.00 (dd, J = 15.9, 8.4 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 147.1 (C), 137.6 (C), 128.5 (2 $\times$ CH), 127.9 (2 $\times$ CH), 126.4 (CH), 119.9 (CH), 83.3 (2 $\times$ C), 74.2 (CH₂), 70.2 (CH₂), 41.2 (CH), 25.0 (2 $\times$ CH₃), 24.8 (2 $\times$ CH₃), 14.2 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₁₈H₂₅BO₃ [M + H]⁺: 301.2050; Found: 301.1974.

(Z)-4,4,5,5-tetramethyl-2-((4-(4-methylbenzylidene)tetrahydrofuran-3-yl)methyl)-1,3,2-



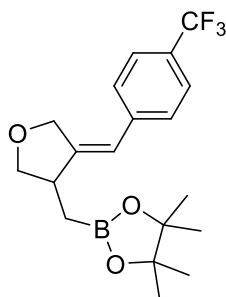
dioxaborolane (2b): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a yellow oil in 51% yield (64 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.14 (d, J = 8.0 Hz, 2H), 7.03 (d, J = 8.0 Hz, 1H), 6.32 (d, J = 2.1 Hz, 2H), 4.68 (d, J = 14.0, 1.8 Hz, 1H), 4.61 (d, J = 14.0, 1.8 Hz, 1H), 4.11 (t, J = 7.8 Hz, 1H), 3.46 (t, J = 7.8 Hz, 1H), 3.04 (dd, J = 14.0, 7.1 Hz, 1H), 2.34 (s, 3H), 1.26 (d, J = 2.6 Hz, 12H), 1.20 (d, J = 5.9 Hz, 1H), 1.02 (dd, J = 15.9, 8.3 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 146.0 (C), 136.1 (C), 134.8 (C), 129.2 (2 $\times$ CH), 127.9 (2 $\times$ CH), 119.7 (CH), 83.3 (2 $\times$ C), 74.2 (CH_2), 70.2 (CH_2), 41.2 (CH), 25.0 (2 $\times$ CH_3), 24.8 (2 $\times$ CH_3), 21.1 (CH_3), 14.0 (br m, $\text{CH}_2\text{-B}$). HRMS (ESI, MeOH) calcd. for $\text{C}_{19}\text{H}_{27}\text{BO}_3$ $[\text{M} + \text{H}]^+$: 315.2320; Found: 315.2126.

(Z)-2-((4-(4-methoxybenzylidene)tetrahydrofuran-3-yl)methyl)-4,4,5,5-tetramethyl-1,3,2-



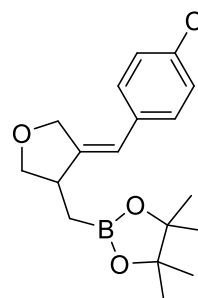
dioxaborolane (2c): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a pale yellow oil in 44% yield (58 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.05 (d, J = 8.7 Hz, 2H), 6.86 (d, J = 8.7 Hz, 2H), 6.27 (d, J = 2.2 Hz, 1H), 4.65 (d, J = 14.0 Hz, 1H), 4.59 (t, J = 14.0, 1.9 Hz, 1H), 4.08 (t, J = 8.0 Hz, 1H), 3.78 (s, 3H), 3.43 (t, J = 8.0 Hz, 1H), 3.07 – 2.93 (m, 1H), 1.24 (d, J = 2.6 Hz, 12H), 1.22 – 1.15 (m, 1H), 0.98 (dd, J = 15.9, 8.3 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 158.2 (C), 144.7 (C), 130.5 (C), 129.2 (2 $\times$ CH), 119.3 (CH), 114.0 (2 $\times$ CH), 83.3 (2 $\times$ C), 74.2 (CH_2), 70.2 (CH_2), 55.3 (CH_3), 41.1 (CH), 25.0 (2 $\times$ CH_3), 24.8 (2 $\times$ CH_3), 14.1 (br m, $\text{CH}_2\text{-B}$). HRMS (ESI, MeOH) calcd. for $\text{C}_{19}\text{H}_{27}\text{BO}_4$ $[\text{M} + \text{Na}]^+$: 353.2310; Found: 353.1898.

(Z)-4,4,5,5-tetramethyl-2-((4-(4-(trifluoromethyl)benzylidene)tetrahydrofuran-3-yl)methyl)-1,3,2-



dioxaborolane (2d): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a yellow oil in 52% yield (76 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.58 (d, J = 8.2 Hz, 2H), 7.21 (d, J = 8.2 Hz, 2H), 6.37 (d, J = 2.3 Hz, 1H), 4.68 (d, J = 14.1 Hz, 1H), 4.61 (dt, J = 14.1, 8.2 Hz, 1H), 4.12 (t, J = 8.1 Hz, 1H), 3.47 (t, J = 8.1 Hz, 1H), 3.11 – 2.99 (m, 1H), 1.25 (d, J = 2.7 Hz, 12H), 1.19 (d, J = 5.8 Hz, 1H), 1.02 (dd, J = 16.0, 8.3 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 150.4 (C), 141.1 (C), 128.5 (C), 128.1 (4 $\times$ CH), 125.5 (q, J = 3.8 Hz, CF_3), 118.9 (CH), 83.5 (2 $\times$ C), 74.2 (CH_2), 70.2 (CH_2), 41.5 (CH), 25.0 (2 $\times$ CH_3), 24.9 (2 $\times$ CH_3), 14.0 (br m, $\text{CH}_2\text{-B}$). HRMS (ESI, MeOH) calcd. for $\text{C}_{19}\text{H}_{24}\text{BF}_3\text{O}_3$ $[\text{M} + \text{H}]^+$: 368.2032; Found: 368.1721.

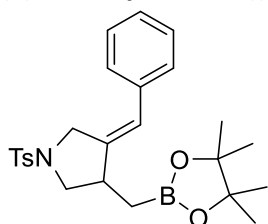
(Z)-4-((4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)dihydrofuran-3(2H)-



ylidene)methyl)benzonitrile (2e): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a white solid in 24% yield (31 mg). M.p. = 108 – 110 $^\circ\text{C}$. ^1H NMR (300 MHz, CDCl_3) δ 7.61 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8.4 Hz, 2H), 6.35 (q, J = 2.3 Hz, 1H), 4.67 (dd, J = 14.7, 1.6 Hz, 1H), 4.59 (dt, J = 14.7, 2.2 Hz, 1H), 4.14 (t, J = 7.4 Hz, 1H), 3.47 (t, J = 8.1 Hz, 1H), 3.11 – 2.98 (m, 1H), 1.24 (d, J = 2.9 Hz, 12H), 1.18 (dd, J = 16.0, 5.8 Hz, 1H), 1.01 (dd, J = 16.0, 8.4 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 152.1 (C), 142.1 (C), 132.4 (2 $\times$ CH), 128.4 (2 $\times$ CH), 119.1 (C), 118.8 (CH), 109.8 (C), 83.6 (2 $\times$ C), 74.2 (CH_2), 70.3 (CH_2), 41.7 (CH), 25.1 (2 $\times$ CH_3), 24.9 (2 $\times$ CH_3),

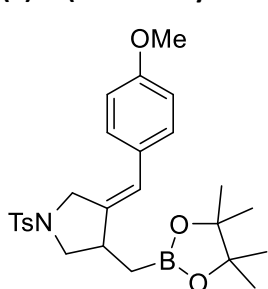
14.0 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₁₉H₂₄BNO₃ [M + Na]⁺: 348.2150; Found: 348.1754.

(Z)-3-benzylidene-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-1-tosylpyrrolidine



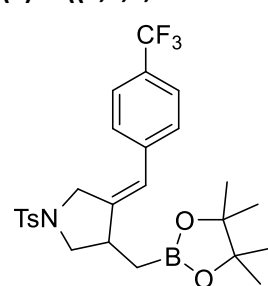
(2f):³⁹ The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a brown solid in 63% yield (114 mg). M.p. = 125 – 127 °C. ¹H NMR (300 MHz, CDCl₃) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.39 – 7.28 (m, 3H), 7.24 – 7.22 (m, 2H), 7.12 (d, *J* = 7.6 Hz, 2H), 6.24 (d, *J* = 2.4 Hz, 1H), 4.26 (dd, *J* = 14.8, 1.6 Hz, 1H), 3.99 (dt, *J* = 14.8, 1.6 Hz, 1H), 3.64 (dd, *J* = 8.8, 7.3 Hz, 1H), 2.96 (m, 1H), 2.80 (t, *J* = 8.8 Hz, 1H), 2.41 (s, 3H), 1.19 (d, *J* = 5.7 Hz, 12H), 1.11 (dd, *J* = 16.0, 5.7 Hz, 1H), 0.93 (dd, *J* = 16.0, 8.1 Hz, 1H).

(Z)-3-(4-methoxybenzylidene)-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-1-tosylpyrrolidine (2g):



The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a brown solid in 63% yield (120 mg). M.p. = 157 – 159 °C. ¹H NMR (300 MHz, CDCl₃) δ 7.72 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.06 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.17 (d, *J* = 2.6 Hz, 1H), 4.23 (d, *J* = 14.5 Hz, 1H), 3.97 (dd, *J* = 14.6, 2.6 Hz, 1H), 3.81 (s, 3H), 3.62 (dd, *J* = 8.6, 7.6 Hz, 1H), 3.05 – 2.90 (m, 1H), 2.79 (t, *J* = 8.6 Hz, 1H), 2.41 (s, 3H), 1.18 (d, *J* = 5.8 Hz, 12H), 1.11 (dd, *J* = 16.0, 5.5 Hz, 1H), 0.93 (dd, *J* = 16.0, 8.0 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 158.5 (C), 143.5 (C), 140.1 (C), 133.2 (C), 129.7 (2 × CH), 129.5 (C), 129.4 (2 × CH), 127.8 (CH), 121.4 (2 × CH), 114.0 (2 × CH), 83.4 (2 × C), 55.3 (CH₃), 53.7 (CH₂), 50.8 (CH₂), 40.3 (CH), 24.9 (2 × CH₃), 24.8 (2 × CH₃), 21.5 (CH₃), 14.1 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₂₆H₃₄BNO₅S [M + H]⁺: 484.2251; Found: 484.2327.

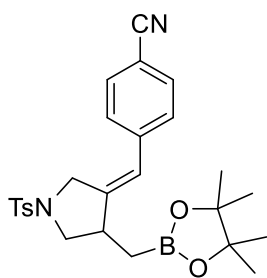
(Z)-3-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-1-tosyl-4-(4-



(trifluoromethyl)benzylidene)pyrrolidine (2h): The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a brown solid in 43% yield (90 mg). M.p. = 112 – 114 °C. ¹H NMR (300 MHz, CDCl₃) δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 6.28 (s, 1H), 4.24 (d, *J* = 14.9 Hz, 1H), 3.97 (d, *J* = 14.9 Hz, 1H), 3.65 (t, *J* = 8.2 Hz, 1H), 3.07 – 2.93 (m, 1H), 2.83 (t, *J* = 8.7 Hz, 1H), 2.39 (s, 3H), 1.17 (d, *J* = 5.0 Hz, 12H), 1.09 (dd, *J* = 13.6, 5.0 Hz, 1H), 0.96 (dd, *J* = 16.1, 7.9 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 145.5 (C), 143.7 (C), 140.3 (C), 140.2 (C), 133.0 (C), 129.9 (2 × CH), 129.8 (2 × CH), 128.3 (2 × CH), 127.9 (2 × CH), 125.5 (q, *J* = 3.6 Hz, CF₃), 120.9 (CH), 83.5 (2 × C), 53.6 (CH₂), 50.9 (CH₂), 40.5 (CH), 24.9 (2 × CH₃), 24.7 (2 × CH₃), 21.5 (CH₃), 14.3 (br m, CH₂-B). HRMS (ESI, MeCN) calcd. for C₂₆H₃₁BF₃NO₄S [M + Na]⁺: 544.4022; Found: 544.1914.

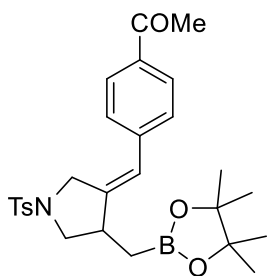
³⁹ T. Xi, Z. Lu, *ACS Catal.*, **2017**, 7, 1181 – 1185.

(Z)-4-((4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-1-tosylpyrrolidin-3-



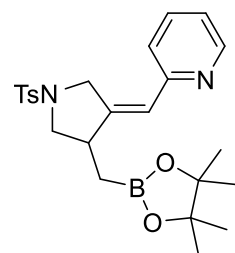
ylidene)methyl)benzonitrile (2i): The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as an orange oil in 61% yield (116 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.72 (d, J = 8.2 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.2 Hz, 2H), 7.19 (d, J = 8.4 Hz, 2H), 6.26 (d, J = 2.4 Hz, 1H), 4.24 (dd, J = 15.1, 1.9 Hz, 1H), 3.96 (dt, J = 15.1, 1.9 Hz, 1H), 3.66 (dd, J = 9.0, 7.4 Hz, 1H), 3.05 – 2.96 (m, 1H), 2.82 (t, J = 9.0 Hz, 1H), 2.42 (s, 3H), 1.18 (d, J = 4.4 Hz, 12H), 1.11 (dd, J = 16.1, 5.5 Hz, 1H), 0.93 (dd, J = 16.1, 8.1 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 146.9 (C), 143.8 (C), 141.2 (C), 132.9 (C), 132.4 (2 $\times$ CH), 129.8 (2 $\times$ CH), 128.5 (2 $\times$ CH), 127.8 (2 $\times$ CH), 120.7 (CH), 118.8 (C), 110.3 (C), 83.5 (2 $\times$ C), 53.5 (CH_2), 50.9 (CH_2), 40.7 (CH), 24.9 (2 $\times$ CH_3), 24.7 (2 $\times$ CH_3), 21.6 (CH_3), 14.0 (br m, $\text{CH}_2\text{-B}$). HRMS (ESI, MeOH) calcd. for $\text{C}_{26}\text{H}_{31}\text{BN}_2\text{O}_4\text{S}$ [$\text{M} + \text{H}$] $^+$: 479.2098; Found: 479.2161.

(Z)-1-(4-((4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-1-tosylpyrrolidin-3-

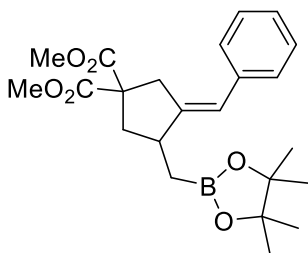


ylidene)methyl)phenyl)ethan-1-one (2j): The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a light brown solid in 68% yield (68 mg). M.p. = 61 – 63 $^\circ\text{C}$. ^1H NMR (300 MHz, CDCl_3) δ 7.92 (d, J = 8.4 Hz, 2H), 7.72 (d, J = 8.3 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.19 (d, J = 8.3 Hz, 2H), 6.28 (d, J = 2.3 Hz, 1H), 4.27 (dd, J = 14.8, 1.4 Hz, 1H), 3.99 (dt, J = 4.3, 1.9 Hz, 1H), 3.66 (dd, J = 9.0, 7.5 Hz, 1H), 3.07 – 2.95 (m, 1H), 2.82 (t, J = 8.7 Hz, 1H), 2.60 (s, 3H), 2.41 (s, 3H), 1.18 (d, J = 5.5 Hz, 12H), 1.12 (dd, J = 16.0, 5.5 Hz, 1H), 0.96 (dd, J = 16.0, 8.0 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 197.5 (C), 145.7 (C), 143.7 (C), 141.4 (C), 135.4 (C), 133.0 (C), 129.8 (2 $\times$ CH), 128.7 (2 $\times$ CH), 128.2 (2 $\times$ CH), 127.9 (2 $\times$ CH), 121.3 (C), 83.5 (2 $\times$ C), 53.6 (CH_2), 51.0 (CH_2), 40.7 (CH), 26.6 (CH_3), 24.9 (2 $\times$ CH_3), 24.8 (2 $\times$ CH_3), 21.6 (CH_3), 14.0 (br m, $\text{CH}_2\text{-B}$). HRMS (ESI, MeOH) calcd. for $\text{C}_{27}\text{H}_{34}\text{BNO}_5\text{S}$ [$\text{M} + \text{Na}$] $^+$: 518.4410; Found: 518.2144.

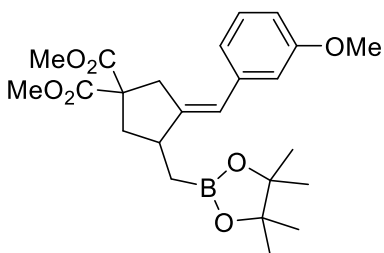
(Z)-2-((4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-1-tosylpyrrolidin-3-



ylidene)methyl)pyridine (2k): The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a brown oil in 41% yield (64 mg). ^1H NMR (300 MHz, CDCl_3) δ 8.57 (s, 1H), 7.74 (d, J = 8.0 Hz, 2H), 7.65 – 7.47 (m, 1H), 7.28 (d, J = 8.0 Hz, 2H), 7.14 – 6.97 (m, 2H), 6.23 (d, J = 2.1 Hz, 1H), 4.55 (t, J = 14.2 Hz, 1H), 4.33 (t, J = 16.1 Hz, 1H), 3.70 – 3.51 (m, 1H), 3.04 – 2.94 (m, 1H), 2.82 – 2.68 (m, 1H), 2.38 (s, 3H), 1.18 (d, J = 5.4 Hz, 12H), 1.12 (dd, J = 16.0, 5.4 Hz, 1H), 0.92 (dd, J = 16.0, 8.5 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 155.8 (C), 149.5 (CH), 148.4 (C), 143.4 (C), 136.2 (CH), 133.2 (C), 129.7 (2 $\times$ CH), 128.0 (2 $\times$ CH), 123.5 (CH), 120.8 (CH), 120.4 (CH), 83.5 (2 $\times$ C), 53.7 (CH_2), 52.7 (CH_2), 40.4 (CH), 24.9 (2 $\times$ CH_3), 24.8 (2 $\times$ CH_3), 21.6 (CH_3), 14.1 (br m, $\text{CH}_2\text{-B}$). HRMS (ESI, MeOH) calcd. for $\text{C}_{24}\text{H}_{31}\text{BN}_2\text{O}_4\text{S}$ [$\text{M} + \text{H}$] $^+$: 455.3920; Found: 455.2157.

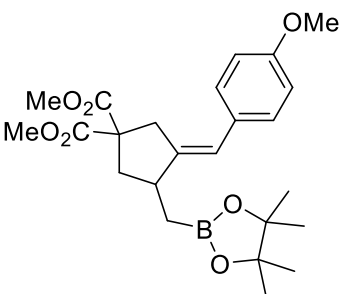
Dimethyl

(E)-3-benzylidene-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)cyclopentane-1,1-dicarboxylate (2l):⁴⁰ The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a brown oil in 58% yield (93 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.35 – 7.28 (m, 4H), 7.18 (t, J = 6.8 Hz, 1H), 6.25 (q, J = 2.3 Hz, 1H), 3.73 (s, 3H), 3.71 (s, 3H), 3.37 (d, J = 17.6 Hz, 1H), 3.20 (dt, J = 17.6, 2.5 Hz, 1H), 2.95 – 2.84 (m, 1H), 2.65 (ddd, J = 12.7, 7.2, 1.3 Hz, 1H), 1.89 (d, J = 12.7, 11.5 Hz, 1H), 1.24 (s, 12H), 1.18 (dd, J = 15.8, 7.7 Hz, 1H), 1.01 (dd, J = 15.8, 5.8 Hz, 1H).

Dimethyl

(E)-3-(3-methoxybenzylidene)-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)cyclopentane-1,1-dicarboxylate (2m):

The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a brown oil in 67% yield (119 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.21 (t, J = 7.9 Hz, 1H), 6.87 (d, J = 7.9 Hz, 1H), 6.80 (s, 1H), 6.72 (dd, J = 7.9, 2.3 Hz, 1H), 6.22 (d, J = 2.0 Hz, 1H), 3.78 (s, 3H), 3.70 (d, J = 1.6 Hz, 6H), 3.36 (d, J = 17.5 Hz, 1H), 3.19 (dt, J = 17.5, 2.1 Hz, 1H), 2.95 – 2.83 (m, 1H), 2.63 (dd, J = 12.7, 7.2 Hz, 1H), 1.89 (t, J = 12.0 Hz, 1H), 1.23 (s, 12H), 1.16 (dd, J = 15.7, 5.6 Hz, 1H), 1.00 (dd, J = 15.7, 7.7 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 172.3 (C), 172.3 (C), 159.5 (C), 147.1 (C), 139.5 (C), 129.2 (CH), 121.5 (CH), 121.0 (CH), 114.1 (CH), 111.6 (CH), 83.2 (2 $\times$ C), 59.1 (C), 55.2 (CH₃), 52.8 (CH₃), 52.7 (CH₃), 41.2 (CH₂), 40.5 (CH), 39.0 (CH₂), 25.0 (2 $\times$ CH₃), 24.8 (2 $\times$ CH₃), 16.0 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₂₄H₃₃BO₇ [M + Na]⁺: 467.3310; Found: 467.2222.

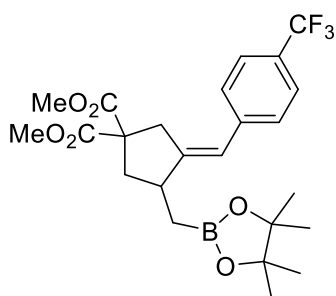
Dimethyl

(E)-3-(4-methoxybenzylidene)-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)cyclopentane-1,1-dicarboxylate (2n):

The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a brown oil in 70% yield (123 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.20 (d, J = 8.6 Hz, 2H), 6.84 (d, J = 8.6 Hz, 2H), 6.17 (d, J = 2.0 Hz, 1H), 3.77 (s, 3H), 3.69 (s, 6H), 3.32 (d, J = 17.4 Hz, 1H), 3.15 (dt, J = 17.4, 2.4 Hz, 1H), 2.94 – 2.82 (m, 1H), 2.62 (ddd, J = 12.6, 7.2, 1.0 Hz, 1H), 1.87 (t, J = 12.0 Hz, 1H), 1.22 (s, 12H), 1.14 (dd, J = 15.7, 5.8 Hz, 1H), 0.98 (dd, J = 15.7, 7.7 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 172.3 (2 $\times$ C), 158.0 (C), 144.4 (C), 130.9 (C), 129.5 (2 $\times$ CH), 120.9 (CH), 113.7 (2 $\times$ CH), 83.1 (2 $\times$ C), 59.1 (C), 55.2 (CH₃), 52.8 (CH₃), 52.7 (CH₃), 41.2 (CH₂), 40.4 (CH), 38.8 (CH₂), 25.0 (2 $\times$ CH₃), 24.7 (2 $\times$ CH₃), 15.7 (br m, CH₂-B). HRMS (ESI, MeCN) calcd. for C₂₄H₃₃BO₇ [M + Na]⁺: 467.3310; Found: 467.2216.

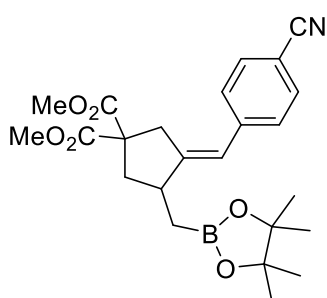
⁴⁰ J. Marco-Martínez, V. López-Carrillo, E. Buñuel, R. Simancas, D. J. Cárdenas, *J. Am. Chem. Soc.*, **2007**, *129*, 1874-1875.

Dimethyl



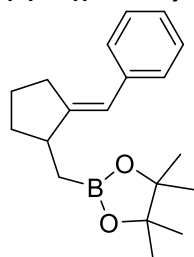
(E)-3-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-4-(4-(trifluoromethyl)benzylidene)cyclopentane-1,1-dicarboxylate (2o):¹⁴ The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a brown oil in 37% yield (35 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.56 (d, J = 8.2 Hz, 2H), 7.36 (d, J = 8.2 Hz, 2H), 6.28 (d, J = 2.2 Hz, 1H), 3.73 (s, 6H), 3.72 (s, 6H), 3.35 (d, J = 17.6 Hz, 1H), 3.19 (dt, J = 17.6, 2.5 Hz, 1H), 3.02 – 2.83 (m, 1H), 2.66 (ddd, J = 12.6, 7.3, 1.3 Hz, 1H), 1.92 (dd, J = 12.6, 11.5 Hz, 1H), 1.24 (d, J = 1.8 Hz, 6H), 1.17 (dd, J = 15.9, 5.8 Hz, 1H), 1.03 (dd, J = 15.9, 7.7 Hz, 1H).

Dimethyl

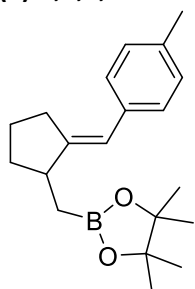


(E)-3-(4-cyanobenzylidene)-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)cyclopentane-1,1-dicarboxylate (2p): The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a light brown oil in 74% yield (123 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.59 (d, J = 8.4 Hz, 1H), 7.34 (d, J = 8.4 Hz, 1H), 6.26 (d, J = 2.3 Hz, 1H), 3.74 (s, 3H), 3.72 (s, 3H), 3.34 (d, J = 17.6 Hz, 1H), 3.18 (dt, J = 17.6, 2.6 Hz, 1H), 2.98 – 2.87 (m, 1H), 2.66 (dd, J = 12.2, 6.8 Hz, 1H), 1.91 (dd, J = 12.6, 11.6 Hz, 1H), 1.23 (d, J = 2.1 Hz, 12H), 1.17 (dd, J = 15.8, 5.7 Hz, 1H), 1.02 (dd, J = 15.8, 7.7 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 172.0 (C), 171.9 (C), 151.4 (C), 142.6 (C), 132.1 (2 $\times$ CH), 128.7 (2 $\times$ CH), 120.4 (CH), 119.1 (C), 109.3 (C), 83.3 (2 $\times$ C), 59.0 (C), 52.9 (CH₃), 52.8 (CH₃), 40.8 (CH), 39.1 (CH₂), 24.9 (2 $\times$ CH₃), 24.7 (2 $\times$ CH₃), 15.6 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₂₄H₃₀BO₆ [M + Na]⁺: 462.3150; Found: 462.2076.

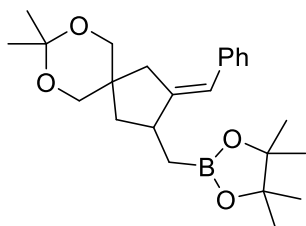
(E)-2-((2-benzylidenecyclopentyl)methyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2q): The compound was purified by column chromatography (cyclohexane/EtOAc 98:2) and was obtained as a yellow oil in 37% yield (49 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.31 (d, J = 4.3 Hz, 4H), 7.15 (td, J = 8.5, 4.3 Hz, 1H), 6.27 (d, J = 2.3 Hz, 1H), 2.80 – 2.51 (m, 3H), 2.07 – 1.77 (m, 3H), 1.73 – 1.51 (m, 1H), 1.26 (d, J = 2.3 Hz, 12H), 1.18 (dd, J = 15.6, 5.7 Hz, 1H), 0.95 (dd, J = 15.6, 8.5 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 152.2 (C), 139.2 (C), 128.2 (4 $\times$ CH), 125.7 (CH), 120.2 (CH), 83.2 (2 $\times$ C), 42.5 (CH), 34.5 (CH₂), 31.4 (CH₂), 25.1 (2 $\times$ CH₃), 24.9 (2 $\times$ CH₃), 24.8 (CH₂), 16.9 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₁₉H₂₇BO₂ [M + H]⁺: 299.2330; Found: 299.2176.



(E)-4,4,5,5-tetramethyl-2-((2-(4-methylbenzylidene)cyclopentyl)methyl)-1,3,2-dioxaborolane (2r): The compound was purified by column chromatography (cyclohexane/EtOAc 98:2) and was obtained as a colorless oil in 22% yield (28 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.21 (d, J = 8.1 Hz, 2H), 7.11 (d, J = 8.1 Hz, 2H), 6.23 (d, J = 2.3 Hz, 1H), 2.80 – 2.45 (m, 3H), 2.33 (s, 3H), 2.03 – 1.75 (m, 2H), 1.69 – 1.51 (m, 2H), 1.26 (d, J = 2.3 Hz, 12H), 1.19 (dd, J = 15.6, 5.5 Hz, 1H), 0.94 (dd, J = 15.6, 8.5 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 151.1 (C), 136.4 (C), 135.2 (C), 129.0 (2 $\times$ CH), 128.1 (2 $\times$ CH), 120.0 (CH), 83.1 (2 $\times$ C), 42.4 (CH), 34.5 (CH₂), 31.3 (CH₂), 25.1 (2 $\times$ CH₃), 24.9 (2 $\times$ CH₃), 24.8 (CH₂), 21.2 (CH₃), 16.7 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₂₀H₂₉BO₂ [M + Na]⁺: 335.2600; Found: 335.2163.

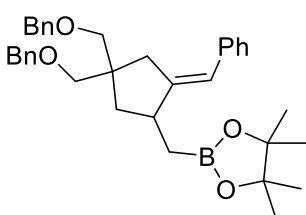


(E)-2-((3-benzylidene-8,8-dimethyl-7,9-dioxaspiro[4.5]decan-2-yl)methyl)-4,4,5,5-



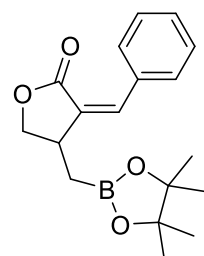
tetramethyl-1,3,2-dioxaborolane (2s): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a yellow oil in 64% yield (51 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.34 – 7.27 (m, 4H), 7.21 – 7.11 (m, 1H), 6.26 (q, J = 2.2 Hz, 1H), 3.74 – 3.50 (m, 4H), 2.85 – 2.82 (m, 1H), 2.77 (d, J = 17.3 Hz, 1H), 2.48 (d, J = 17.3 Hz, 1H), 2.02 (dd, J = 12.5, 7.9 Hz, 1H), 1.43 (s, 3H), 1.41 (s, 3H), 1.37 – 1.31 (m, 1H), 1.24 (d, J = 1.2 Hz, 12H), 1.16 (dd, J = 15.7, 5.1 Hz, 1H), 0.98 (dd, J = 15.7, 8.0 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 149.1 (C), 138.6 (C), 128.4 (2 $\times$ CH), 128.3 (2 $\times$ CH), 126.0 (CH), 121.6 (CH), 98.0 (C), 83.2 (2 $\times$ C), 70.0 (CH_2), 68.4 (CH_2), 40.9 (C), 40.4 (CH_2), 39.6 (CH), 39.0 (CH_2), 25.1 (2 $\times$ CH_3), 24.9 (3 $\times$ CH_3), 23.1 (CH_3), 16.7 (br m, CH_2 -B). HRMS (ESI, MeOH) calcd. for $\text{C}_{24}\text{H}_{35}\text{BO}_4$ [$\text{M} + \text{Na}$] $^+$: 421.3500; Found: 421.2358.

(E)-2-((2-benzylidene-4,4-bis((benzyloxy)methyl)cyclopentyl)methyl)-4,4,5,5-tetramethyl-



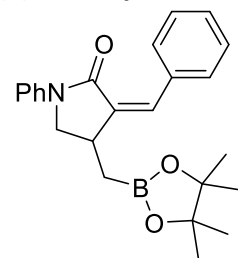
1,3,2-dioxaborolane (2t): The compound was purified by column chromatography (cyclohexane/EtOAc 98:2) and was obtained as a pale yellow oil in 58% yield (124 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.32 – 7.27 (m, 15H), 6.23 (d, J = 2.2 Hz, 1H), 4.50 (d, J = 1.9 Hz, 4H), 3.47 – 3.40 (m, 4H), 2.89 (s, 1H), 2.55 (dt, J = 17.3, 2.2 Hz, 2H), 2.05 (dd, J = 12.7, 7.9 Hz, 1H), 1.24 (d, J = 2.1 Hz, 13H), 1.18 (d, J = 6.2 Hz, 1H), 0.95 (dd, J = 15.5, 8.2 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 150.4 (C), 139.1 (C), 139.0 (C), 138.8 (C), 128.5 (2 $\times$ CH), 128.4 (2 $\times$ CH), 128.2 (2 $\times$ CH), 127.6 (2 $\times$ CH), 127.5 (2 $\times$ CH), 127.5 (2 $\times$ CH), 127.4 (2 $\times$ CH), 125.8 (CH), 120.9 (CH), 83.2 (2 $\times$ C), 75.2 (CH_2), 73.4 (CH_2), 73.3 (CH_2), 72.9 (CH_2), 46.9 (C), 40.0 (CH), 39.5 (CH_2), 38.1 (CH_2), 25.1 (2 $\times$ CH_3), 24.9 (2 $\times$ CH_3), 16.7 (br m, CH_2 -B). HRMS (ESI, MeOH) calcd. for $\text{C}_{35}\text{H}_{43}\text{BO}_4$ [M] $^+$: 539.5350; Found: 539.3326.

(Z)-3-benzylidene-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)dihydrofuran-



2(3H)-one (2u): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a colorless oil in 66% yield (83 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.81 (d, J = 7.8 Hz, 2H), 7.43 – 7.29 (m, 3H), 6.92 (d, J = 2.1 Hz, 1H), 4.54 (t, J = 8.4 Hz, 1H), 3.98 (dd, J = 8.7, 6.5 Hz, 1H), 3.39 (d, J = 6.5 Hz, 1H), 1.25 (d, J = 2.1 Hz, 12H), 1.13 (dd, J = 16.1, 8.3 Hz, 2H). ^{13}C NMR (75 MHz, CDCl_3) δ 169.2 (C), 138.6 (CH), 133.8 (C), 130.7 (2 $\times$ CH), 130.4 (C), 129.3 (CH), 128.1 (2 $\times$ CH), 83.7 (2 $\times$ C), 72.1 (CH_2), 38.3 (CH), 25.0 (2 $\times$ CH_3), 24.8 (2 $\times$ CH_3), 15.9 (br m, CH_2 -B). HRMS (ESI, MeCN) calcd. for $\text{C}_{18}\text{H}_{23}\text{BO}_4$ [$\text{M} + \text{Na}$] $^+$: 337.1880; Found: 337.1588.

(Z)-3-benzylidene-1-phenyl-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-

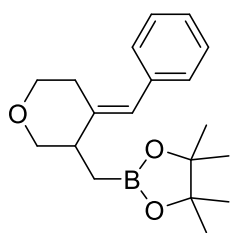


yl)methyl)pyrrolidin-2-one (2v): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a pale yellow oil in 77% yield (120 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.82 (d, J = 7.1 Hz, 2H), 7.68 (dd, J = 8.6, 0.9 Hz, 2H), 7.41 – 7.27 (m, 5H), 7.15 (t, J = 7.4 Hz, 1H), 6.80 (d, J = 2.1 Hz, 1H), 4.06 (dd, J = 9.2, 8.2 Hz, 1H), 3.56 (dd, J = 9.2, 5.3 Hz, 1H), 3.35 – 3.20 (m, 1H), 1.37 (dd, J = 16.1, 5.6 Hz, 1H), 1.26 (s, 12H), 1.20 (dd, J = 16.1, 8.4 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ

166.1 (C), 139.9 (C), 137.5 (C), 134.7 (C), 134.6 (CH), 130.5 (2 $\times$ CH), 128.7 (2 $\times$ CH), 128.3 (CH), 127.8 (2 $\times$ CH), 124.5 (CH), 120.1 (2 $\times$ CH), 83.5 (2 $\times$ C), 53.2 (CH_2), 34.7 (CH), 25.0 (2 $\times$ CH_3), 24.8

(2 × CH₃), 17.3 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₂₄H₂₈BNO₃ [M + H]⁺: 390.3020; Found: 390.2226.

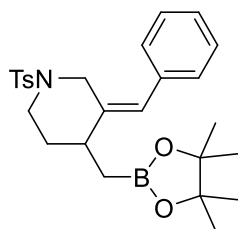
(E)-2-((4-benzylidenetetrahydro-2H-pyran-3-yl)methyl)-4,4,5,5-tetramethyl-1,3,2-



dioxaborolane (2w): The compound was purified by column chromatography (cyclohexane/EtOAc 98:2) and was obtained as a yellow oil in 9% yield (11 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.30 (t, *J* = 7.3 Hz, 2H), 7.22 – 7.15 (m, 3H), 6.34 (s, 1H), 3.87 (dd, *J* = 10.7, 4.0 Hz, 1H), 3.73 – 3.64 (m, 1H), 3.63 – 3.54 (m, 1H), 3.42 (dd, *J* = 10.7, 7.0 Hz, 1H), 2.74 – 2.57 (m, 2H), 2.43 – 2.32 (m, 1H), 1.23 (s, 12H), 1.15 (dd, *J* = 15.6, 8.0 Hz, 1H), 0.96 (dd, *J* = 15.6, 7.2 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 142.6 (C), 138.0 (C),

129.1 (2 × CH), 128.2 (2 × CH), 126.2 (CH), 122.0 (CH), 83.3 (2 × C), 75.5 (CH₂), 69.2 (CH₂), 40.9 (CH), 29.4 (CH₂), 25.1 (2 × CH₃), 25.0 (2 × CH₃), 12.5 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₁₉H₂₇BNO₃ [M + Na]⁺: 337.2320; Found: 337.1951.

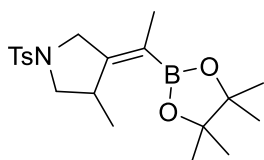
(Z)-3-benzylidene-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-1-tosylpiperidine



(2x): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a brown oil in 26% yield (23 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.58 (d, *J* = 8.2 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 3H), 7.30 – 7.30 (m, 5H), 6.39 (s, 1H), 4.31 (d, *J* = 12.4 Hz, 1H), 3.62 – 3.50 (m, 1H), 3.18 (d, *J* = 12.4 Hz, 1H), 2.88 – 2.78 (m, 1H), 2.42 (s, 3H), 1.97 – 1.84 (m, 1H), 1.61 – 1.47 (m, 2H), 1.22 (s, 12H), 1.11 (dd, *J* = 15.7, 7.5 Hz, 1H), 0.88 (dd, *J* = 15.7, 7.3 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ

143.5 (C), 138.5 (C), 136.9 (C), 133.4 (C), 129.7 (2 × CH), 129.1 (2 × CH), 128.5 (2 × CH), 128.0 (2 × CH), 126.9 (CH), 124.5 (CH), 83.4 (2 × C), 47.0 (CH₂), 45.7 (CH₂), 38.2 (CH), 34.5 (CH₂), 25.0 (4 × CH₃), 21.6 (CH₃), 14.8 (br m, CH₂-B). HRMS (ESI, MeOH) calcd. for C₂₆H₃₄BNO₄S [M + Na]⁺: 490.4310; Found: 490.2205.

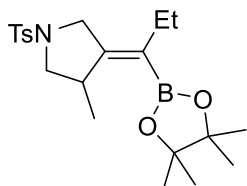
(Z)-3-methyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethylidene)-1-tosylpyrrolidine



(4a):³⁷ The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a white solid in 71% yield (108 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 4.05 (dd, *J* = 15.6, 1.2 Hz, 1H), 3.49 (dd, *J* = 15.6, 1.2 Hz, 1H), 3.27 (t, *J* = 8.2 Hz, 2H), 2.95 (dd, *J* = 8.9, 6.1 Hz, 1H), 2.40 (s, 3H),

1.55 (s, 3H), 1.20 (s, 12H), 1.10 (d, *J* = 6.1 Hz, 3H).

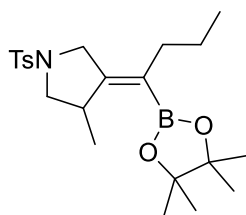
(Z)-3-methyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propylidene)-1-



tosylpyrrolidine (4b): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a white solid in 61% yield (92 mg). M.p. = 132 – 134 °C. ¹H NMR (300 MHz, CDCl₃) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 4.09 (d, *J* = 15.3 Hz, 1H), 3.56 (d, *J* = 15.3 Hz, 1H), 3.25 (t, *J* = 7.4 Hz, 2H), 2.96 (dd, *J* = 8.6, 6.4 Hz, 1H), 2.41 (s, 3H), 1.93 (q, *J* = 7.4 Hz, 2H), 1.21 (s, 12H), 1.09 (d, *J* = 6.9 Hz, 3H), 0.86 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 155.5 (C), 143.6 (C), 132.5 (C), 129.7 (2 × CH), 128.0 (2 × CH), 83.1 (2 × C), 55.1 (CH₂), 50.1 (CH₂), 37.7 (CH), 25.4 (CH₂), 25.0 (2 × CH₃), 24.7 (2 × CH₃), 21.9 (CH₃), 21.6 (CH₃), 13.9 (CH₃). HRMS (ESI, MeOH) calcd. for C₂₁H₃₂BNO₄S [M + H]⁺:

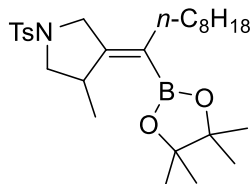
406.3600; Found: 406.2220.

(Z)-3-methyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butylidene)-1-tosylpyrrolidine



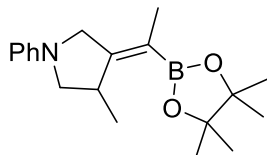
(4c): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a colorless oil in 59% yield (47 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.69 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 4.09 (d, J = 15.3 Hz, 1H), 3.58 (d, J = 15.3 Hz, 1H), 3.26 (d, J = 8.6 Hz, 1H), 2.96 (dd, J = 8.9, 6.2 Hz, 1H), 2.41 (s, 3H), 1.90 (t, J = 7.6 Hz, 2H), 1.28 (dd, J = 14.8, 7.4 Hz, 2H), 1.21 (s, 12H), 1.09 (d, J = 7.0 Hz, 3H), 0.82 (t, J = 7.4 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 156.0 (C), 143.6 (C), 132.6 (C), 129.7 (2 $\times$ CH), 128.0 (2 $\times$ CH), 83.1 (2 $\times$ C), 55.2 (CH_2), 50.4 (CH_2), 37.8 (CH), 34.3 (CH_2), 25.0 (2 $\times$ CH_3), 24.7 (2 $\times$ CH_3), 22.7 (CH_2), 22.0 (CH_3), 21.6 (CH_3), 14.2 (CH_3). HRMS (ESI, MeOH) calcd. for $\text{C}_{22}\text{H}_{34}\text{BNO}_4\text{S}$ [$\text{M} + \text{H}$] $^+$: 420.3870; Found: 420.2372.

(Z)-3-methyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonylidene)-1-



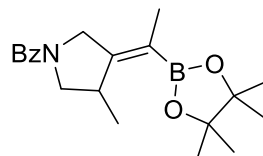
tosylpyrrolidine (4d): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a colorless oil in 45% yield (51 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.70 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 4.09 (d, J = 15.3 Hz, 1H), 3.57 (d, J = 15.3 Hz, 1H), 3.25 (t, J = 8.8 Hz, 2H), 2.96 (dd, J = 8.8, 6.1 Hz, 1H), 2.42 (s, 3H), 1.90 (d, J = 6.7 Hz, 1H), 1.21 (br s, 25H), 1.09 (d, J = 7.0 Hz, 3H), 0.89 (t, J = 6.8 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 155.6 (C), 143.6 (C), 132.6 (C), 129.7 (2 $\times$ CH), 128.1 (2 $\times$ CH), 83.2 (2 $\times$ C), 55.2 (CH_2), 50.4 (CH_2), 37.8 (CH), 32.3 (CH_2), 32.0 (CH_2), 29.7 (CH_2), 29.5 (CH_2), 29.3 (CH_2), 25.0 (2 $\times$ CH_3), 24.7 (2 $\times$ CH_3), 22.8 (CH_2), 22.0 (CH_3), 21.6 (CH_3), 14.3 (CH_3). HRMS (ESI, MeOH) calcd. for $\text{C}_{27}\text{H}_{44}\text{BNO}_4\text{S}$ [M] $^+$: 490.5220; Found: 490.3175.

(Z)-3-methyl-1-phenyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-



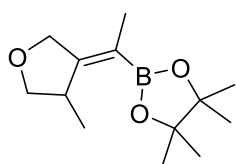
yl)ethylidene)pyrrolidine (4e): The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as colorless oil in 65% yield (82 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.30 – 7.22 (m, 2H), 6.71 (t, J = 7.3 Hz, 1H), 6.65 (d, J = 7.8 Hz, 2H), 4.18 (d, J = 16.0 Hz, 1H), 3.76 (d, J = 16.0 Hz, 1H), 3.54 – 3.40 (m, 1H), 3.32 – 3.22 (m, 2H), 1.73 (s, 3H), 1.29 (d, J = 2.3 Hz, 12H), 1.19 (d, J = 7.0 Hz, 2H). ^{13}C NMR (75 MHz, CDCl_3) δ 160.2 (C), 148.8 (C), 129.3 (2 $\times$ CH), 116.4 (CH), 112.4 (2 $\times$ CH), 83.1 (2 $\times$ C), 77.4 (C), 55.5 (CH_2), 52.2 (CH_2), 37.6 (CH), 25.2 (2 $\times$ CH_3), 24.9 (2 $\times$ CH_3), 23.1 (CH_3), 17.1 (CH_3). HRMS (ESI, MeOH) calcd. for $\text{C}_{19}\text{H}_{28}\text{BNO}_2$ [$\text{M} + \text{H}$] $^+$: 314.2480; Found: 314.2275.

(Z)-(3-methyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethylidene)pyrrolidin-1-



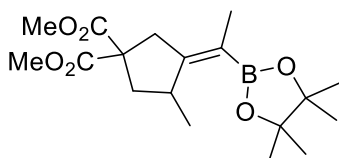
yl)(phenyl)methanone (4f): The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as colorless oil in 75% yield (102 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.52 – 7.45 (m, 2H), 7.43 – 7.37 (m, 3H), 4.56 (d, J = 18.5 Hz, 1H), 4.13 (d, J = 18.5 Hz, 1H), 4.12 – 3.90 (m, 1H), 3.61 (dd, J = 10.6, 6.1 Hz, 1H), 3.40 – 3.19 (m, 1H), 1.70 (s, 3H), 1.24 (d, J = 2.1 Hz, 12H), 1.02 (d, J = 7.0 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 170.1 (C), 157.0 (C), 136.7 (C), 129.9 (2 $\times$ CH), 128.4 (2 $\times$ CH), 127.3 (2 $\times$ CH), 83.2 (2 $\times$ C), 56.7 (CH_2), 49.0 (CH_2), 38.2 (CH), 25.1 (2 $\times$ CH_3), 24.8 (2 $\times$ CH_3), 21.6 (CH_3), 17.0 (CH_3). HRMS (ESI, MeOH) calcd. for $\text{C}_{20}\text{H}_{28}\text{BNO}_3$ [M] $^+$: 342.2580; Found: 342.2238.

(Z)-4,4,5,5-tetramethyl-2-(1-(4-methyldihydrofuran-3(2H)-ylidene)ethyl)-1,3,2-dioxaborolane



(4g):¹⁴ The compound was purified by column chromatography (cyclohexane/EtOAc 98:2) and was obtained as a colorless oil in 15% yield (29 mg). ¹H NMR (300 MHz, CDCl₃) δ 4.48 (d, *J* = 15.0 Hz, 1H), 4.23 (d, *J* = 15.0 Hz, 1H), 3.80 (dd, *J* = 8.3, 5.2 Hz, 1H), 3.71 (d, *J* = 8.3 Hz, 1H), 3.22 (quin, *J* = 6.5 Hz 1H), 1.61 (d, *J* = 0.9 Hz, 3H), 1.27 (d, *J* = 1.1 Hz, 12H), 1.12 (d, *J* = 7.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 161.9 (C), 83.1 (2 × C), 76.1 (CH₂), 70.7 (CH₂), 38.6 (CH), 25.2 (2 × CH₃), 24.8 (2 × CH₃), 21.1 (CH₃), 16.9 (CH₃).

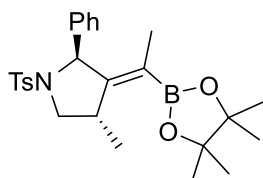
Dimethyl



(E)-3-methyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethylidene)cyclopentane-1,1-dicarboxylate (4h):⁴¹

The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a colorless oil in 18% yield (25 mg). ¹H NMR (300 MHz, CDCl₃) δ 3.74 (s, 3H), 3.70 (s, 3H), 3.27 – 3.23 (m, 1H), 3.16 (d, *J* = 17.8 Hz, 1H), 2.88 (d, *J* = 17.8 Hz, 1H), 2.57 (dd, *J* = 13.3, 8.3 Hz, 1H), 2.09 (dd, *J* = 13.3, 3.1 Hz, 1H), 1.67 (d, *J* = 1.2 Hz, 3H), 1.24 (s, 12H), 1.00 (d, *J* = 7.1 Hz, 3H).

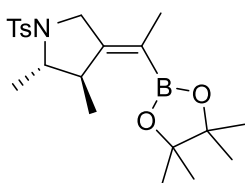
(Z)-4-methyl-2-phenyl-3-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethylidene)-1-



tosylpyrrolidine (4i): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a white solid in 72% yield (68 mg). M.p. = 144 – 146 °C. ¹H NMR (300 MHz, CDCl₃) δ 7.20 – 7.11 (m, 7H), 6.97 (d, *J* = 8.0 Hz, 2H), 5.59 (br s, 1H), 3.57 – 3.41 (m, 3H), 2.29 (s, 3H), 1.27 (s, 3H), 1.24 (d, *J* = 4.6 Hz, 12H), 1.15 (d, *J* = 6.2 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 161.7 (C), 142.3

(C), 140.5 (C), 137.3 (C), 129.1 (2 × CH), 128.9 (2 × CH), 128.3 (2 × CH), 127.4 (CH), 126.9 (2 × CH), 83.3 (2 × C), 66.4 (CH), 54.2 (CH₂), 38.4 (CH), 25.2 (2 × CH₃), 24.8 (2 × CH₃), 23.4 (CH₃), 21.5 (CH₃), 18.1 (CH₃). HRMS (ESI, MeOH) calcd. for C₂₆H₃₄BNO₄S [M + Na]⁺: 490.4310; Found: 490.2184.

(Z)-2,3-dimethyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethylidene)-1-

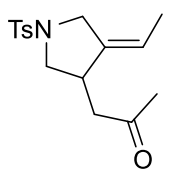


tosylpyrrolidine (4j): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a colorless oil in 54% yield (42 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.75 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 4.04 (dd, *J* = 15.6, 1.0 Hz, 1H), 3.88 (dt, *J* = 15.6, 1.4 Hz, 1H), 3.69 (q, *J* = 6.5 Hz, 1H), 2.93 (q, *J* = 7.0 Hz, 1H), 2.40 (s, 3H), 1.60 (s, 3H), 1.21 (d, *J* = 2.5 Hz, 12H), 1.15 (d, *J* = 6.5 Hz, 3H),

0.67 (d, *J* = 7.0 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 156.8 (C), 143.2 (C), 136.7 (C), 129.7 (2 × CH), 127.3 (2 × CH), 83.2 (2 × CH), 63.7 (CH), 49.1 (CH₂), 45.6 (CH), 25.0 (2 × CH₃), 24.8 (2 × CH₃), 21.9 (CH₃), 21.6 (CH₃), 21.2 (CH₃), 17.1 (CH₃). HRMS (ESI, MeOH) calcd. for C₂₁H₃₂BNO₄S [M + H]⁺: 406.3600; Found: 406.2221.

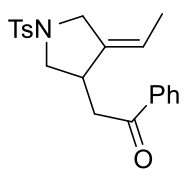
⁴¹ R. E. Kinder, R. A. Widenhoefer, *Org. Lett.*, **2006**, *8*, 1967 – 1969.

(Z)-1-(4-benzylidene-1-tosylpyrrolidin-3-yl)propan-2-one (6a): The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a brown oil in 57% yield (84 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.71 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.30 (m, 4H), 7.11 (d, *J* = 7.3 Hz, 2H), 6.26 (s, 1H), 4.24 (d, *J* = 15.0 Hz, 1H), 3.97 (dd, *J* = 15.0, 2.3 Hz, 1H), 3.36 (dd, *J* = 9.4, 6.8 Hz, 1H), 3.24 (s, 1H), 3.04 (dd, *J* = 9.4, 4.4 Hz, 1H), 2.71 (dd, *J* = 10.2, 6.9 Hz, 2H), 2.42 (s, 3H), 2.16 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 206.7 (C), 143.9 (C), 139.6 (C), 136.3 (C), 132.7 (C), 129.9 (2 × CH), 128.7 (2 × CH), 128.1 (2 × CH), 127.8 (2 × CH), 127.3 (CH), 123.5 (CH), 52.3 (CH₂), 50.5 (CH₂), 47.4 (CH₂), 39.9 (CH), 30.3 (CH₃), 21.6 (CH₃). HRMS (ESI, MeOH) calcd. for C₂₁H₂₃NO₃S [M + H]⁺: 370.4790; Found: 370.1484.

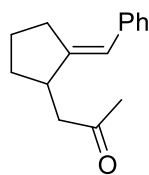


(Z)-1-(4-ethylidene-1-tosylpyrrolidin-3-yl)propan-2-one (6b):⁴² The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a yellow oil in 60% yield (37 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.71 (d, *J* = 8.3 Hz, 2H), 7.34 (d, *J* = 8.3 Hz, 2H), 5.27 – 5.22 (m, 1H), 3.85 (d, *J* = 14.0 Hz, 1H), 3.65 (d, *J* = 14.0 Hz, 1H), 3.36 (dd, *J* = 9.2, 6.6 Hz, 1H), 3.06 – 2.97 (s, 1H), 2.93 (dd, *J* = 9.2, 5.2 Hz, 1H), 2.60 – 2.48 (m, 2H), 2.44 (s, 3H), 2.12 (s, 3H), 1.54 – 1.50 (m, 3H).

(Z)-2-(4-ethylidene-1-tosylpyrrolidin-3-yl)-1-phenylethan-1-one (6c): The compound was purified by column chromatography (cyclohexane/EtOAc 9:1) and was obtained as a yellow oil in 69% yield (51 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.88 (d, *J* = 7.4 Hz, 2H), 7.70 (d, *J* = 8.1 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 5.42 – 5.21 (m, 1H), 3.89 (d, *J* = 14.0 Hz, 1H), 3.72 (d, *J* = 14.0 Hz, 1H), 3.47 (dd, *J* = 9.5, 6.8 Hz, 1H), 3.25 – 3.15 (m, 1H), 3.10 – 2.90 (m, 3H), 2.40 (s, 3H), 1.53 (d, *J* = 6.8 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 198.3 (C), 143.7 (C), 138.8 (C), 136.7 (C), 133.4 (CH), 132.7 (C), 129.8 (2 × CH), 128.7 (2 × CH), 128.1 (2 × CH), 127.9 (2 × CH), 117.8 (CH), 53.7 (CH₂), 49.5 (CH₂), 42.6 (CH₂), 38.4 (CH), 21.6 (CH₃), 14.6 (CH₃). HRMS (ESI, MeOH) calcd. for C₂₁H₂₃NO₃S [M + H]⁺: 370.4790; Found: 370.1483.



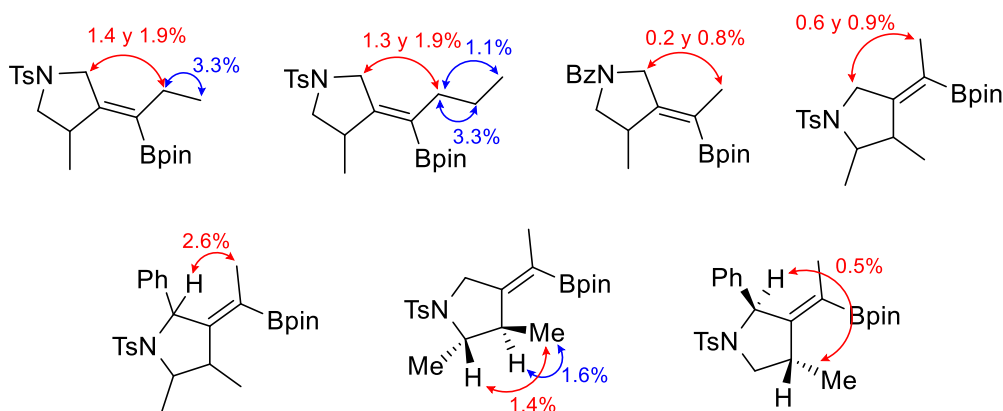
(E)-1-(2-benzylidenecyclopentyl)propan-2-one (6d): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a colorless oil in 24% yield (11 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.33 – 7.27 (m, 4H), 7.21 – 7.14 (m, 1H), 6.22 (q, *J* = 2.3 Hz, 1H), 3.12 – 2.97 (m, 1H), 2.80 (dd, *J* = 16.6, 4.9 Hz, 1H), 2.69 – 2.38 (m, 3H), 2.20 (s, 3H), 2.00 (dt, *J* = 11.7, 6.8 Hz, 1H), 1.90 – 1.76 (m, 1H), 1.74 – 1.55 (m, 1H), 1.35 – 1.22 (m, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 208.4 (C), 149.2 (C), 138.6 (C), 128.3 (2 × CH), 128.2 (2 × CH), 126.1 (CH), 121.1 (CH), 49.3 (CH₂), 41.7 (CH), 32.5 (CH₂), 31.5 (CH₂), 30.6 (CH₃), 25.0 (CH₂). HRMS (ESI, MeOH) calcd. for C₁₅H₁₈O [M + H]⁺: 214.1358; Found: 214.1351.



⁴² J. E. Lee, S. H. Hong, Y. K. Chung, *Tetrahedron Lett.* **1997**, 38, 1781 – 1784.

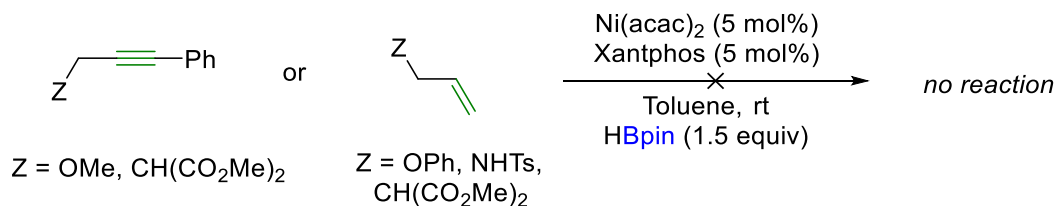
IX. nOe experiments

The *Z/E* configuration of the double bond of alkenylboronates was determined by nOe experiments. Also, these experiments were carried out to determine which diastereomer was obtained.

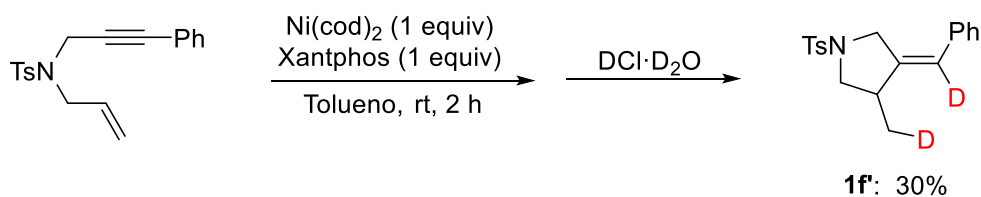
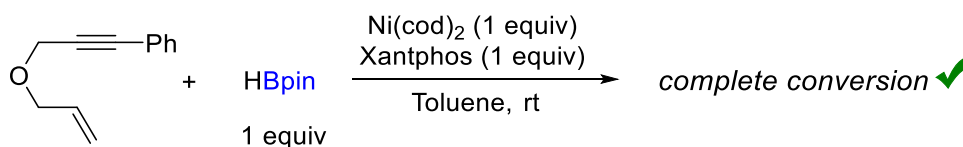
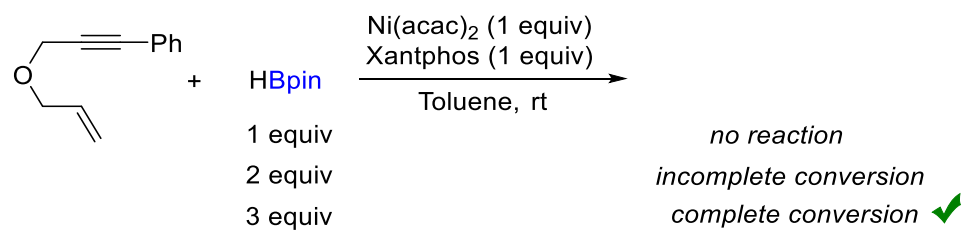


X. Mechanistic studies

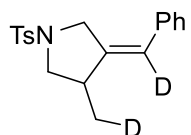
- Reaction with simple alkenes and alkynes:



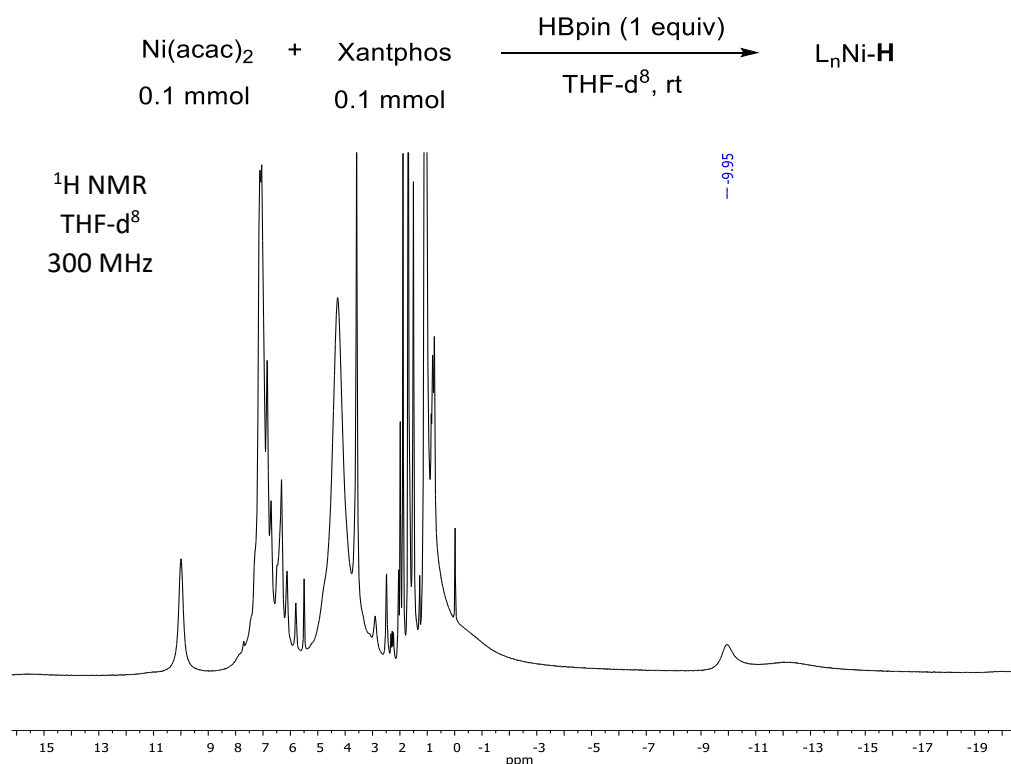
- Stoichiometric reactions



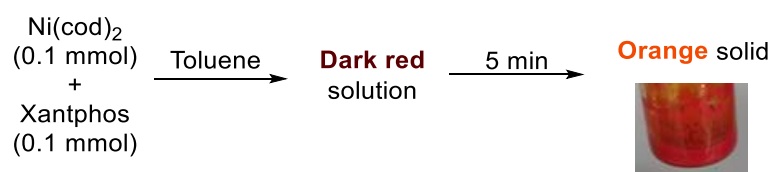
(Z)-3-(methyl-*d*)-4-(phenylmethylene-*d*)-1-tosylpyrrolidine (1f'): The product was obtained as a yellow oil in 30% yield (20 mg). ^1H NMR (300 MHz, CDCl_3) δ 7.72 (d, J = 8.2 Hz, 2H), 7.33 (dd, J = 15.4, 7.7 Hz, 5H), 7.14 (d, J = 7.2 Hz, 2H), 4.24 (d, J = 14.9 Hz, 1H), 4.05 (d, J = 14.9 Hz, 1H), 3.55 (dd, J = 8.9, 7.2 Hz, 1H), 2.95 – 2.80 (m, 1H), 2.77 – 2.67 (m, 1H), 2.41 (s, 3H), 1.17 (d, J = 6.6 Hz, 2H). D NMR (77 MHz, CDCl_3) δ 6.26 (s, 1D), 1.18 (s, 1D). ^{13}C NMR (75 MHz, CDCl_3) δ 143.8 (C), 141.9 (C), 136.7 (C), 133.2 (C), 129.9 (2 $\times$ CH), 128.7 (2 $\times$ CH), 128.2 (2 $\times$ CH), 127.9 (2 $\times$ CH), 127.1 (CH), 122.2 (CD), 54.0 (CH_2), 50.9 (CH_2), 39.2 (CH), 21.7 (CH_3), 16.8 (t, J = 19.0, CH_2D). HRMS (ESI, MeCN) calcd. for $\text{C}_{19}\text{H}_{19}\text{D}_2\text{NO}_2\text{S}$ [$\text{M} + \text{Na}$] $^-$: 353.1419; Found: 352.1303.



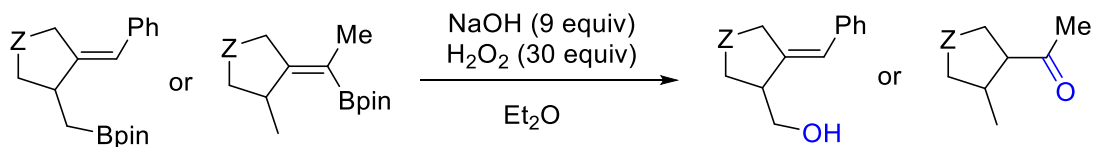
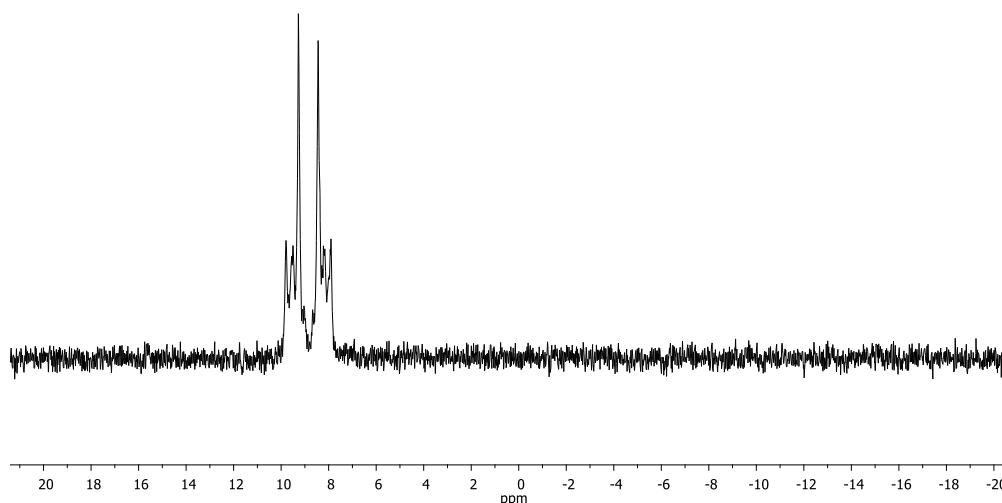
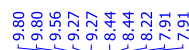
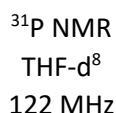
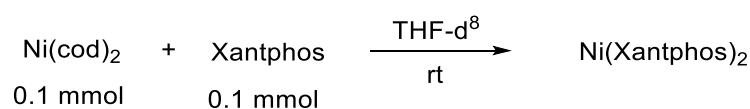
- Nickel hydride



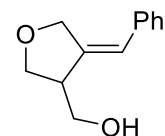
- Nickel complexes⁴³



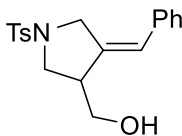
⁴³ W. Goertz, W. Keim, D. Vogt, U. Englert, M. D. K. Boele, L. A. van der Veen, P. C. J. Kamer, P. W. N. M. van Leeuwen, *J. Chem. Soc., Dalton Trans.* **1998**, 2981 – 2988.



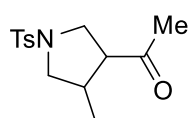
(Z)-(4-benzylidenetetrahydrofuran-3-yl)methanol (7a):³⁹ The product was obtained as a colorless oil in 86% yield (80 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.34 (t, *J* = 7.3 Hz, 2H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.13 (d, *J* = 7.3 Hz, 2H), 6.44 (d, *J* = 1.8 Hz, 1H), 4.68 (dt, *J* = 14.1, 2.0 Hz, 1H), 4.57 (dd, *J* = 14.1, 2.0 Hz, 1H), 3.94 (qd, *J* = 8.9, 5.1 Hz, 2H), 3.73 (d, *J* = 6.2 Hz, 1H), 3.09 – 2.97 (m, 1H), 2.19 (br s, 1H).



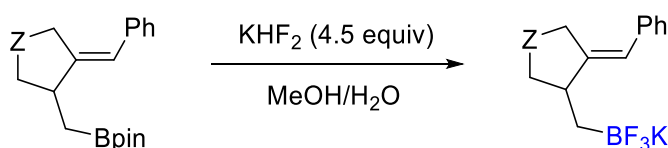
(Z)-(4-benzylidene-1-tosylpyrrolidin-3-yl)methanol (7b):³⁹ The product was obtained as a white solid in 80% yield (78 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.73 (d, *J* = 8.2 Hz, 2H), 7.35 (m, 4H), 7.26 (m, 1H), 7.14 (d, *J* = 8.2 Hz, 2H), 6.37 (s, 1H), 4.22 (d, *J* = 14.8 Hz, 1H), 4.02 (d, *J* = 14.8 Hz, 1H), 3.65 (t, *J* = 5.6 Hz, 2H), 3.38 (dd, *J* = 9.6, 4.0 Hz, 1H), 3.28 (dd, *J* = 9.6, 6.8 Hz, 1H), 2.99 (m, 1H), 2.42 (s, 3H), 1.70 (t, *J* = 5.6 Hz, 1H).



1-(4-methyl-1-tosylpyrrolidin-3-yl)ethan-1-one (10):⁴¹ The product was obtained as a colorless oil in 83% yield (59 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.69 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 1H), 3.55 (dd, *J* = 10.0, 8.0 Hz, 1H), 3.39 (dd, *J* = 9.7, 7.7 Hz, 1H), 3.29 (dd, *J* = 10.0, 8.0 Hz, 1H), 2.87 (dd, *J* = 9.7, 7.7 Hz, 1H), 2.66 (q, *J* = 8.1 Hz, 1H), 2.43 (s, 3H), 2.30 (dt, *J* = 14.5, 7.2 Hz, 1H), 2.12 (s, 3H), 1.02 (d, *J* = 6.7 Hz, 3H).

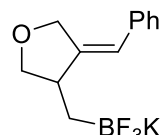


- General procedure for the synthesis of trifluoroborates salts:

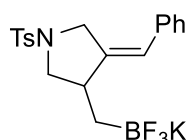


The alkylboronate (1 equiv, 0.4 mmol) was solved in methanol (0.2 M, 2 mL). To the solution was added KHF₂ (4.5 equiv, 4.5 M aqueous solution) dropwise. The reaction mixture was stirred at 25 °C for 1.5 h. Then, the solvent was removed under vacuum and the solid residue was triturated with acetone (20 mL). The liquid phase was filtered, and the residual inorganic salts were washed with additional acetone. The combined solution was concentrated under vacuum to give white solids. The solids were washed with ether (3 x 20 mL) to remove pinacol and dried under vacuum, affording the desired product.

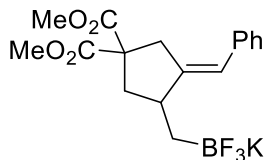
Potassium (Z)-((4-benzylidenetetrahydrofuran-3-yl)methyl)trifluoroborate (8a): The product was obtained as a white solid in 84 % yield (94 mg). ¹H NMR (300 MHz, DMSO-d₆) δ 7.32 (t, *J* = 7.5 Hz, 2H), 7.16 (dd, *J* = 11.3, 7.5 Hz, 3H), 6.24 (d, *J* = 2.1 Hz, 1H), 4.57 (d, *J* = 14.4 Hz, 1H), 4.37 (d, *J* = 14.4 Hz, 1H), 3.97 (dd, *J* = 8.1, 7.9 Hz, 1H), 3.16 (t, *J* = 8.8 Hz, 1H), 2.62 (m, 1H), 0.60 – 0.45 (m, 1H), 0.06 – -0.15 (m, 1H). ¹³C NMR (75 MHz, DMSO-d₆) δ 150.7 (C), 137.8 (C), 128.4 (2 × CH), 127.6 (2 × CH), 125.7 (CH), 117.6 (CH), 74.2 (CH₂), 69.4 (2 × CH₂), 43.0 (q, *J* = 2.3 Hz, CH). ¹⁹F NMR (282 MHz, DMSO-d₆) δ -136.24. HRMS (ESI, MeCN) calcd. for C₁₂H₁₃BF₃KO [M - K]⁺: 241.0397; Found: 241.1026.



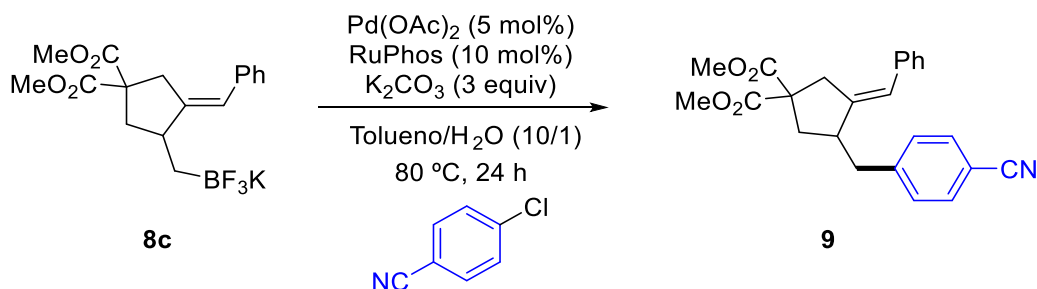
Potassium (Z)-3-benzylidene-1-tosyl-4-((trifluoroboranyl)methyl)pyrrolidine (8b):³⁹ The product was obtained as a white solid in 72 % yield (79 mg). ¹H NMR (300 MHz, DMSO-d₆) δ 7.66 (d, *J* = 7.9 Hz, 2H), 7.37 (m, 4H), 7.18 (m, 3H), 6.22 (s, 1H), 4.19 (d, *J* = 15.4 Hz, 1H), 3.76 (d, *J* = 15.4 Hz, 1H), 3.55 (d, *J* = 7.7 Hz, 1H), 2.37 (s, 3H), 0.48 (br s, 1H), -0.20 (br s, 1H).



Potassium dimethyl (E)-3-benzylidene-4-((trifluoroboranyl)methyl)cyclopentane-1,1-dicarboxylate (8c): The product was obtained as a light brown solid in 78 % yield (79 mg). M.p. = 70 – 72 °C. ¹H NMR (300 MHz, DMSO) δ 7.32 (t, *J* = 7.6 Hz, 2H), 7.25 (d, *J* = 7.3 Hz, 2H), 7.16 (t, *J* = 7.0 Hz, 1H), 6.22 (d, *J* = 2.1 Hz, 1H), 3.64 (s, 3H), 3.63 (s, 3H), 3.57 (t, *J* = 7.1 Hz, 1H), 3.19 (d, *J* = 17.5 Hz, 1H), 2.95 (d, *J* = 17.5 Hz, 1H), 2.60 – 2.54 (m, 1H), 1.62 (t, *J* = 12.1 Hz, 1H), 0.68 – 0.52 (m, 1H), 0.01 – -0.18 (m, 1H). ¹³C NMR (75 MHz, DMSO) δ 172.1 (2 × C), 150.3 (C), 138.3 (C), 128.2 (2 × CH), 127.9 (2 × CH), 125.6 (CH), 119.5 (CH), 58.4 (C), 52.6 (CH₃), 52.5 (CH₃), 42.0 (CH), 41.4 (CH₂), 38.4 (CH₂). ¹⁹F NMR (282 MHz, DMSO-d₆) δ – 135.35. HRMS (ESI, MeOH) calcd. for C₁₇H₁₉BF₃KO₄ [M - K]: 355.2385; Found: 355.1335.

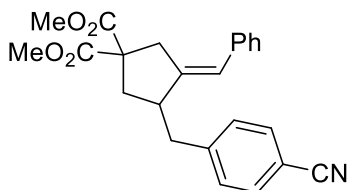


- General procedure for Suzuki-Miyaura Cross-Coupling Reaction of alkyltrifluoroborates:⁴⁴



A vial was charged with Pd(OAc)₂ (0.008 mmol), RuPhos (0.015 mmol), 4-chlorobenzonitrile (0.23 mmol), the potassium trifluoroborate compound **6c** (0.15 mmol) and K₂CO₃ (0.45 mmol). The vial was sealed by a septum, dried under vacuum and backfilled with Ar. To the vial were added toluene (1 mL) and H₂O (0.1 mL), and then the reaction was heated to 80 °C for 24 h. The reaction mixture was allowed to cool to rt. The organic layer was separated, and the aqueous layer was washed with EtOAc. The combined organic layers were concentrated under vacuum and purified by silica gel column chromatography to yield the product.

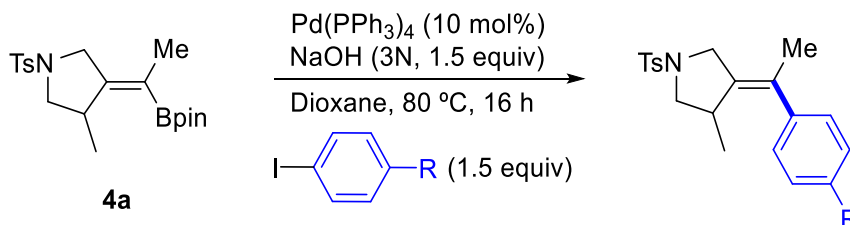
Dimethyl (E)-3-benzylidene-4-(4-cyanobenzyl)cyclopentane-1,1-dicarboxylate (9): The compound was purified by column chromatography (cyclohexane/EtOAc 95:5) and was obtained as a colorless oil in 79% yield (46 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.39 – 7.33 (m, 4H), 7.31 – 7.19 (m, 3H), 6.32 (s, 1H), 3.73 (s, 3H), 3.68 (s, 3H), 3.38 (d, *J* = 17.5 Hz, 1H), 3.28 – 3.15 (m, 2H), 3.12 – 3.04 (m, 1H), 2.69 (dd, *J* = 13.0, 9.4 Hz, 1H), 2.37 (dd, *J* = 13.0, 7.3 Hz, 1H), 1.85 (dd, *J* = 13.0, 10.0 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 172.0 (C), 171.9 (C), 145.9 (C), 143.6 (C), 137.5 (C), 132.4 (2 × CH), 129.9 (2 × CH), 128.5 (4 × CH), 126.7 (CH), 123.3



⁴⁴ S. D. Dreher, S.-E. Lim, D. L. Sandrock, G. A. Molander, *J. Org. Chem.*, **2009**, 74, 3626 – 3631.

(CH), 119.0 (C), 110.3 (C), 59.1 (C), 53.0 (2 × CH₃), 45.4 (CH), 40.9 (CH₂), 39.2 (CH₂), 38.8 (CH₂). HRMS (ESI, MeOH) calcd. for C₂₄H₂₃NO₄ [M + H]⁺: 390.4510; Found: 390.1707.

- General procedure for Suzuki-Miyaura Cross-Coupling Reaction of alkenylboronates.¹⁴

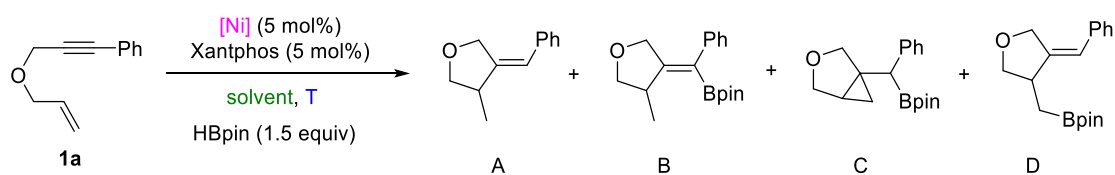


A vial was charged with Pd(PPh₃)₄ (0.015 mmol), the corresponding iodoarene (0.23 mmol) and the alkenylboronate **4a** (0.15 mmol). The vial was sealed by a septum, dried under vacuum and backfilled with Ar. To the vial were added dioxane (1 mL) and NaOH (3 M, 0.1 mL), and then the reaction was heated to 80 °C for 16 h. The reaction mixture was allowed to cool to rt. The solvent was removed under vacuum and the product was purified by column chromatography in silica gel (cyclohexane/EtOAc 9:1).

(E)-3-methyl-4-(1-phenylethylidene)-1-tosylpyrrolidine (11a): The product was obtained as a brown oil in 99 % yield (52 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.75 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.25 (m, 1H), 7.23 – 7.21 (m, 2H), 7.07 (d, *J* = 7.8 Hz, 2H), 4.02 (d, *J* = 14.0 Hz, 1H), 3.80 (d, *J* = 14.0 Hz, 1H), 3.17 (dd, *J* = 9.2, 6.5 Hz, 1H), 3.06 (dd, *J* = 9.2, 2.5 Hz, 1H), 2.87 – 2.71 (m, 1H), 2.45 (s, 3H), 1.85 (s, 3H), 0.76 (d, *J* = 6.9 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 143.7 (C), 142.9 (C), 136.4 (C), 133.0 (C), 129.9 (C), 129.8 (2 × CH), 128.4 (2 × CH), 128.0 (2 × CH), 127.0 (2 × CH), 126.8 (CH), 55.6 (CH₂), 50.6 (CH₂), 35.8 (CH), 22.0 (CH₃), 21.7 (CH₃), 19.4 (CH₃). HRMS (ESI, MeOH) calcd. for C₂₀H₂₃NO₂S [M + H]⁺: 342.4690; Found: 342.1511.

(E)-3-(1-(4-chlorophenyl)ethylidene)-4-methyl-1-tosylpyrrolidine (11b): The product was obtained as a yellow oil in 98 % yield (44 mg). ¹H NMR (300 MHz, CDCl₃) δ 7.74 (d, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.25 (d, *J* = 8.3 Hz, 2H), 7.00 (d, *J* = 8.3 Hz, 2H), 4.00 (d, *J* = 14.1 Hz, 1H), 3.77 (d, *J* = 14.1 Hz, 1H), 3.16 (dd, *J* = 9.2, 6.4 Hz, 1H), 3.06 (dd, *J* = 9.2, 2.6 Hz, 1H), 2.85 – 2.66 (m, 1H), 2.45 (s, 3H), 1.82 (s, 3H), 0.76 (d, *J* = 6.9 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 143.7 (C), 141.3 (C), 137.2 (C), 133.0 (C), 132.6 (C), 129.8 (2 × CH), 129.0 (2 × CH), 128.8 (C), 128.7 (2 × CH), 128.0 (2 × CH), 55.6 (CH₂), 50.6 (CH₂), 35.8 (CH), 21.9 (CH₃), 21.7 (CH₃), 19.4 (CH₃). HRMS (ESI, MeOH) calcd. for C₂₀H₂₂ClNO₂S [M + H]⁺: 376.9110; Found: 376.1116.

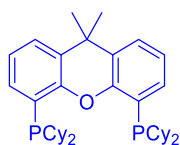
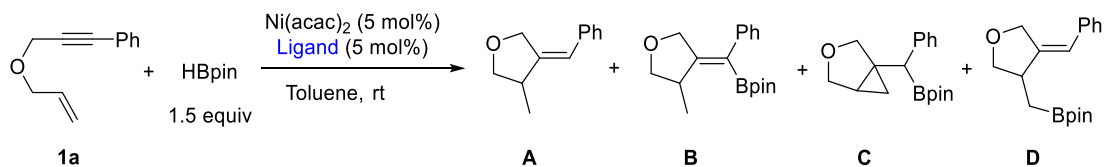
XII. Optimization of borylative cyclization of enynes



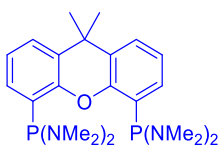
	Nickel salt	Solvent	T (°C)	Yield (%)			
				A	B	C	D
1	Ni(cod) ₂	Toluene	23	6	9	6	36
2	Ni(acac) ₂	Toluene	23	3	9	7	38
3	Ni(py) ₄ Cl ₂	Toluene	23	1	-	-	3
4	NiCl ₂	Toluene	23	-	-	-	-
5	Ni(acac) ₂	Toluene	50	9	7	7	35
6	Ni(acac) ₂	THF	23	16	7	6	34
7	Ni(acac) ₂	<i>i</i> -Pr ₂ O	23	6	6	7	37
8	Ni(acac) ₂	Dioxane	23	16	8	5	30
9	Ni(acac) ₂	DMF	23	15	-	5	31
10 ^a	Ni(py) ₄ Cl ₂	THF	23	-	7	6	36

^a MeMgCl (10 mol%)

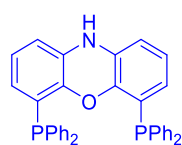
Other ligands:



A = 6%
C = 36%

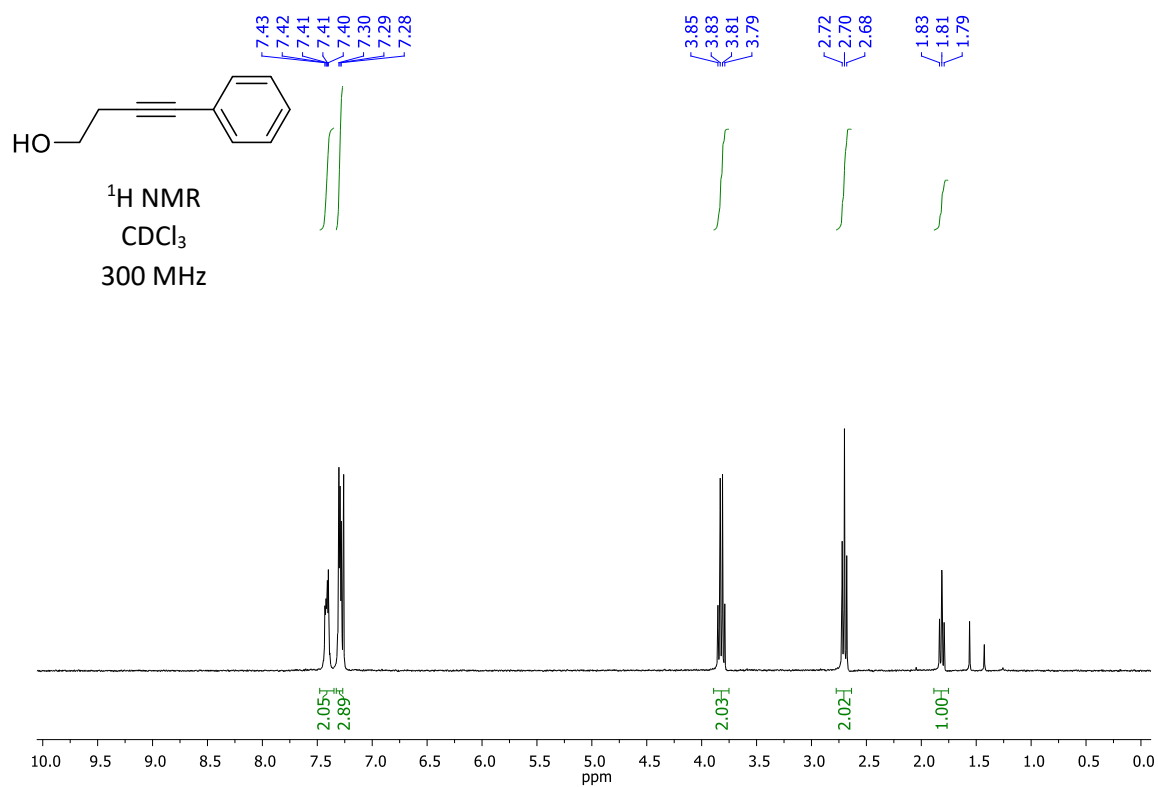
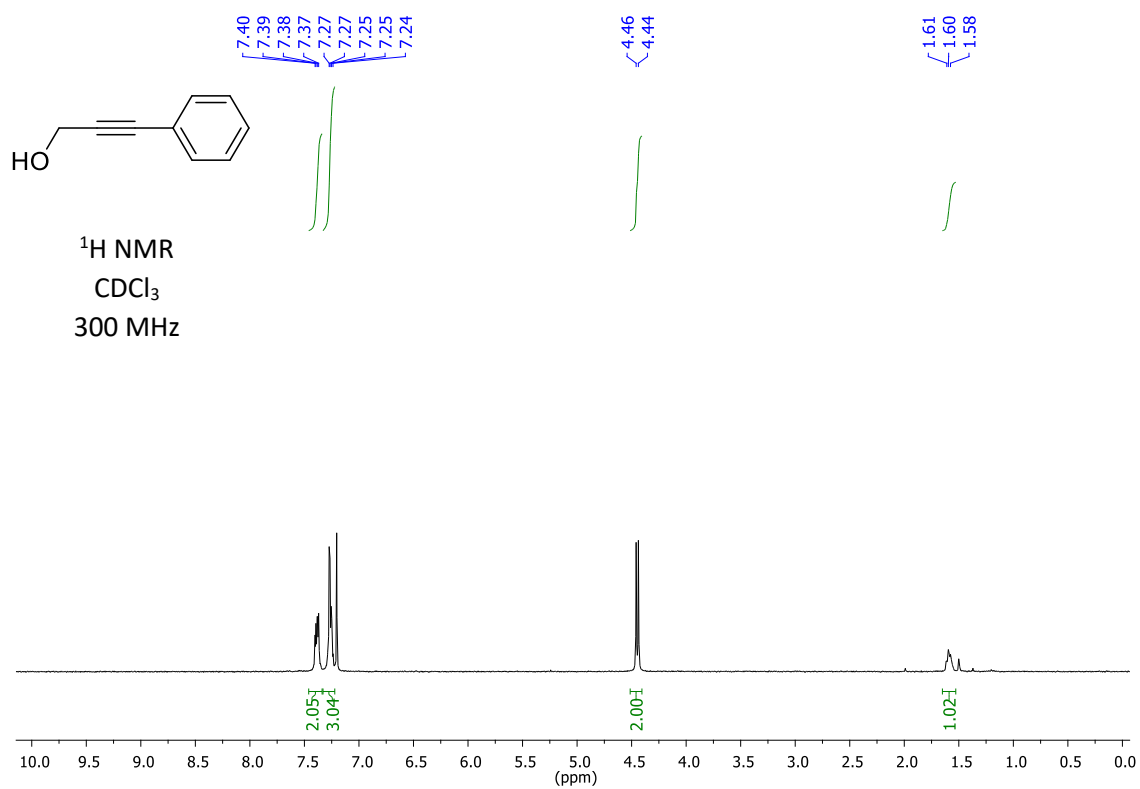


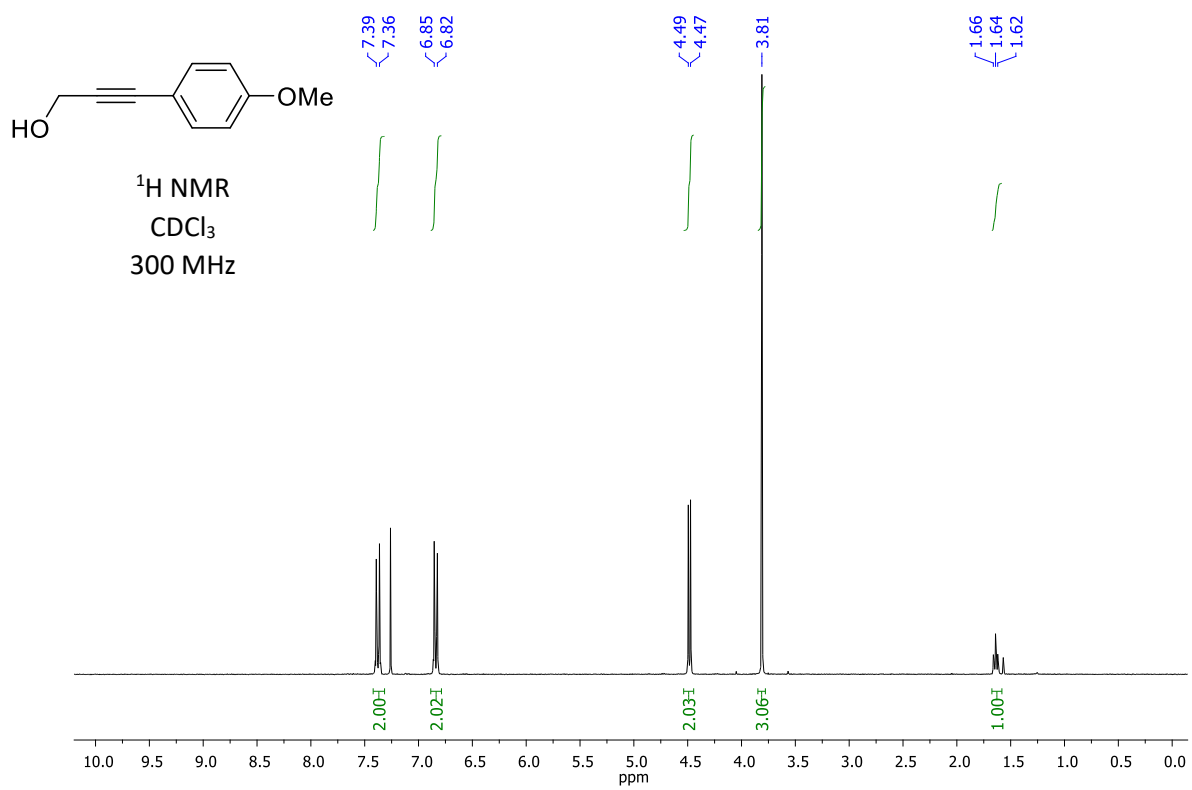
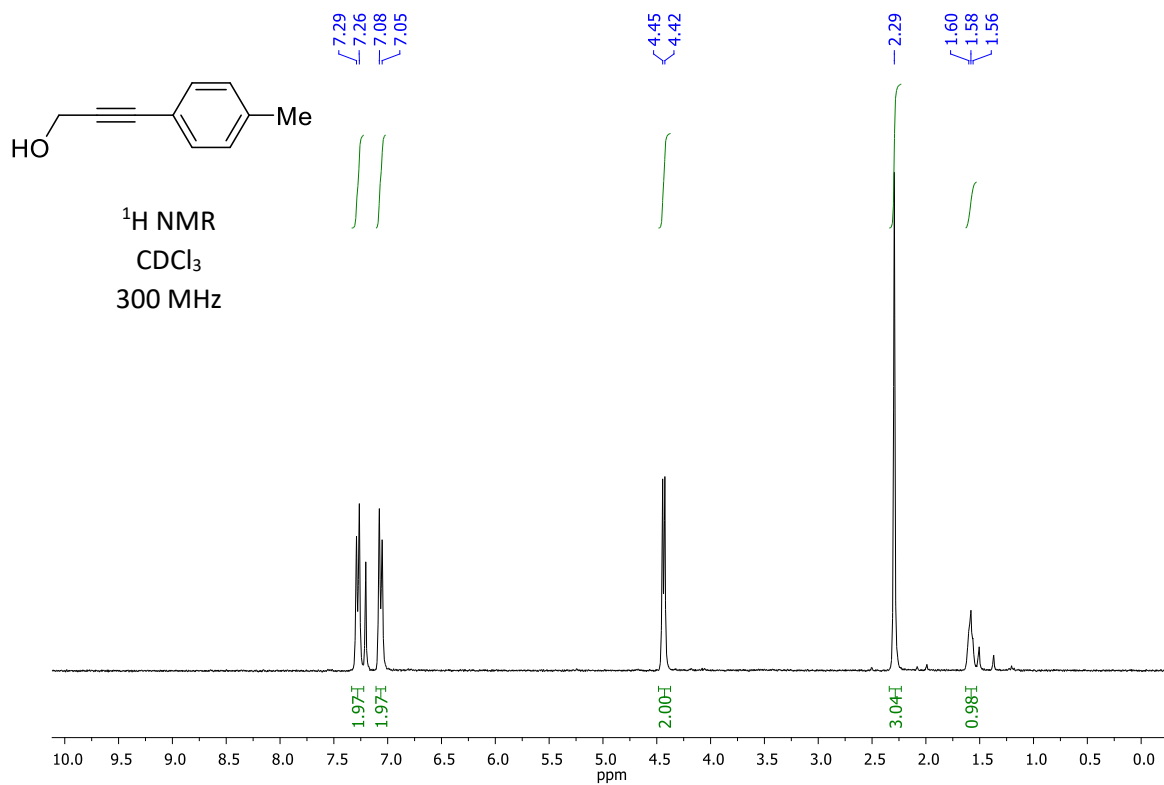
A = 20%
B < 2%
C = 7%
D = 5%

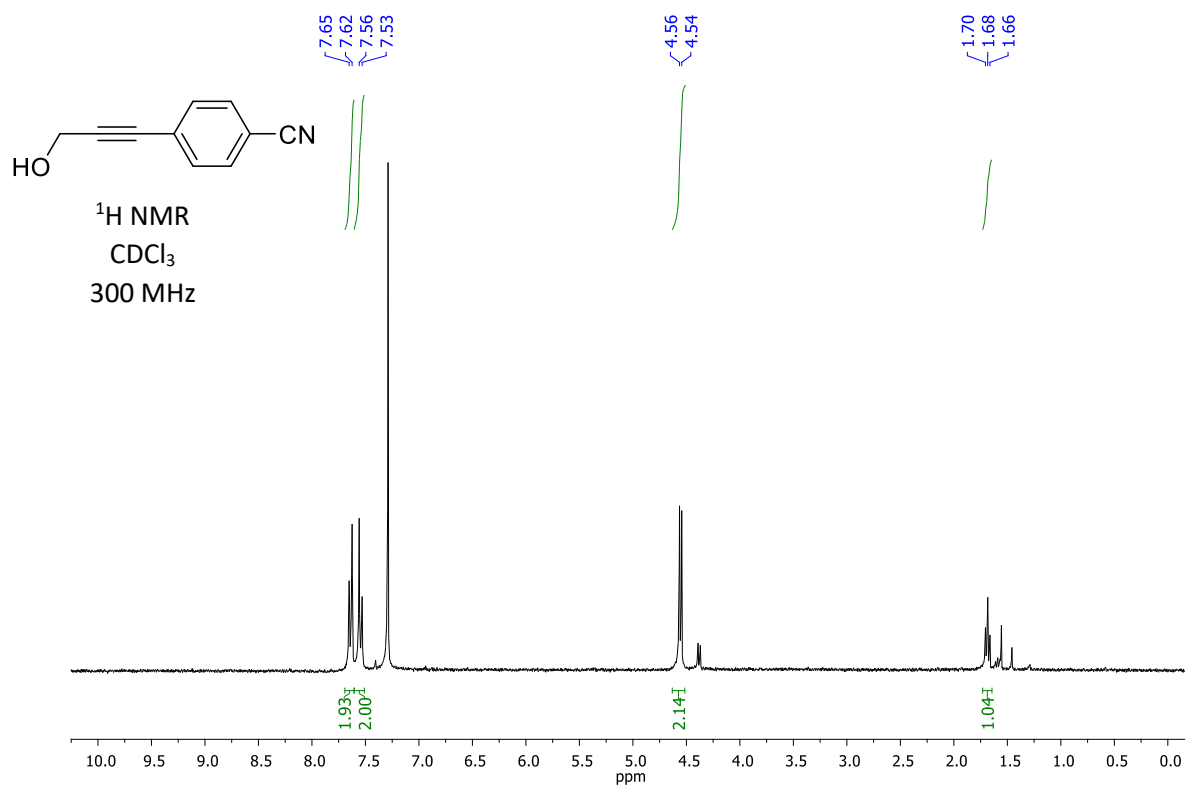
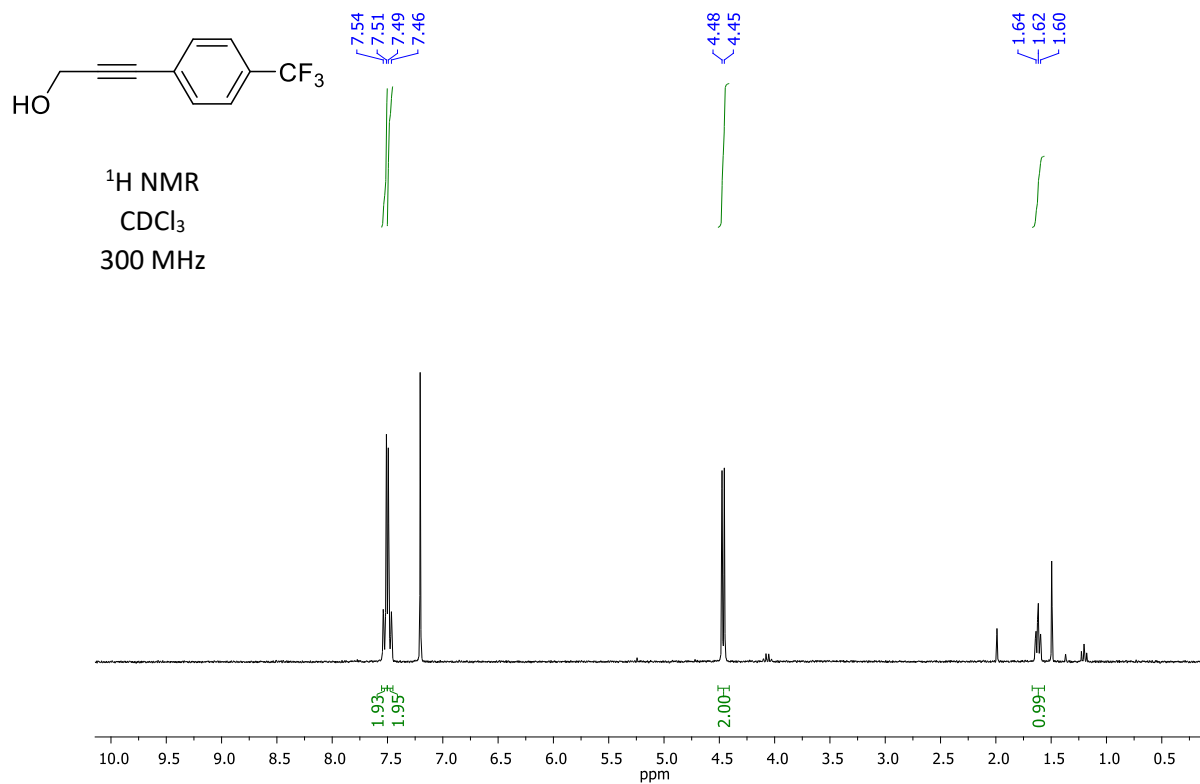


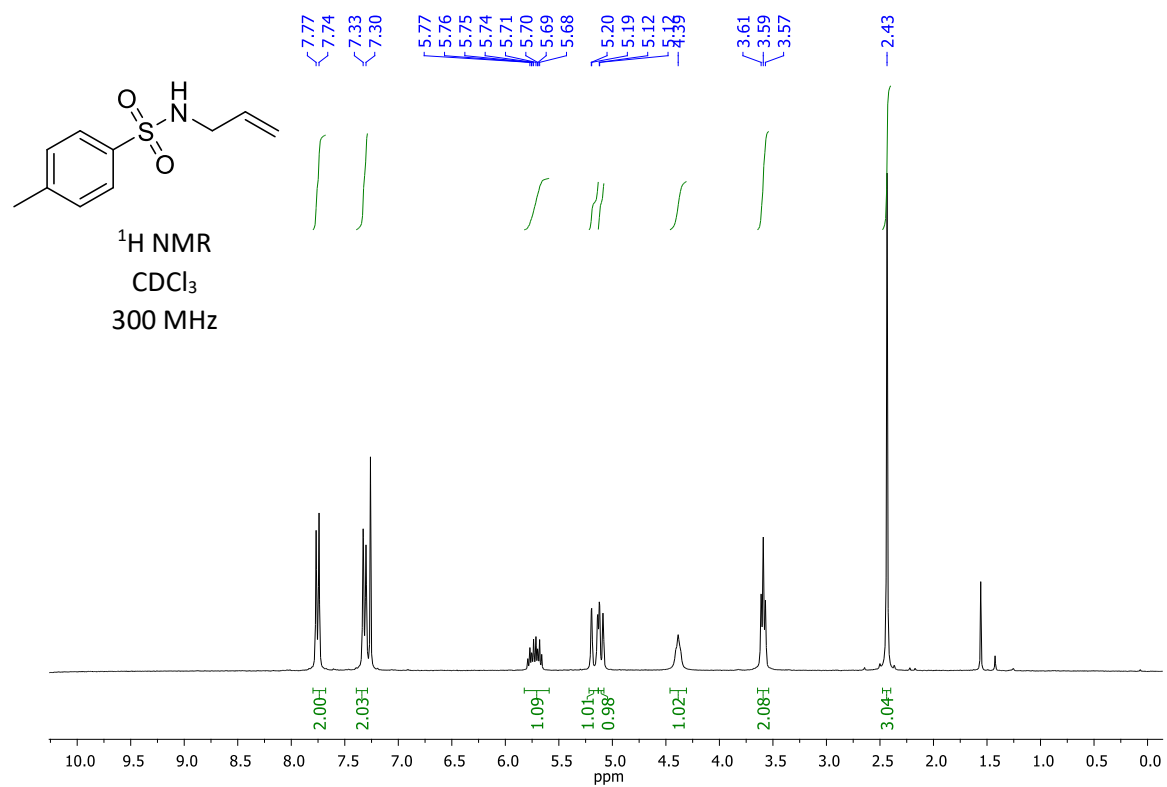
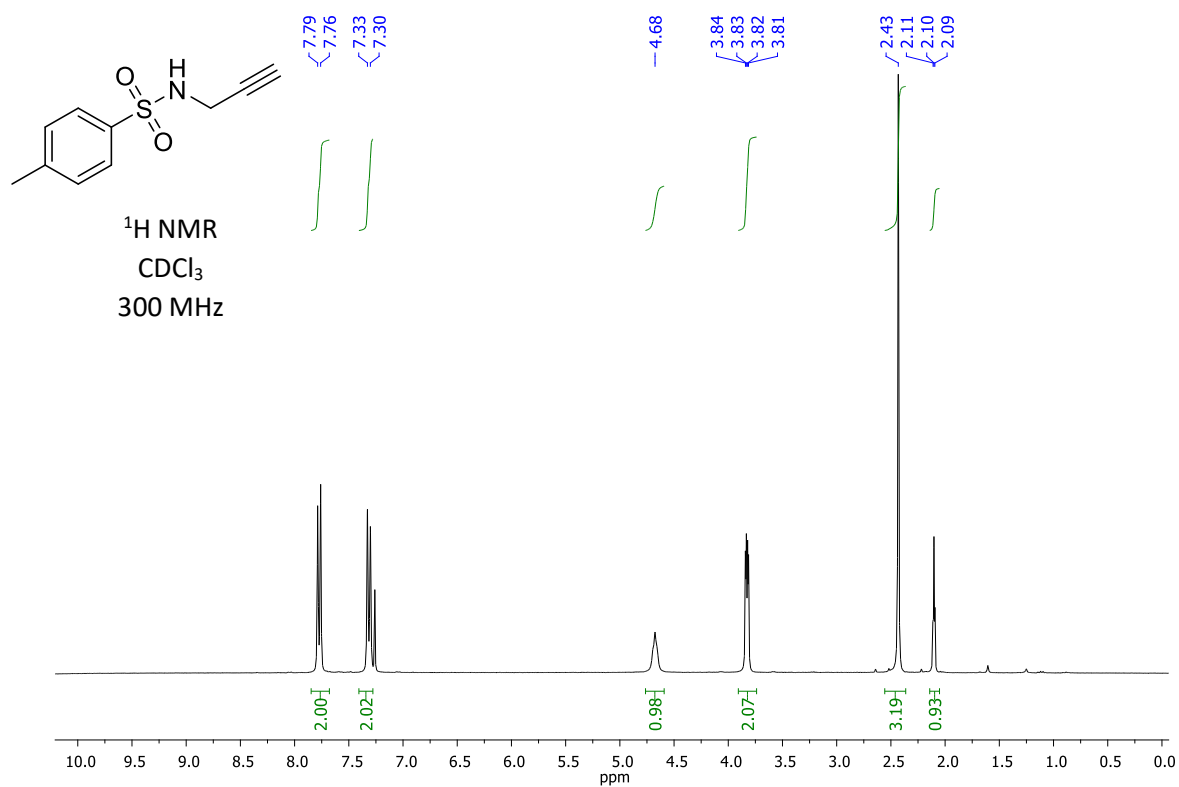
A = 12%
B = 11%
C = 7%
D = 15%

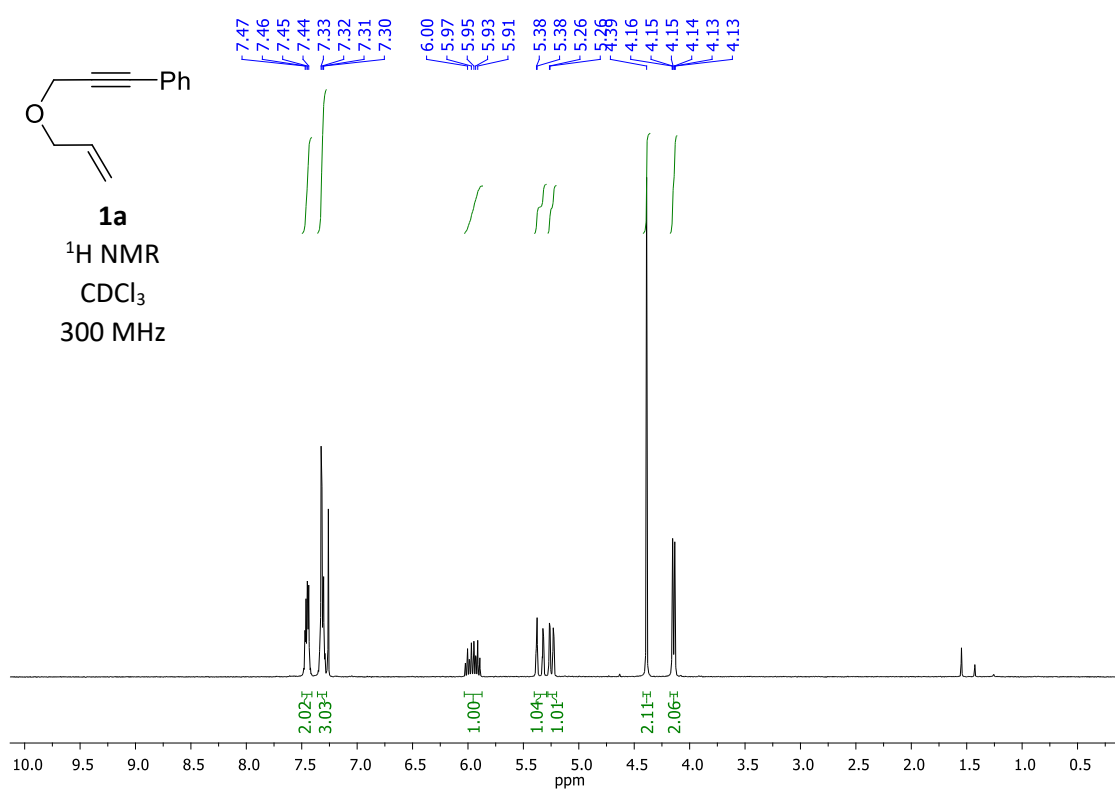
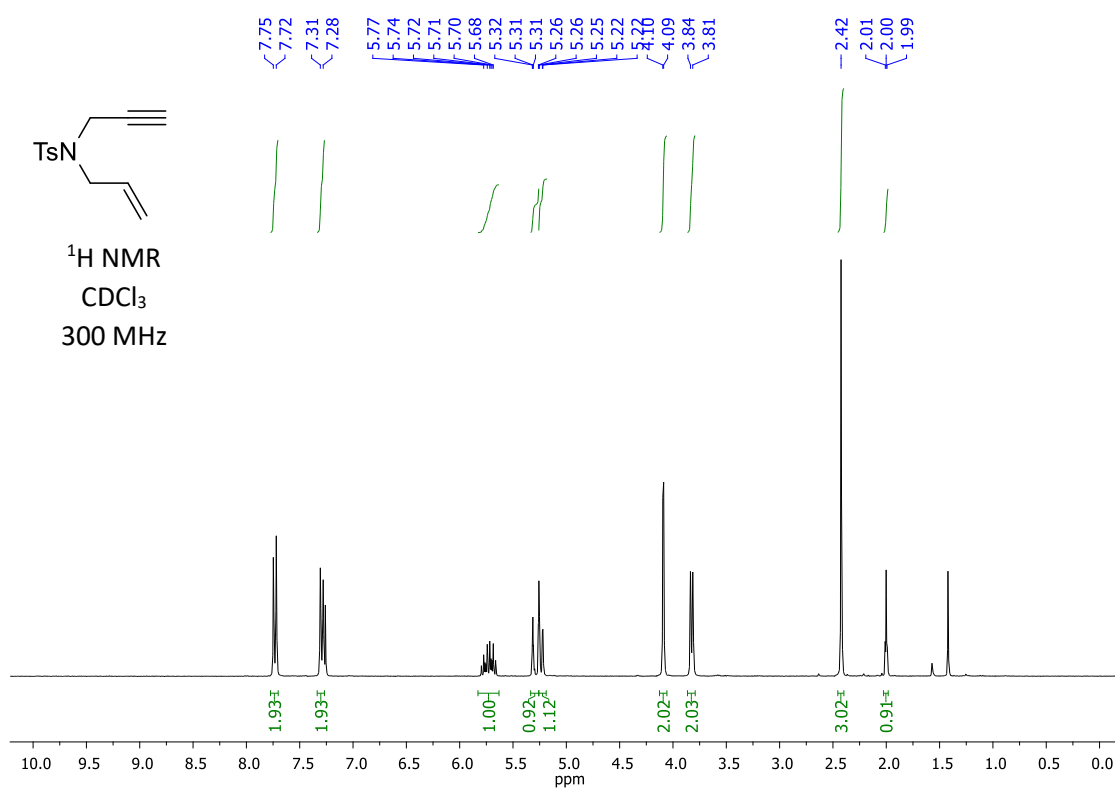
XIII. NMR Spectra

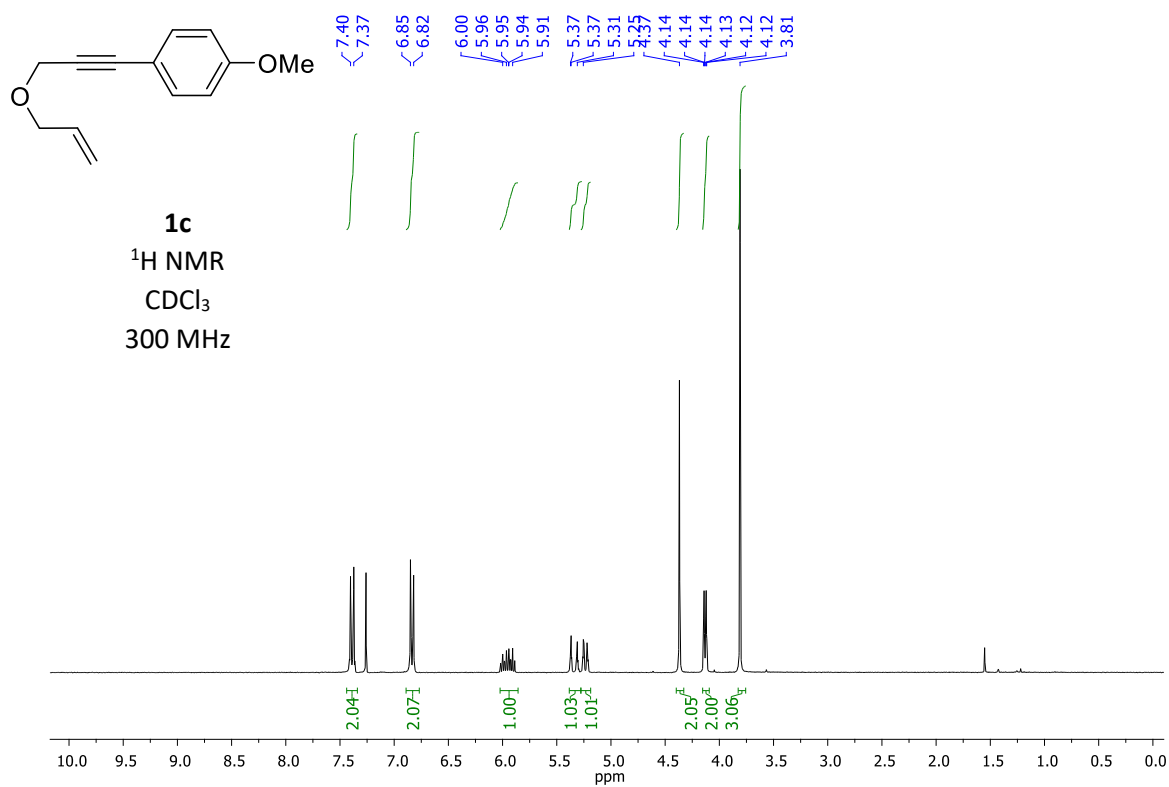
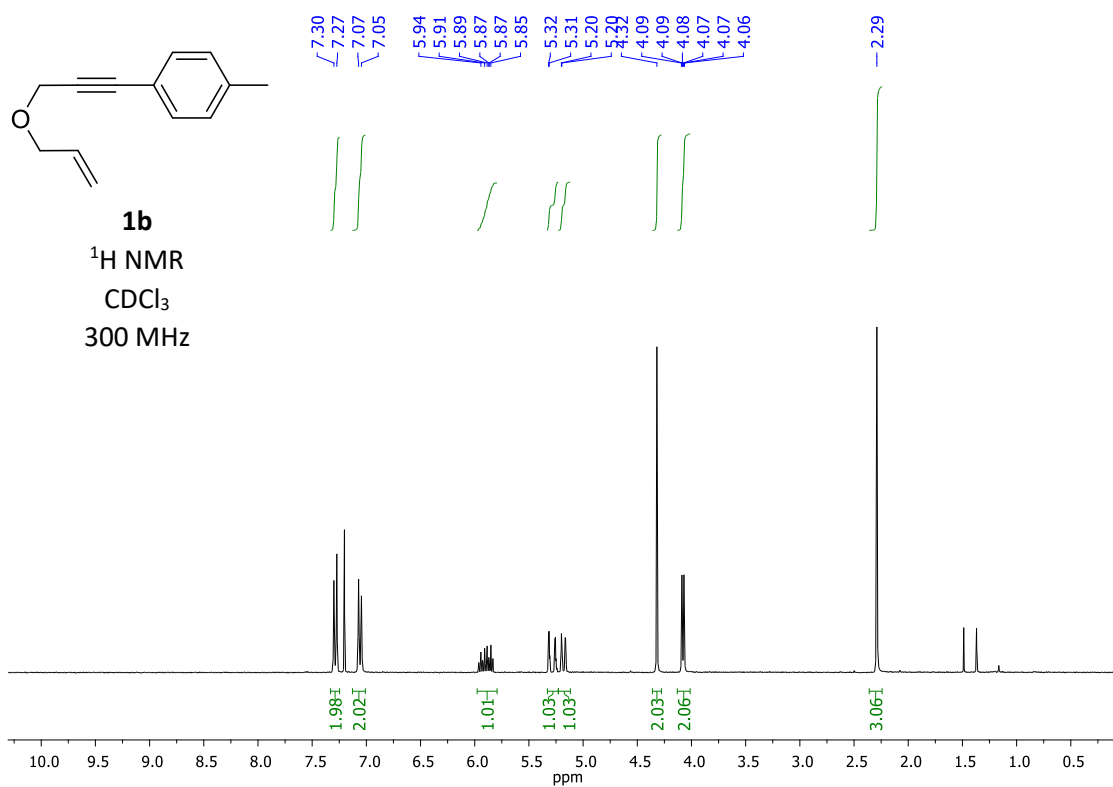


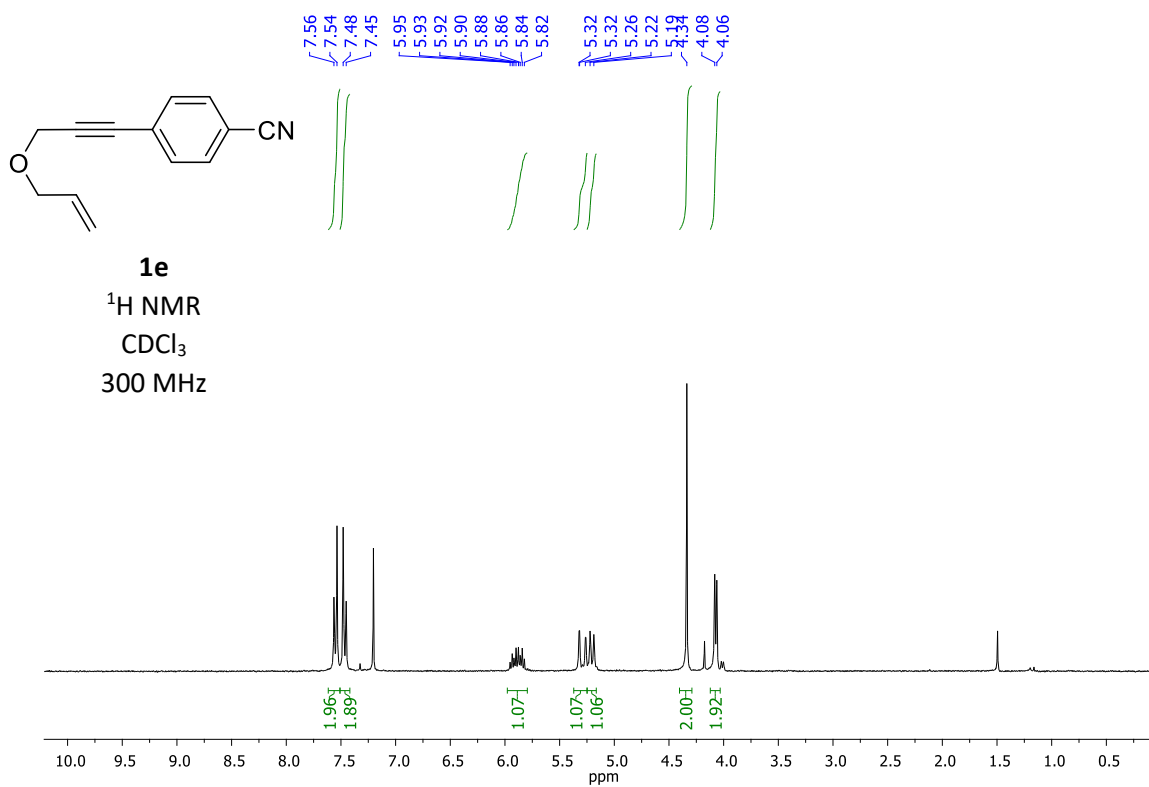
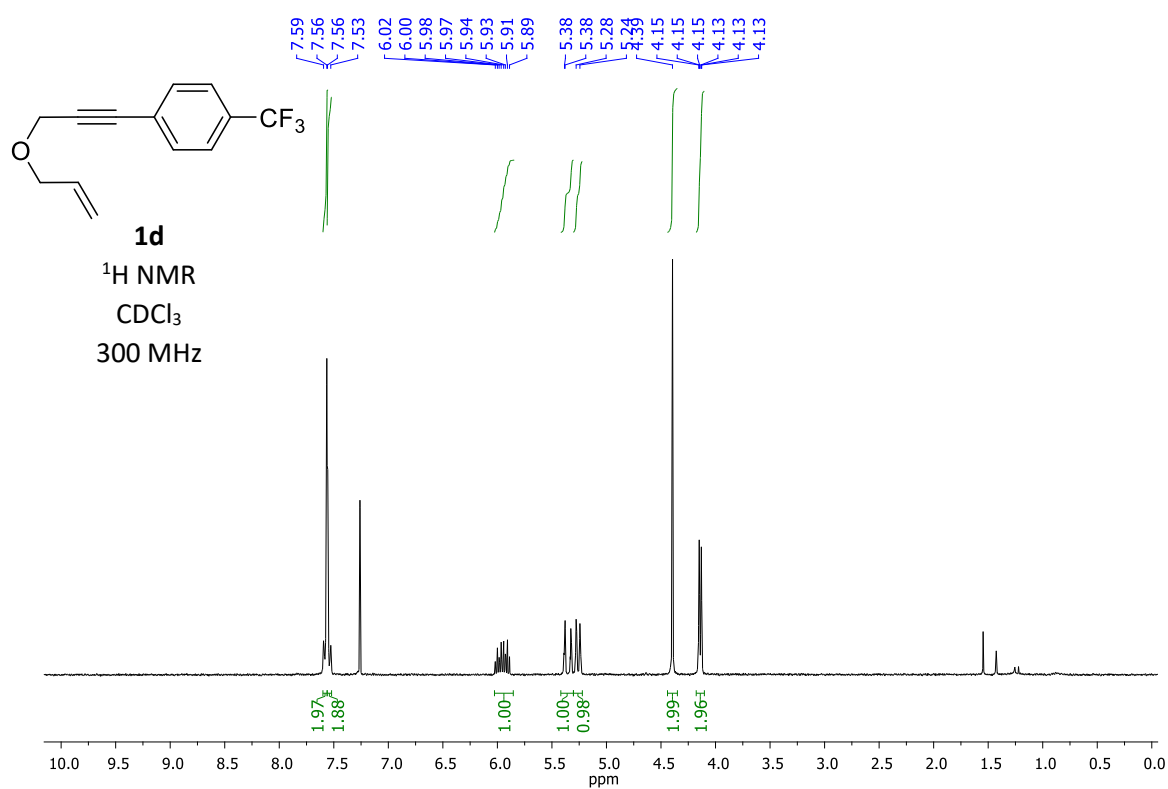


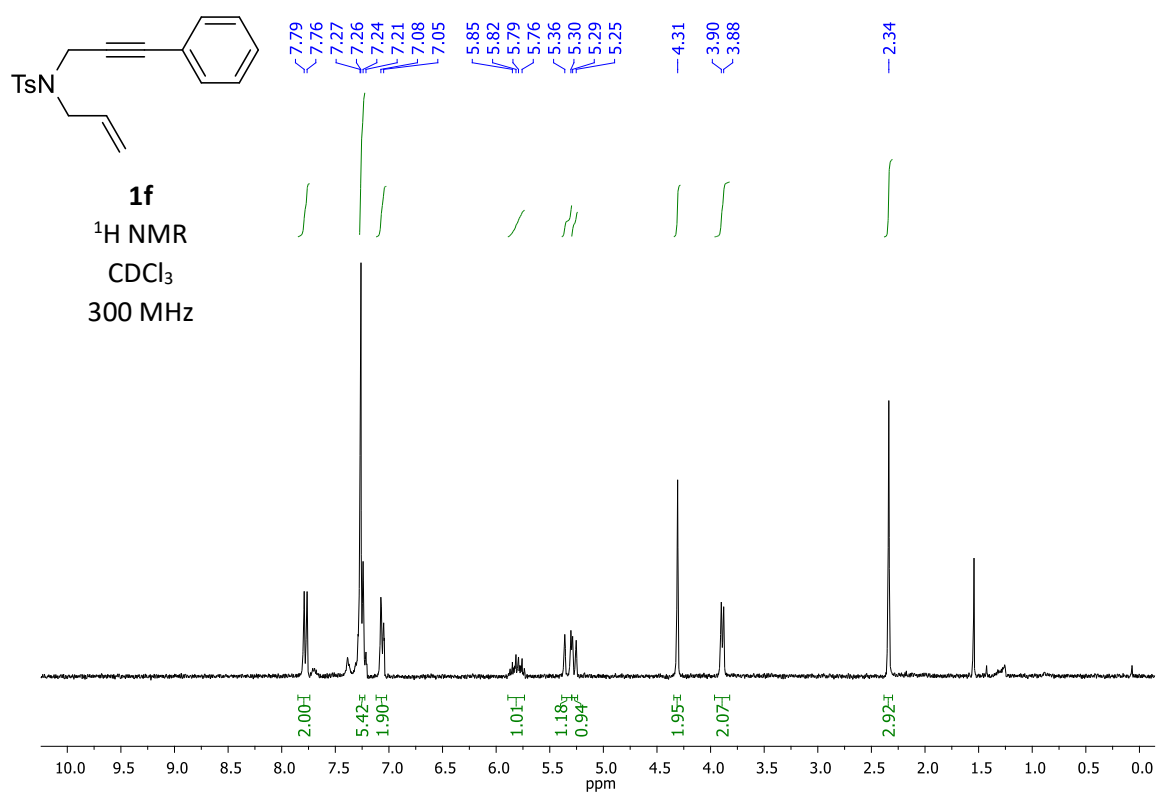
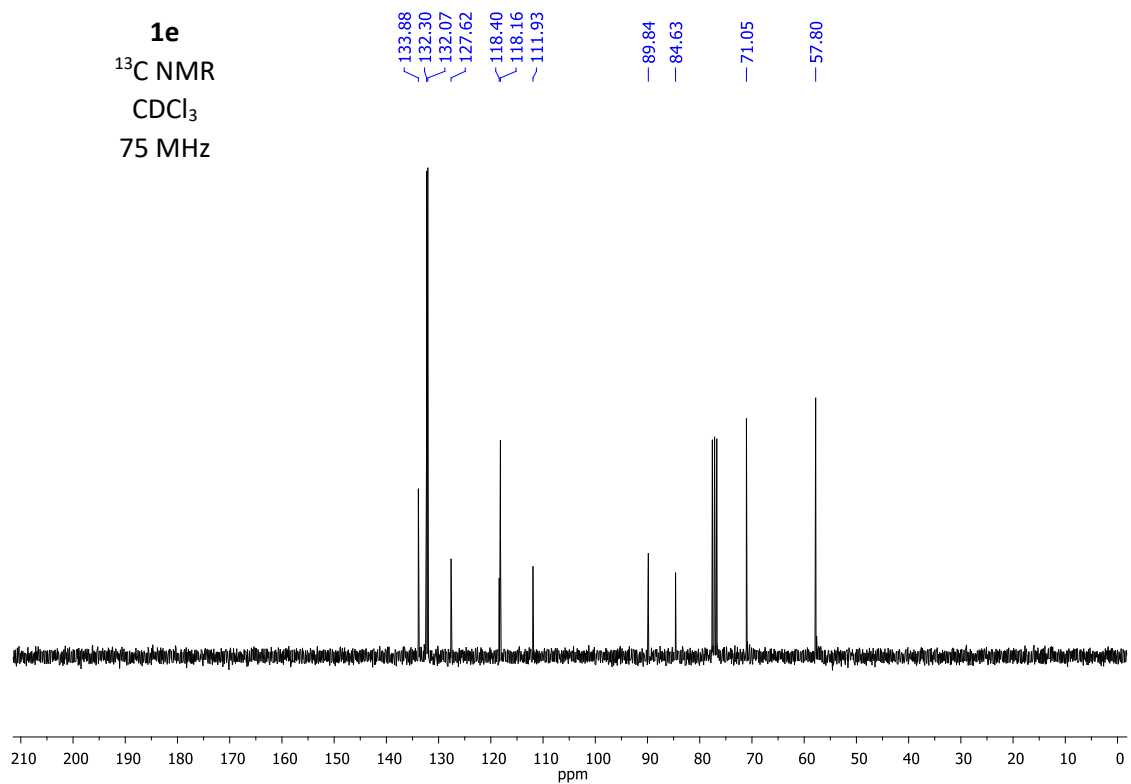


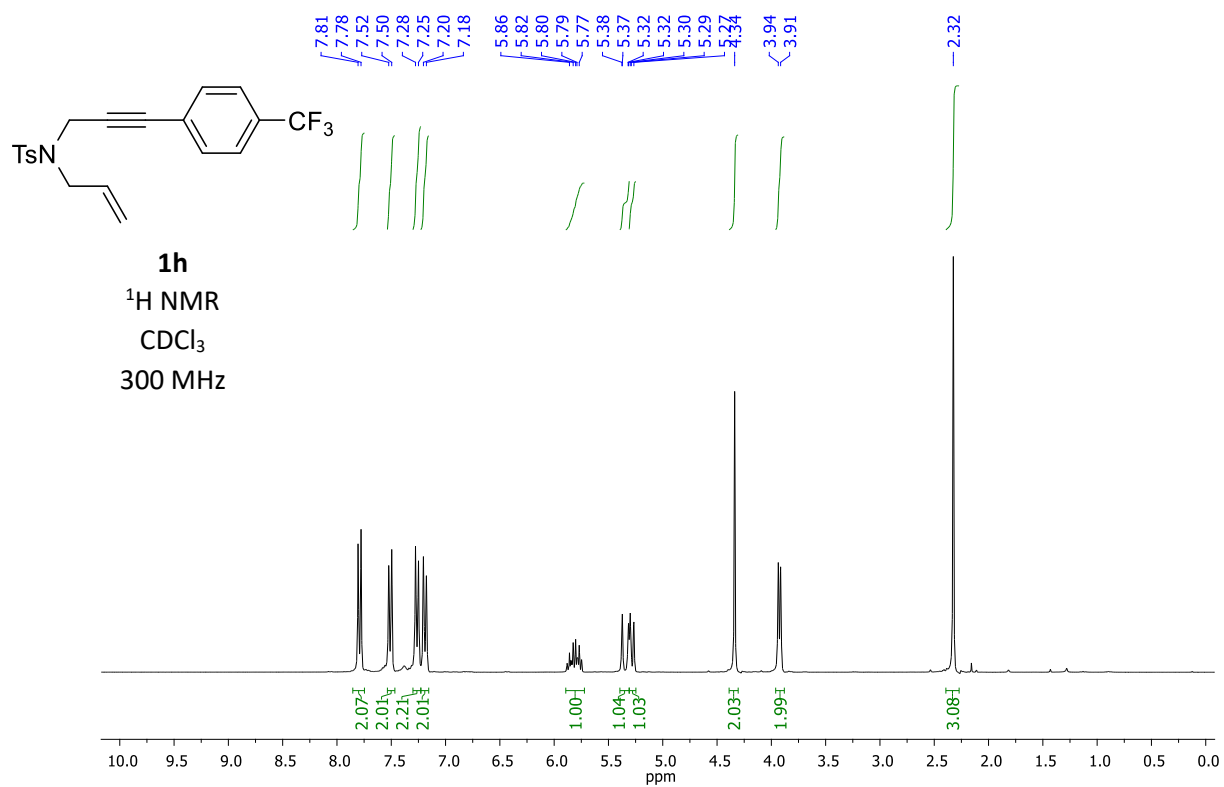
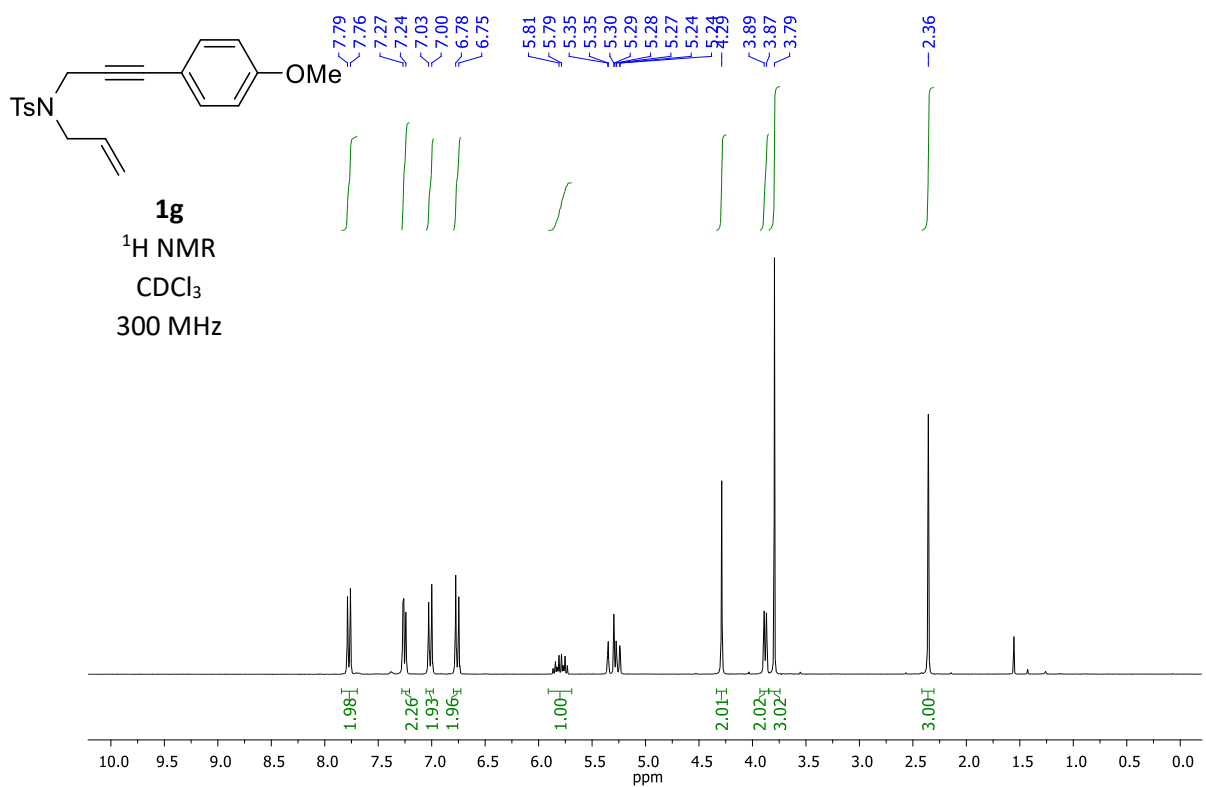


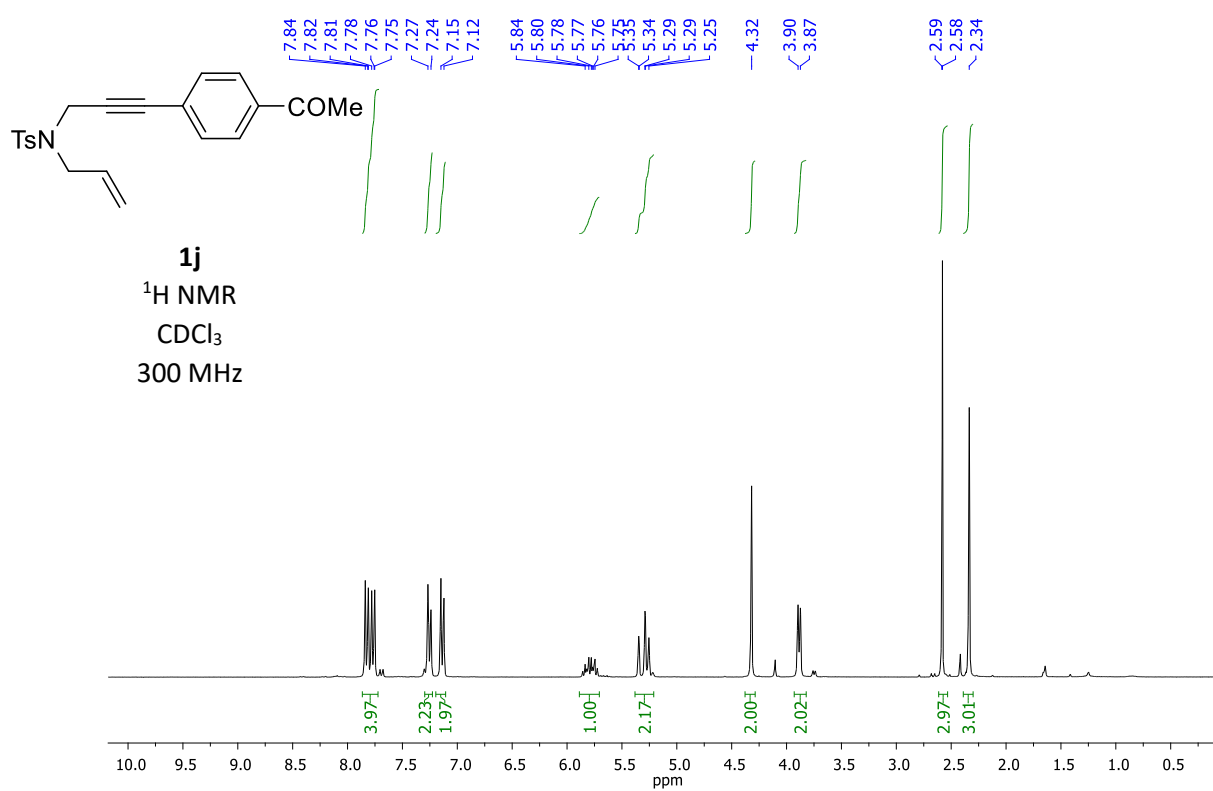
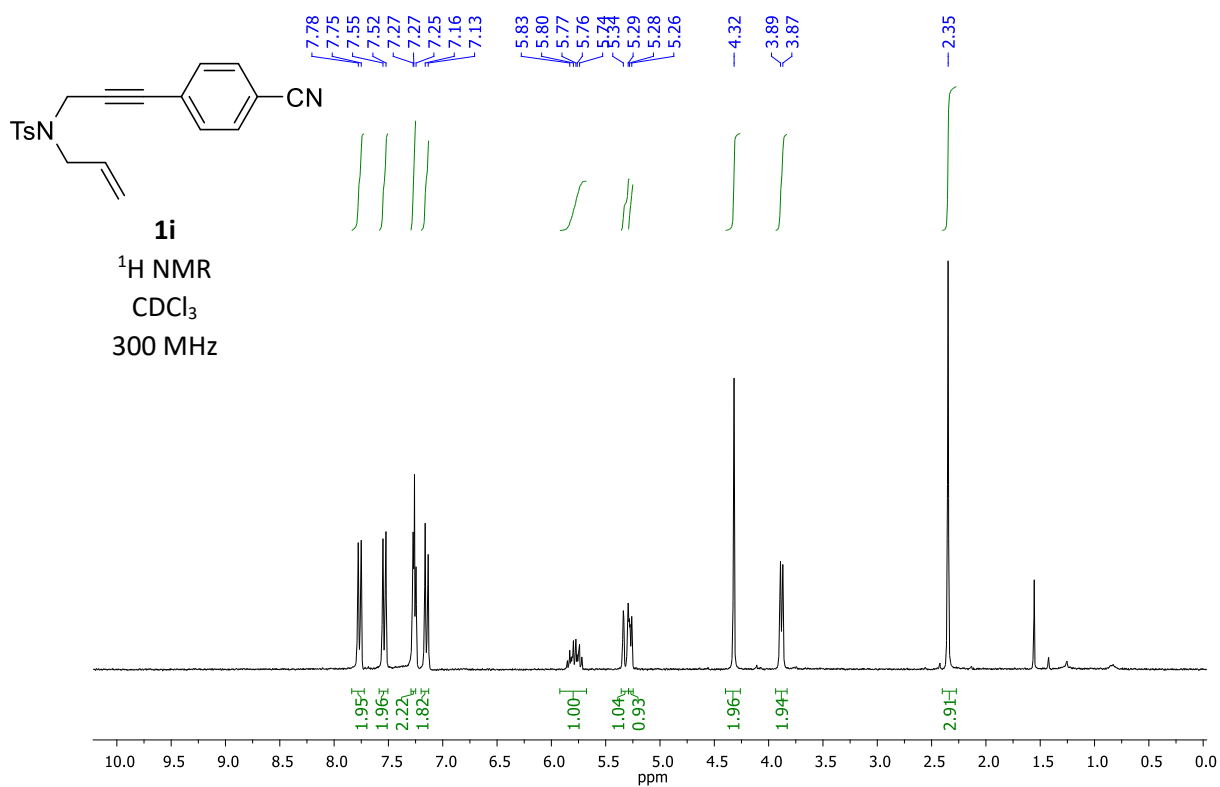


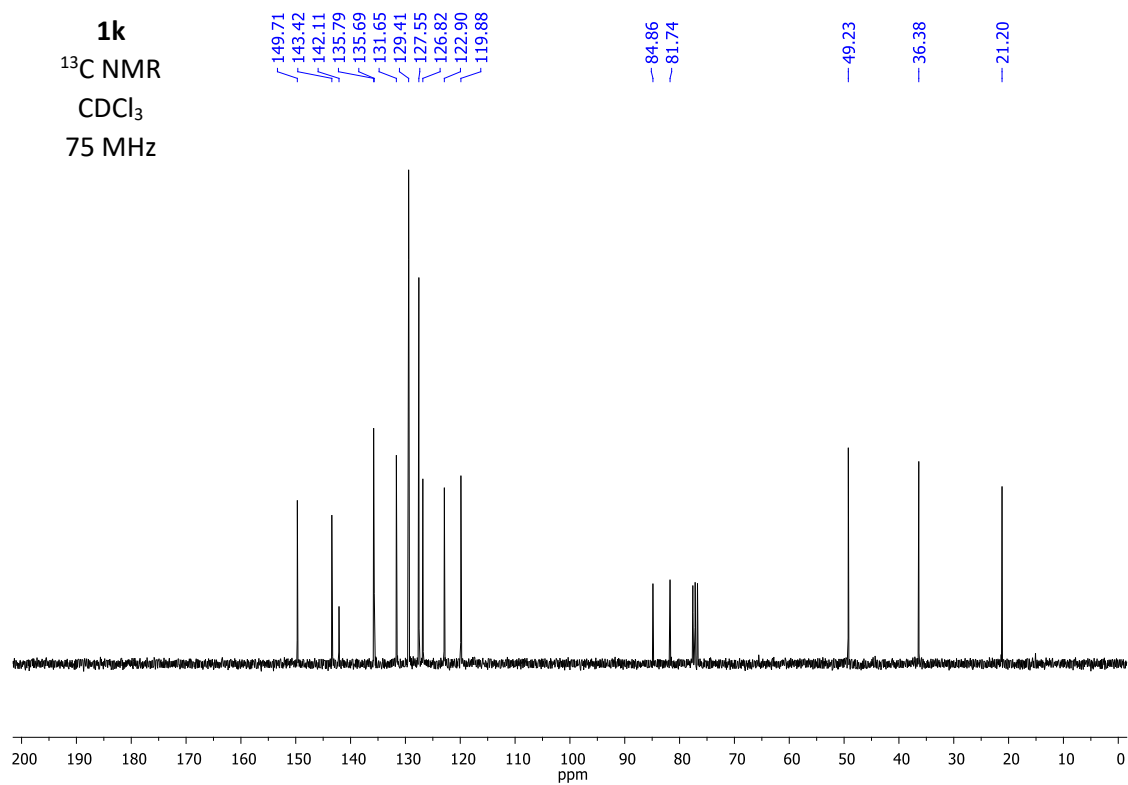
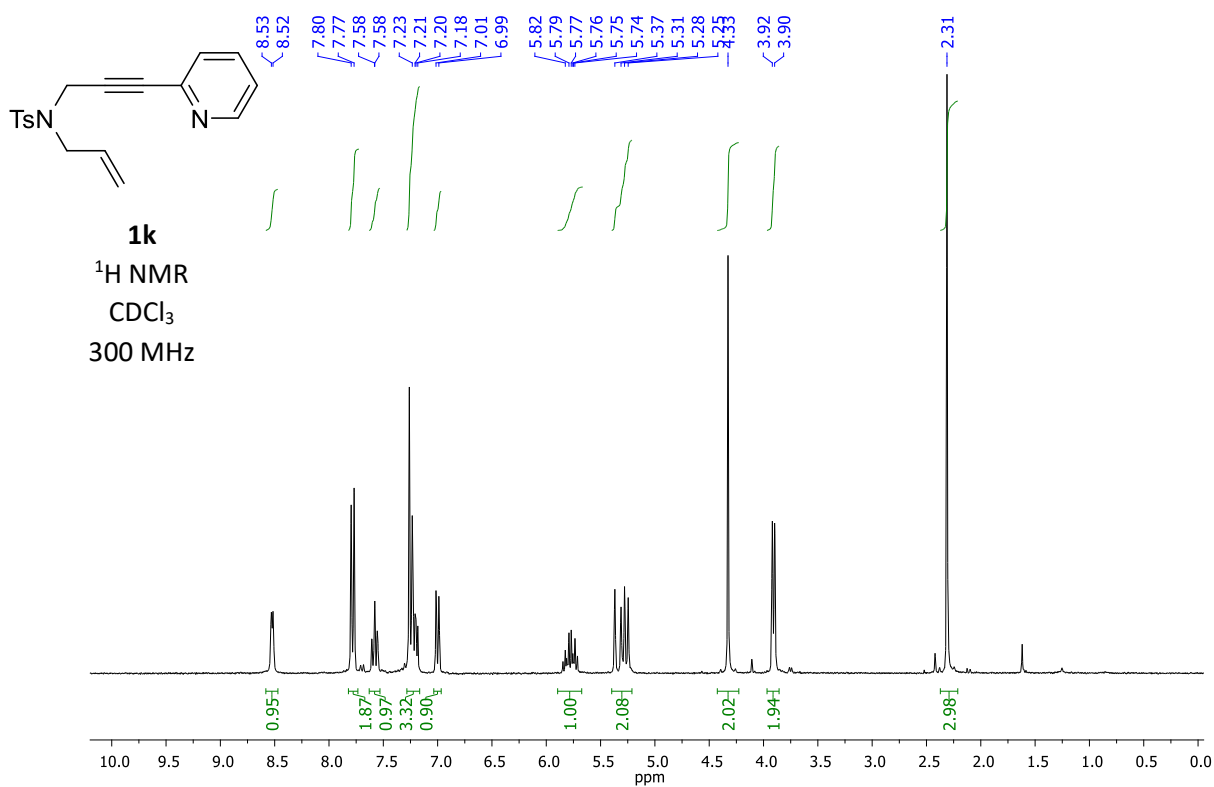


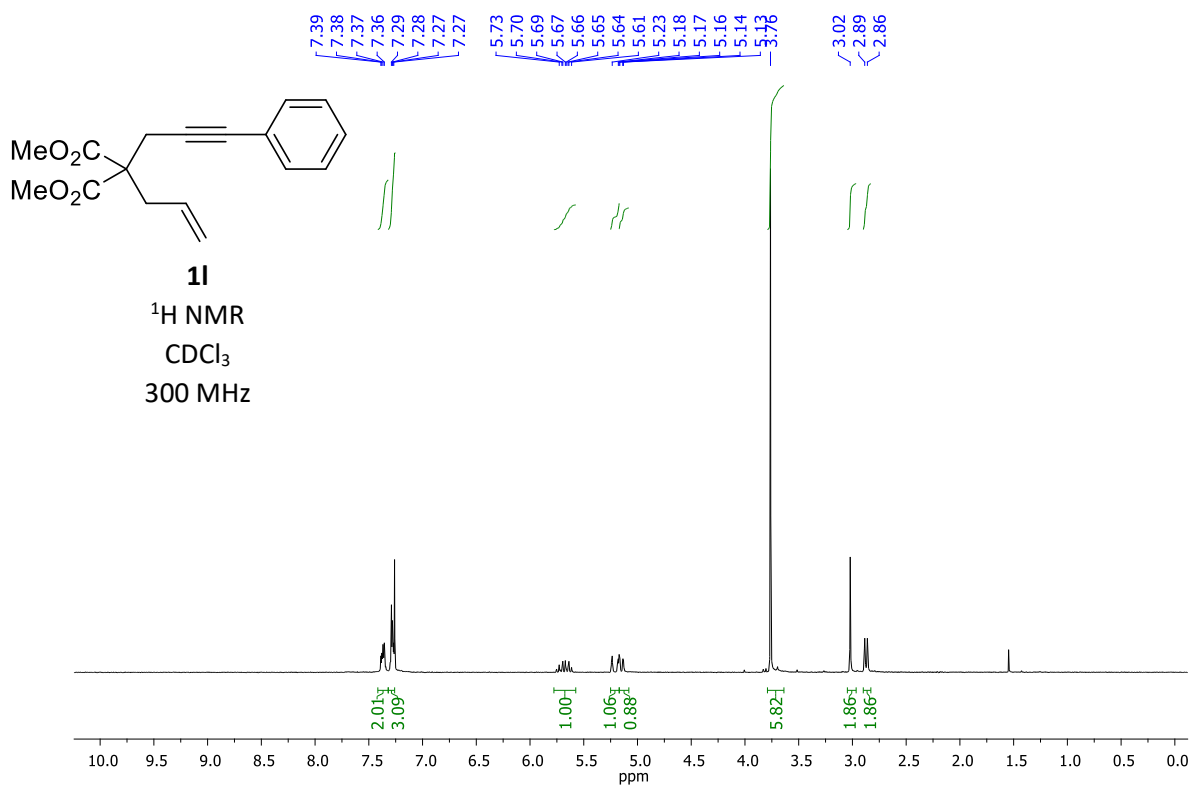
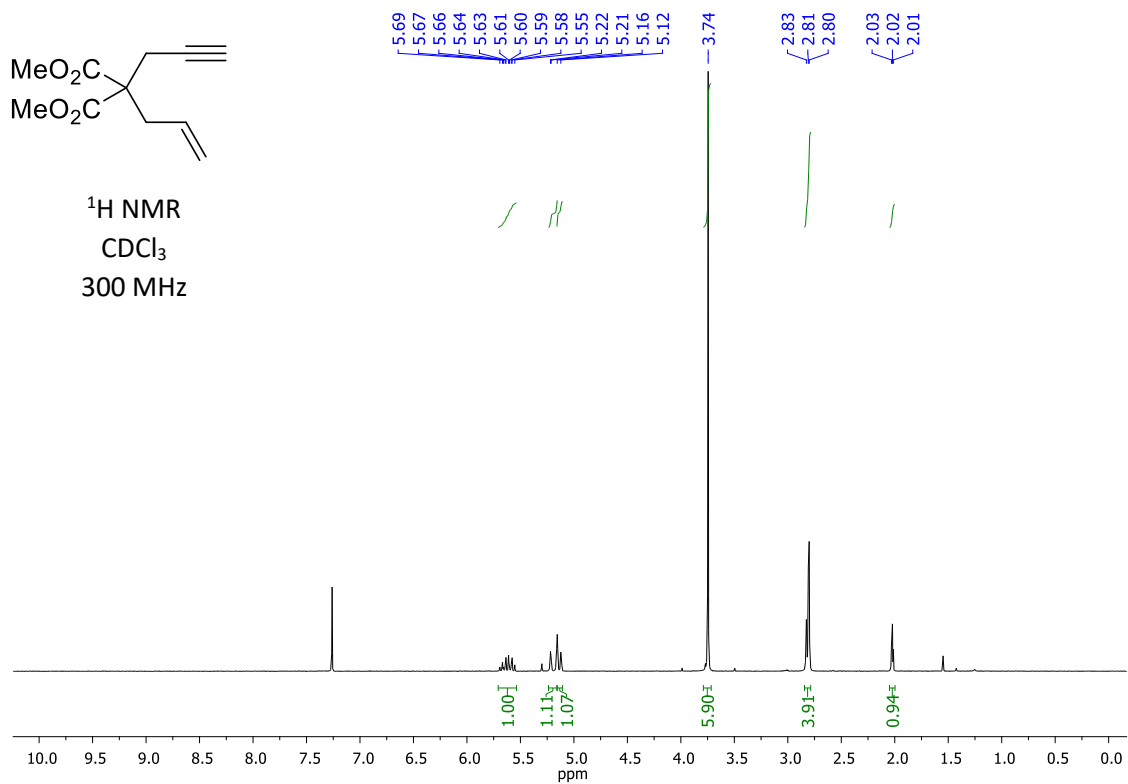


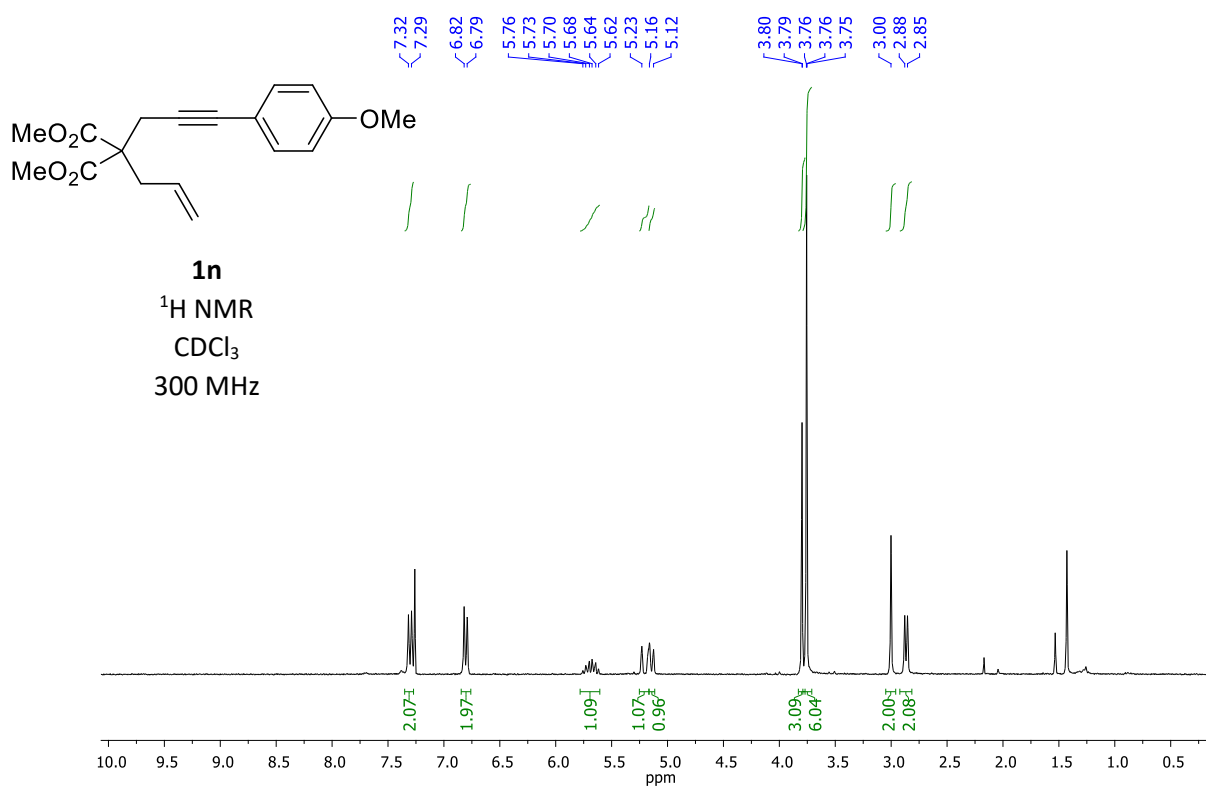
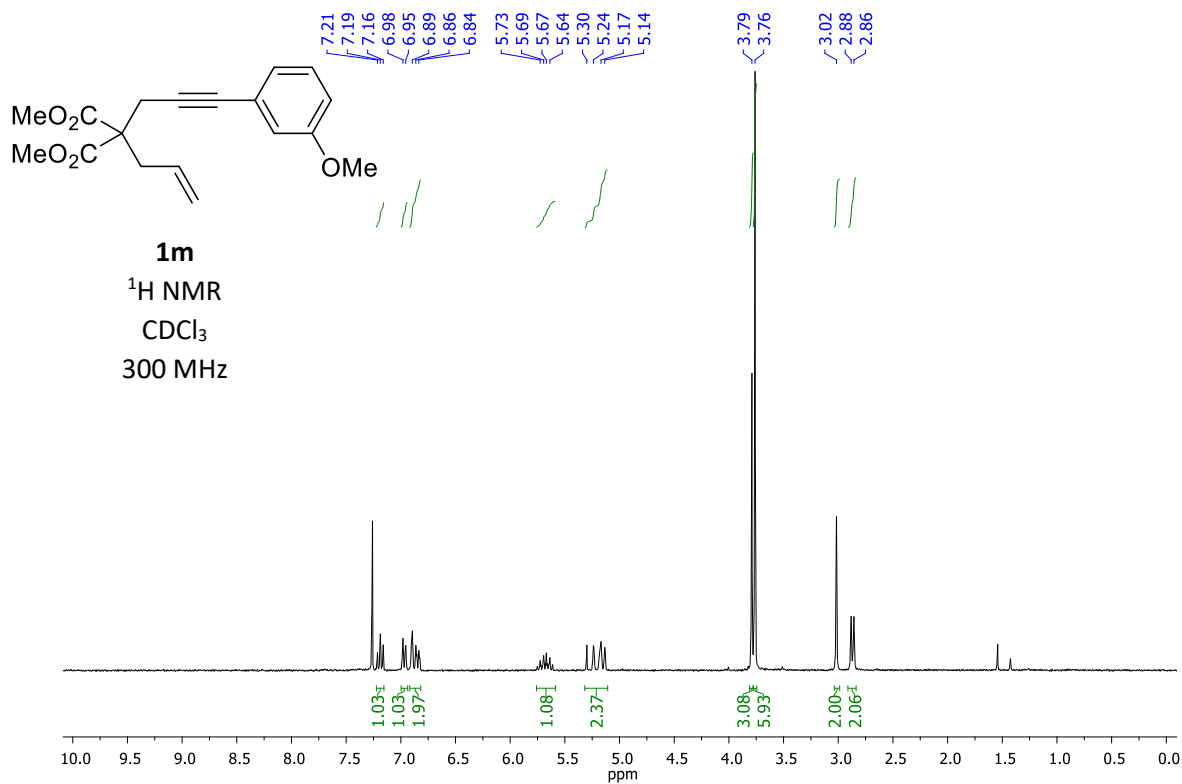


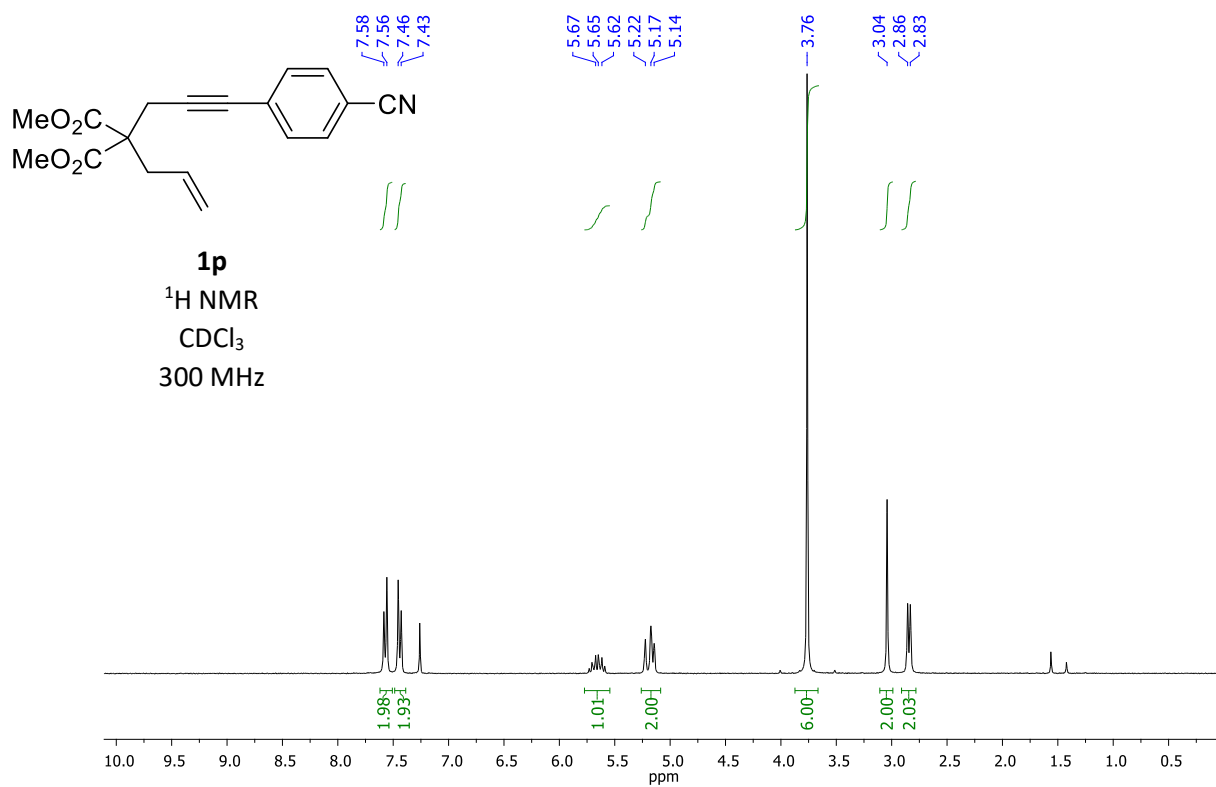
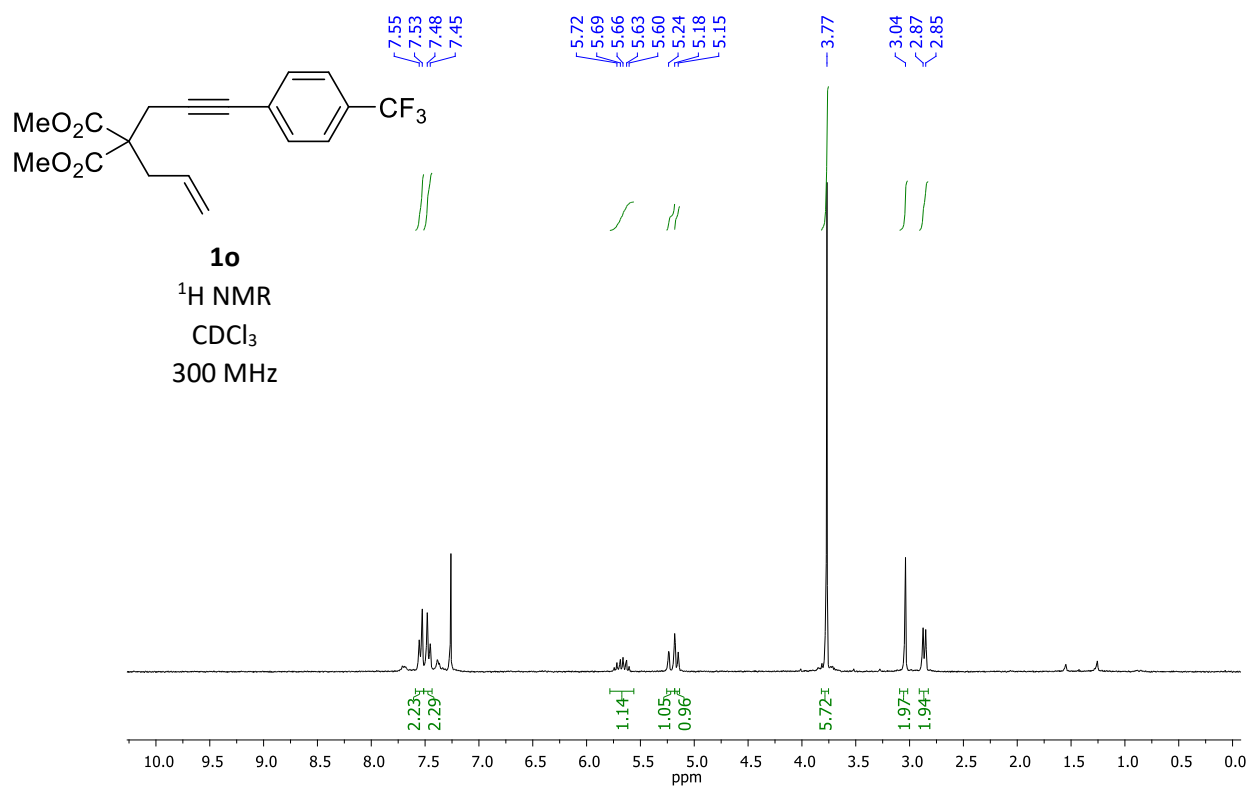


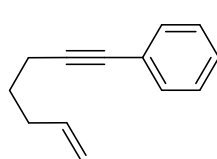




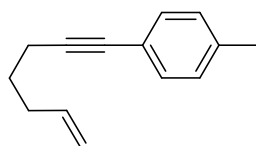
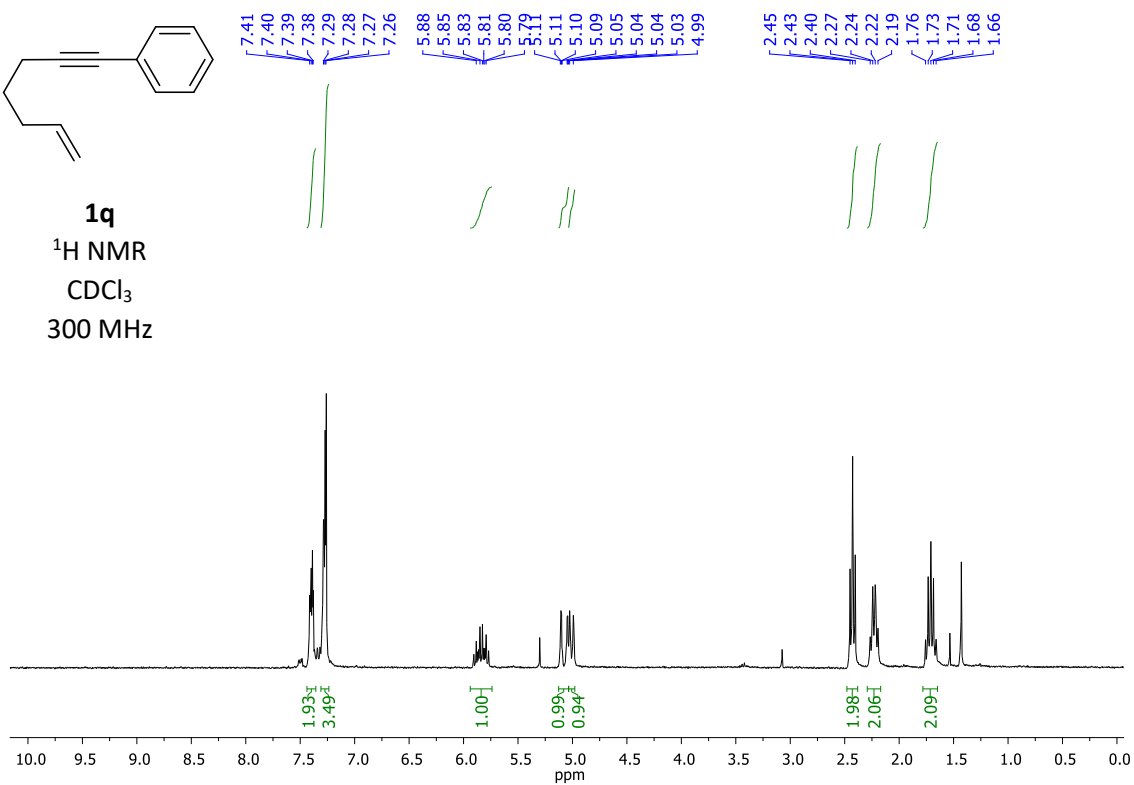




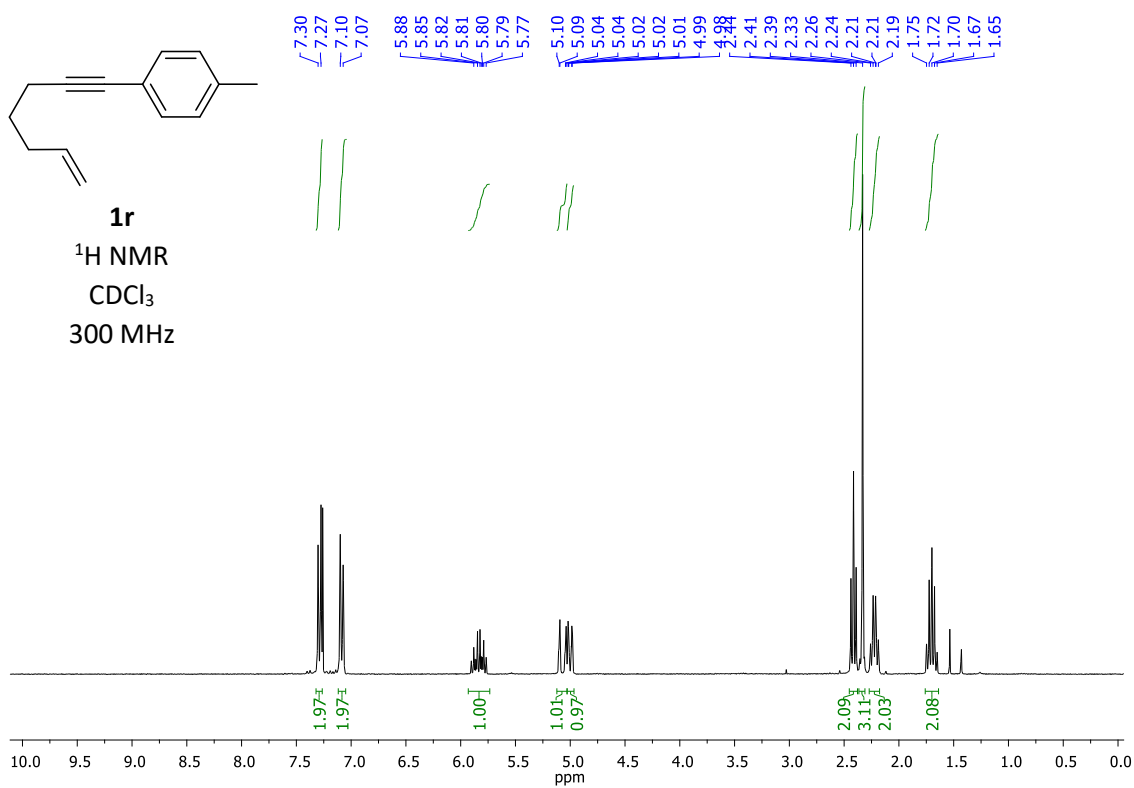


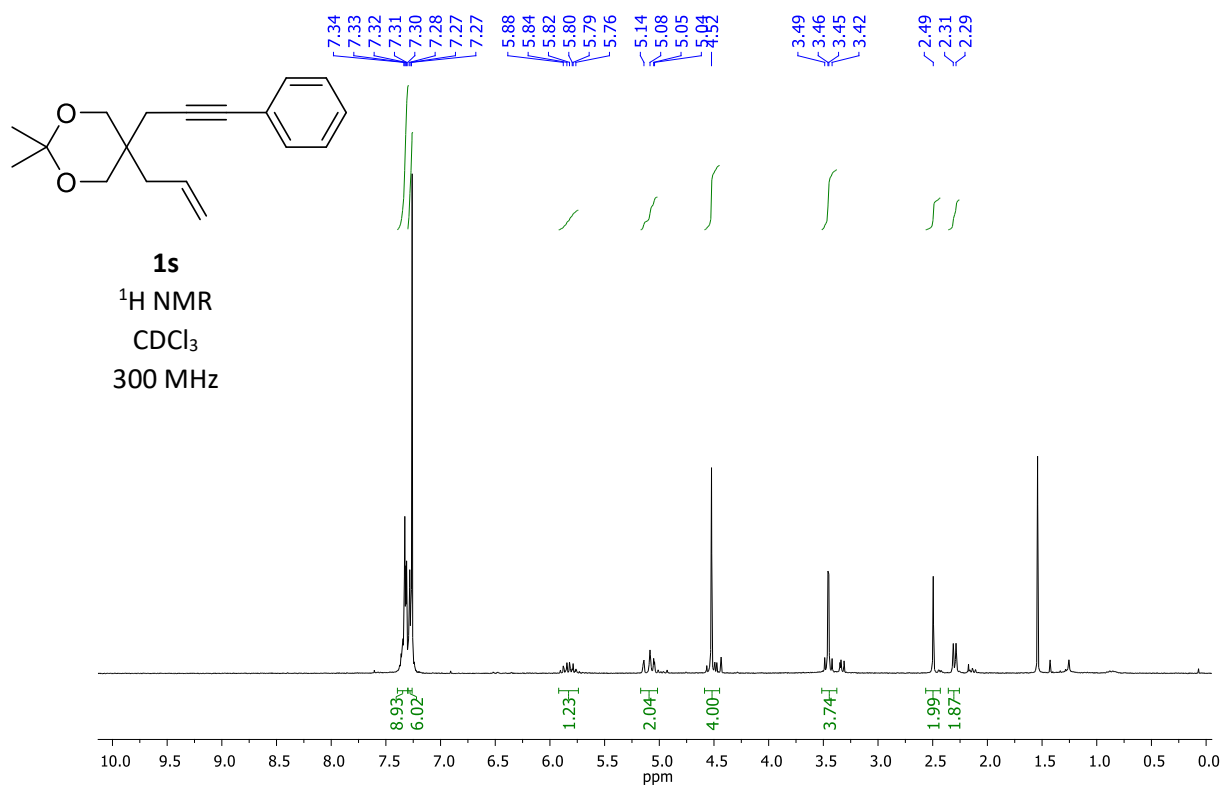
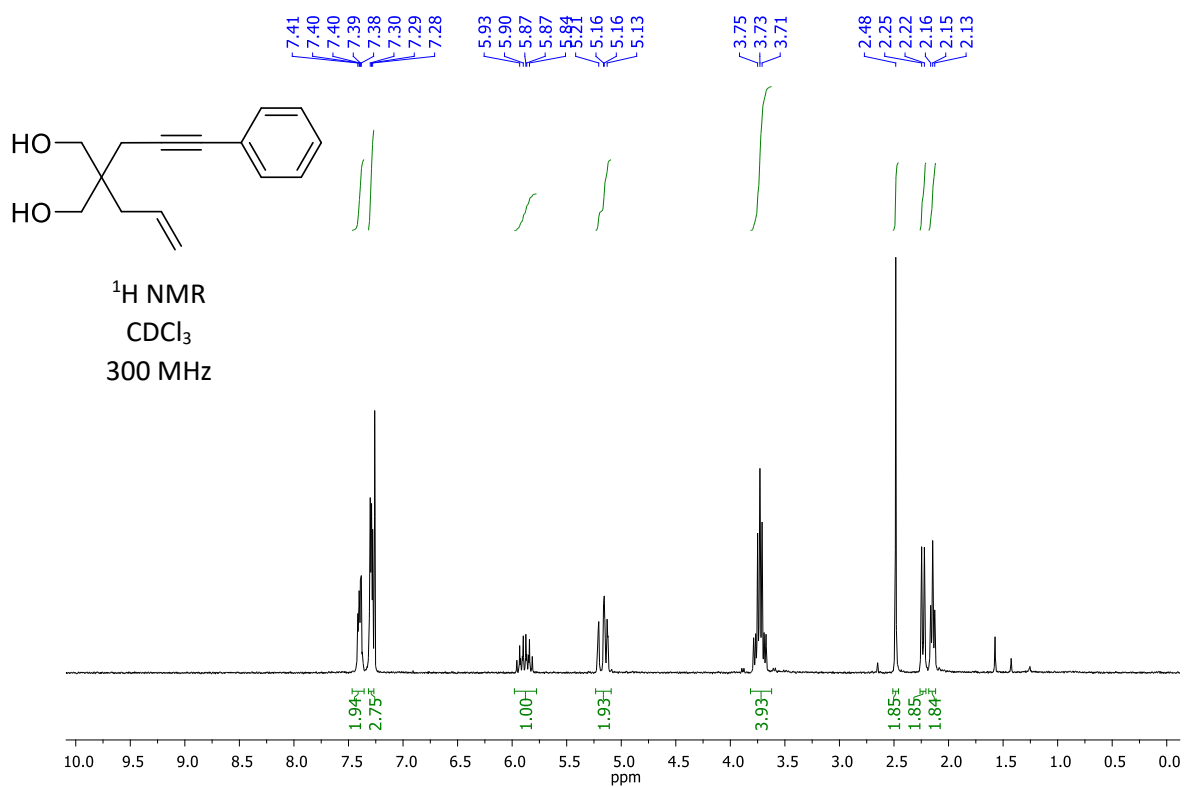


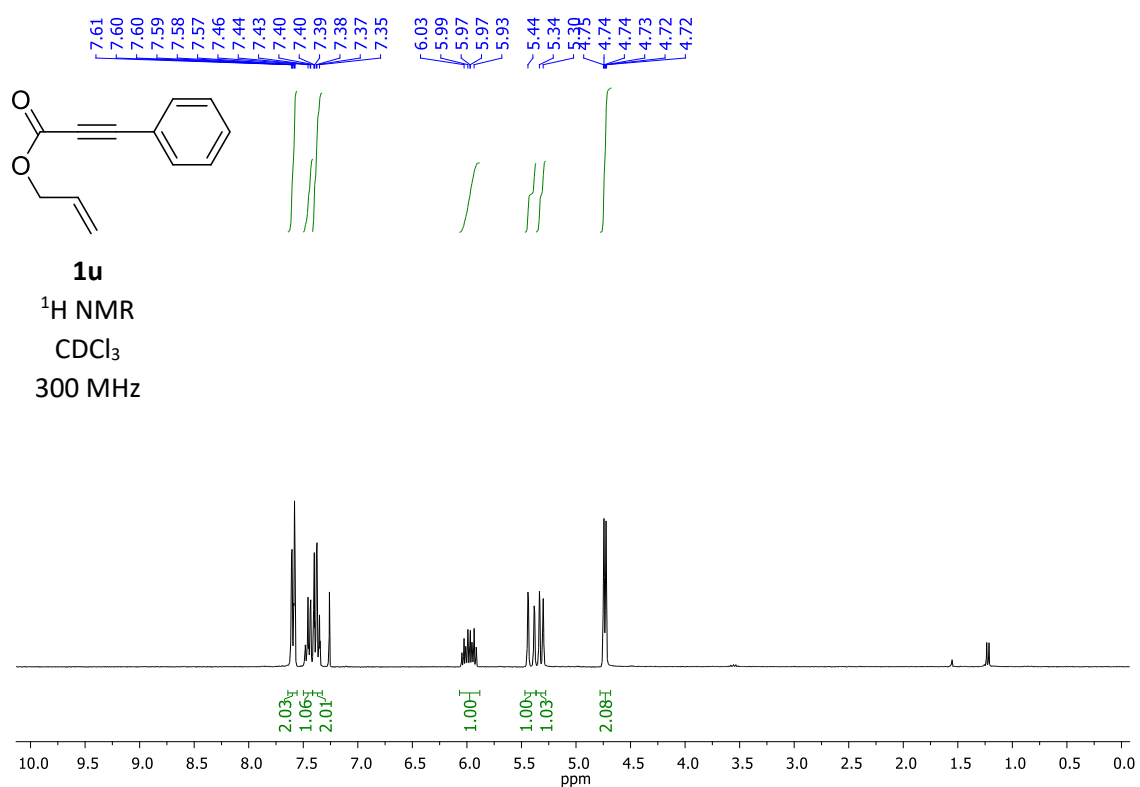
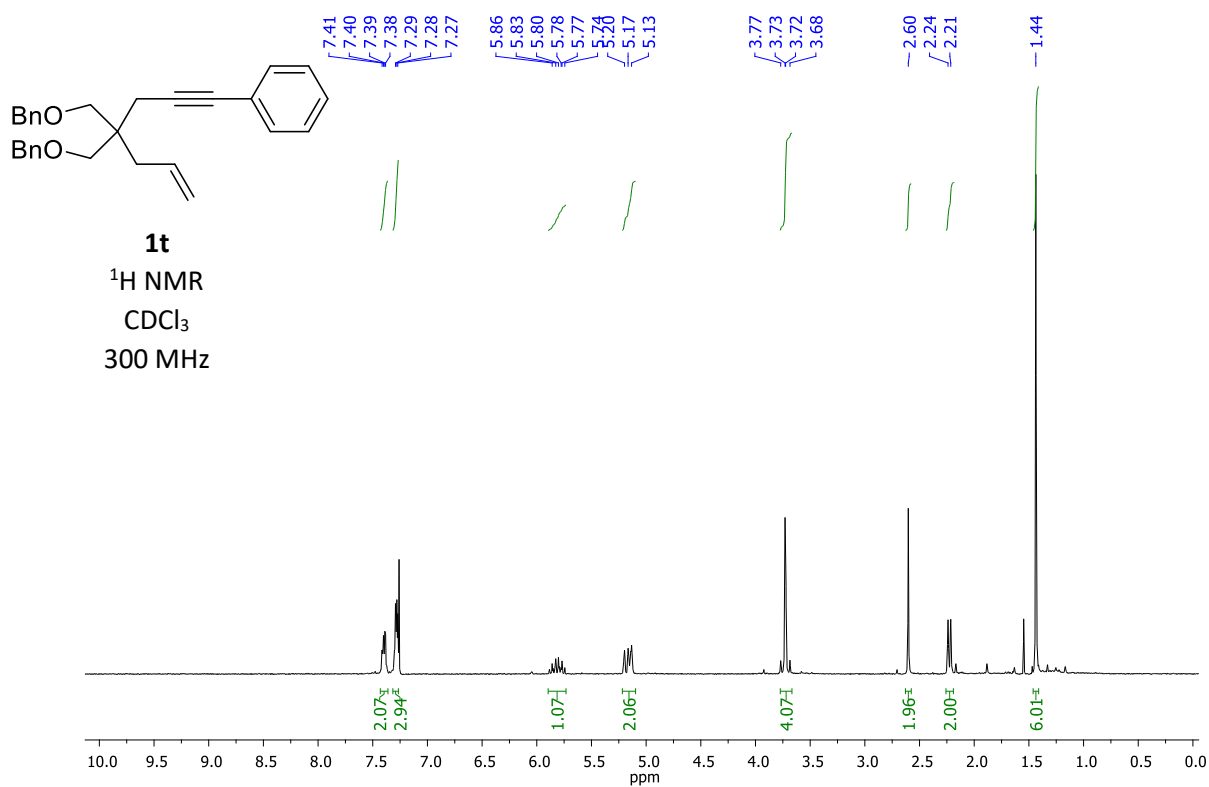
1q
¹H NMR
 CDCl₃
 300 MHz

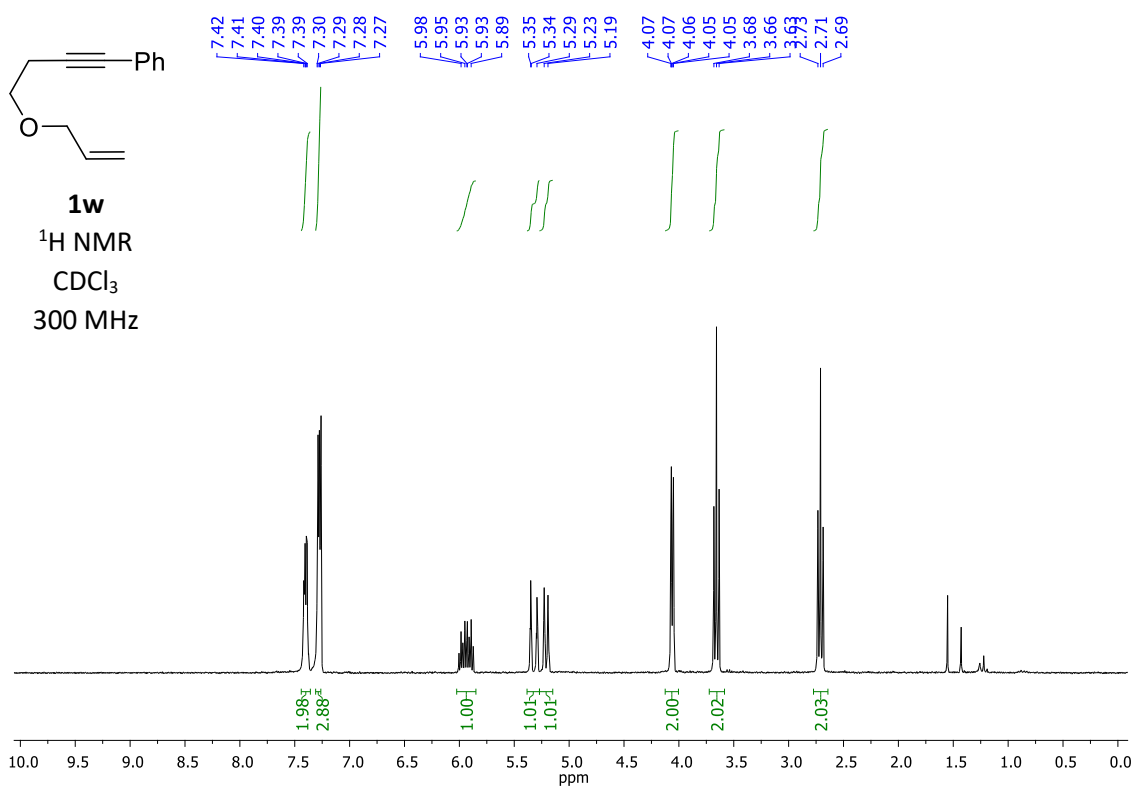
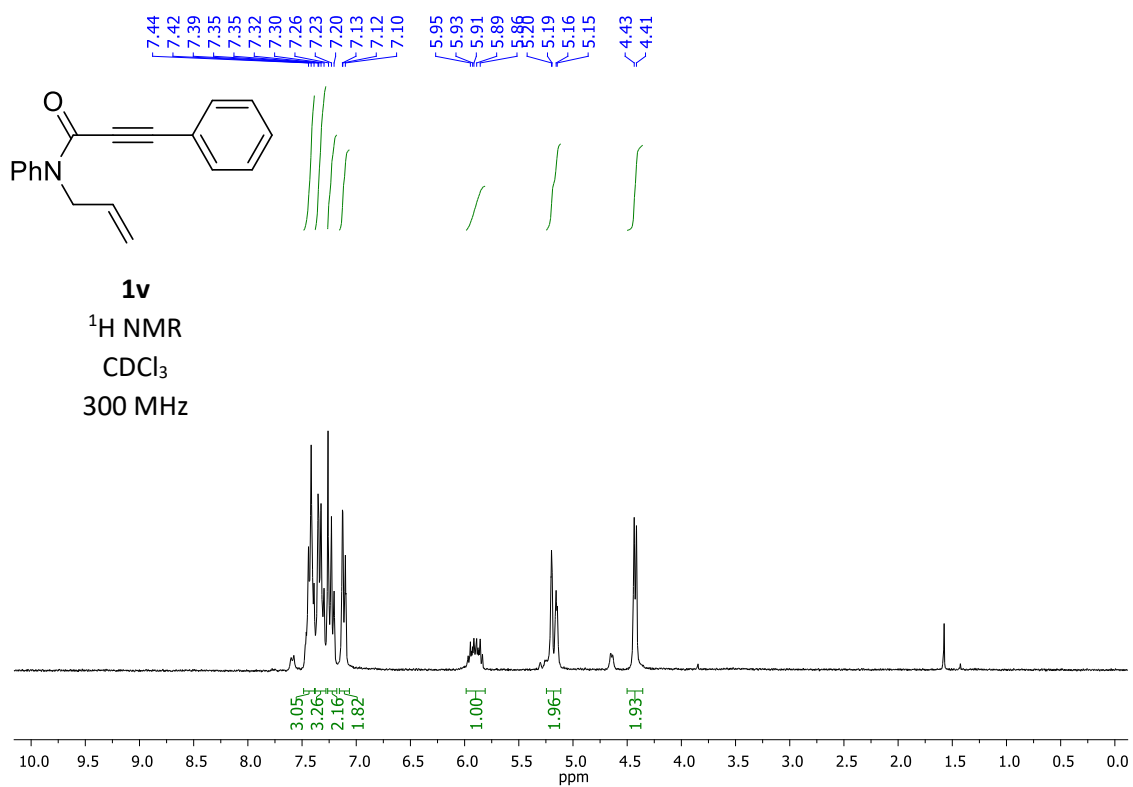


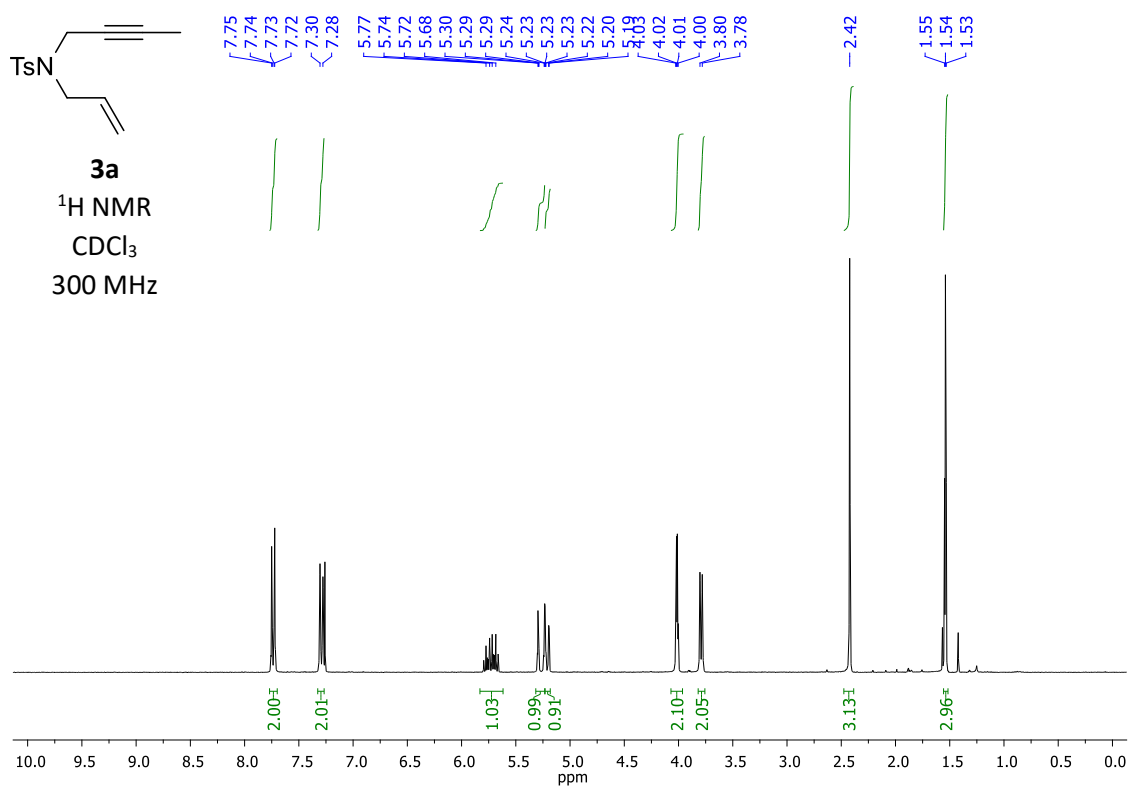
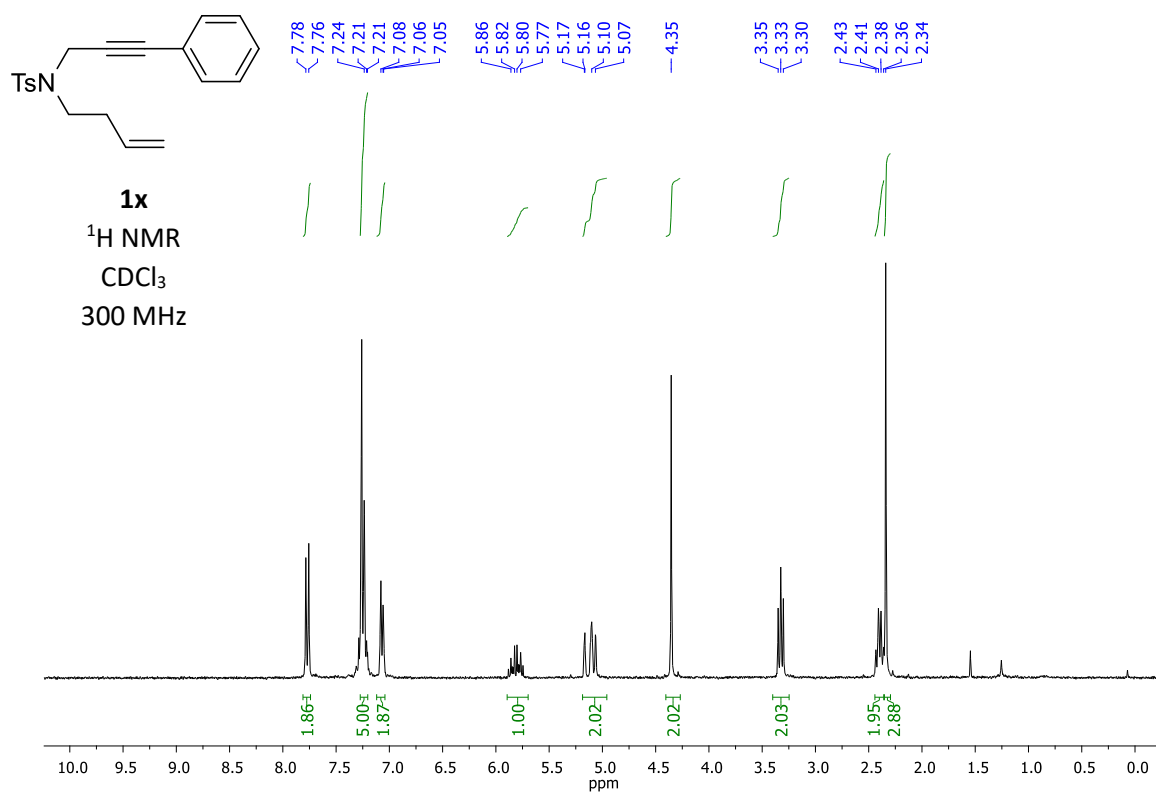
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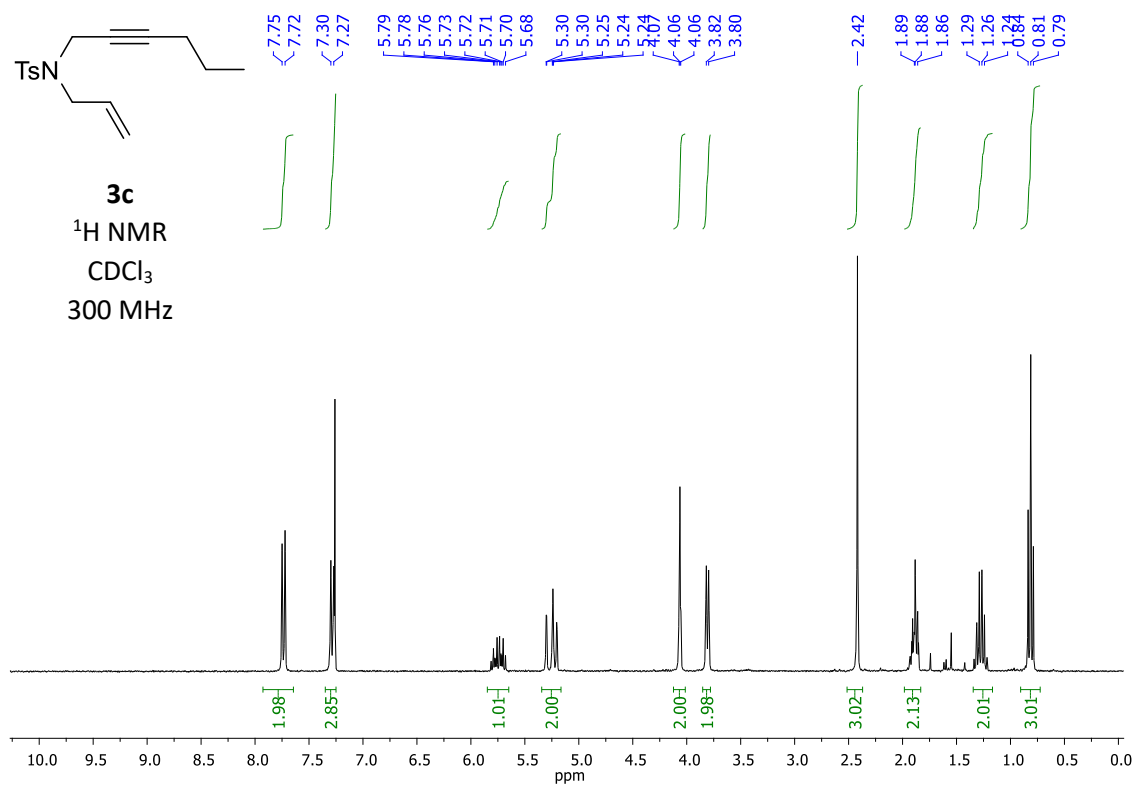
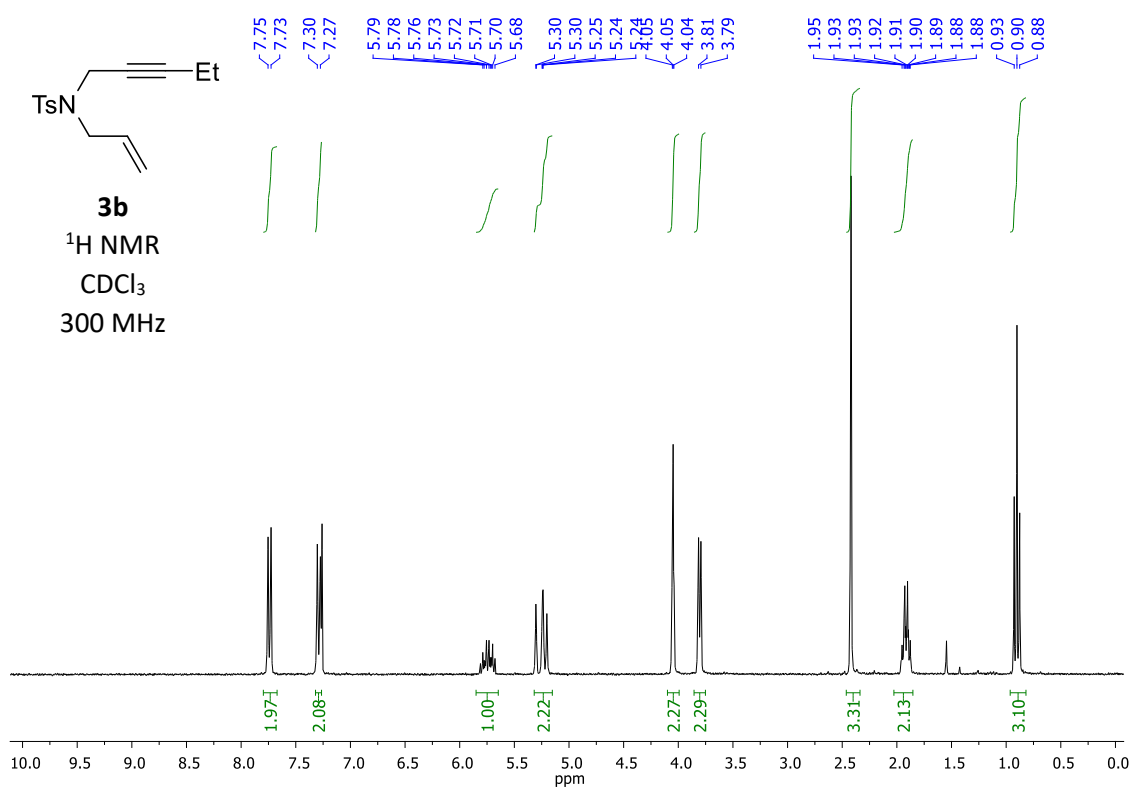


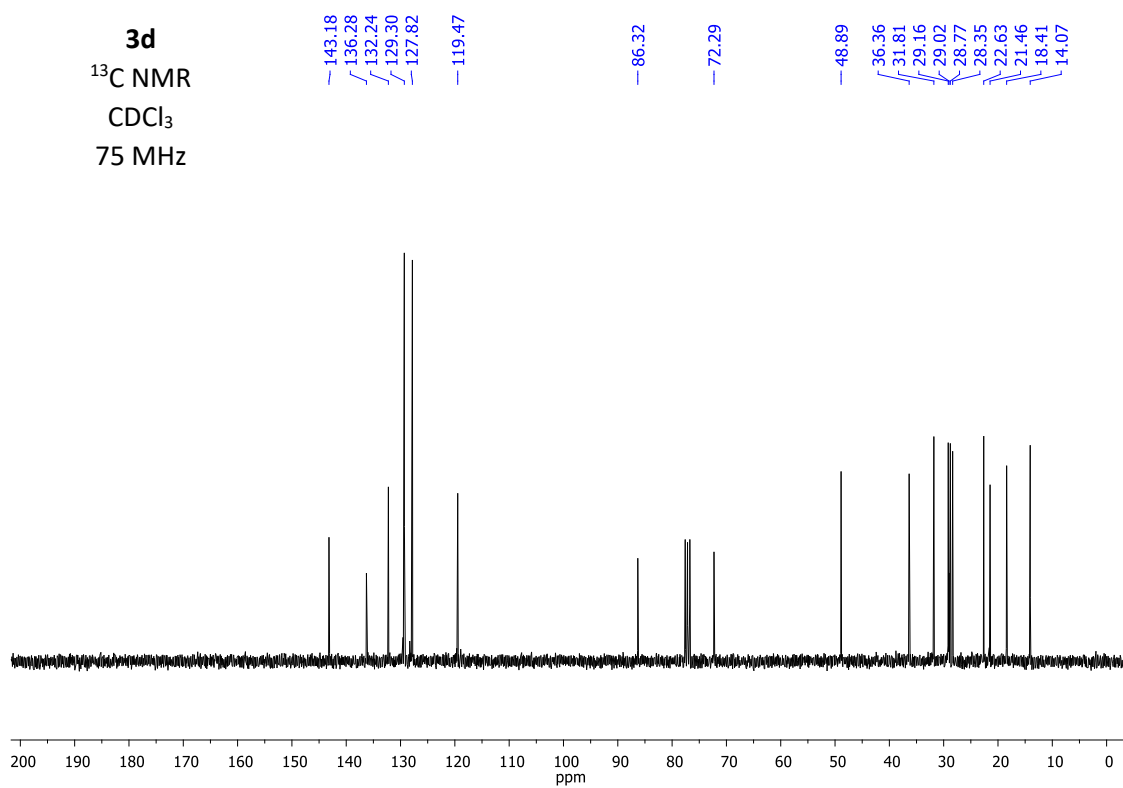
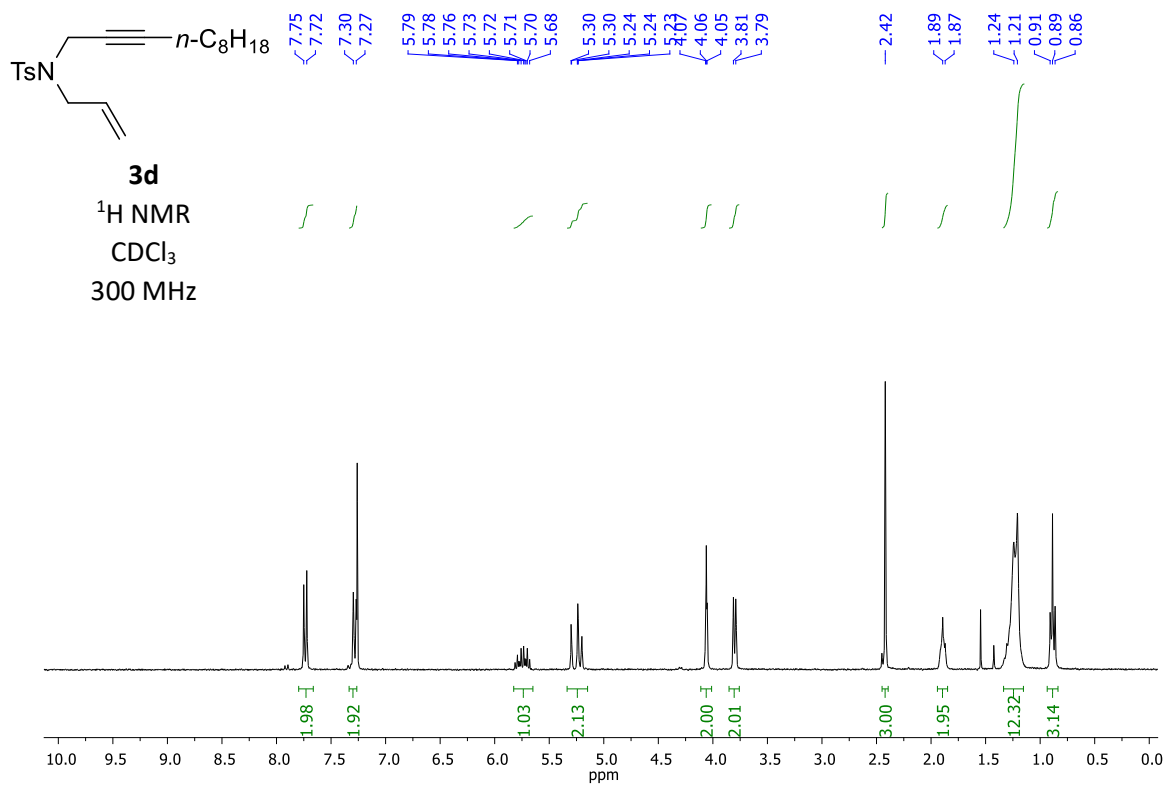


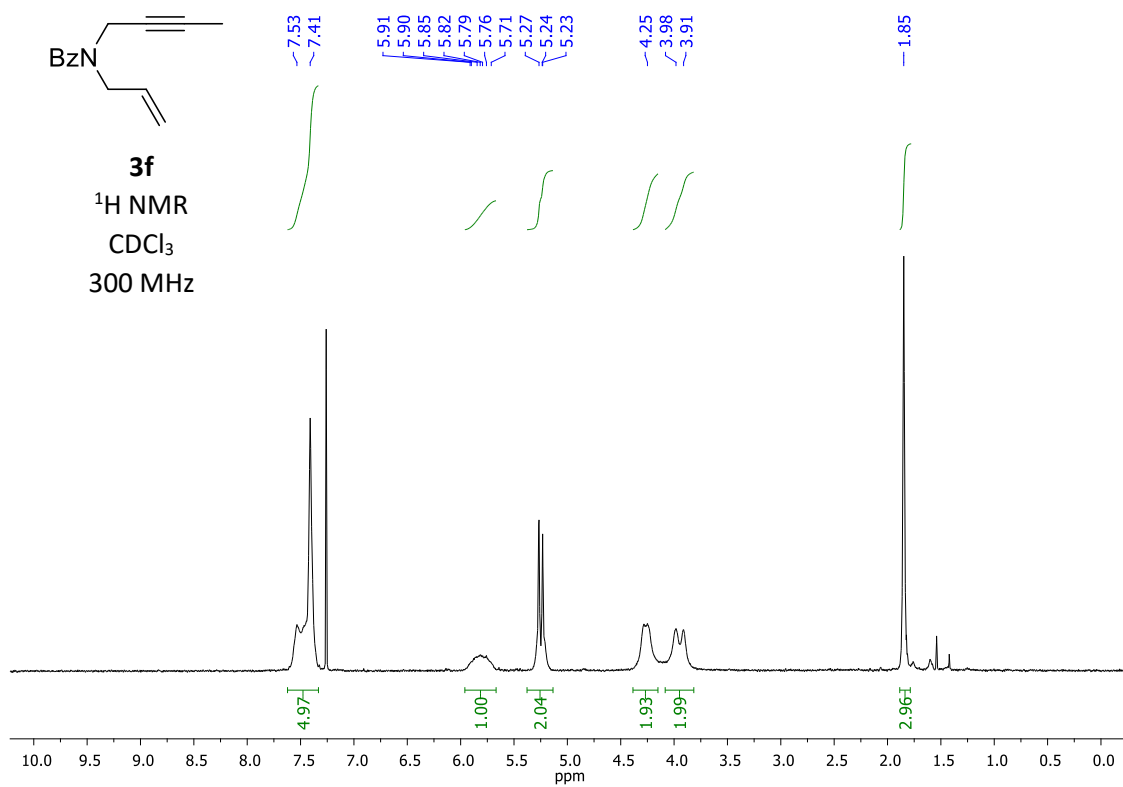
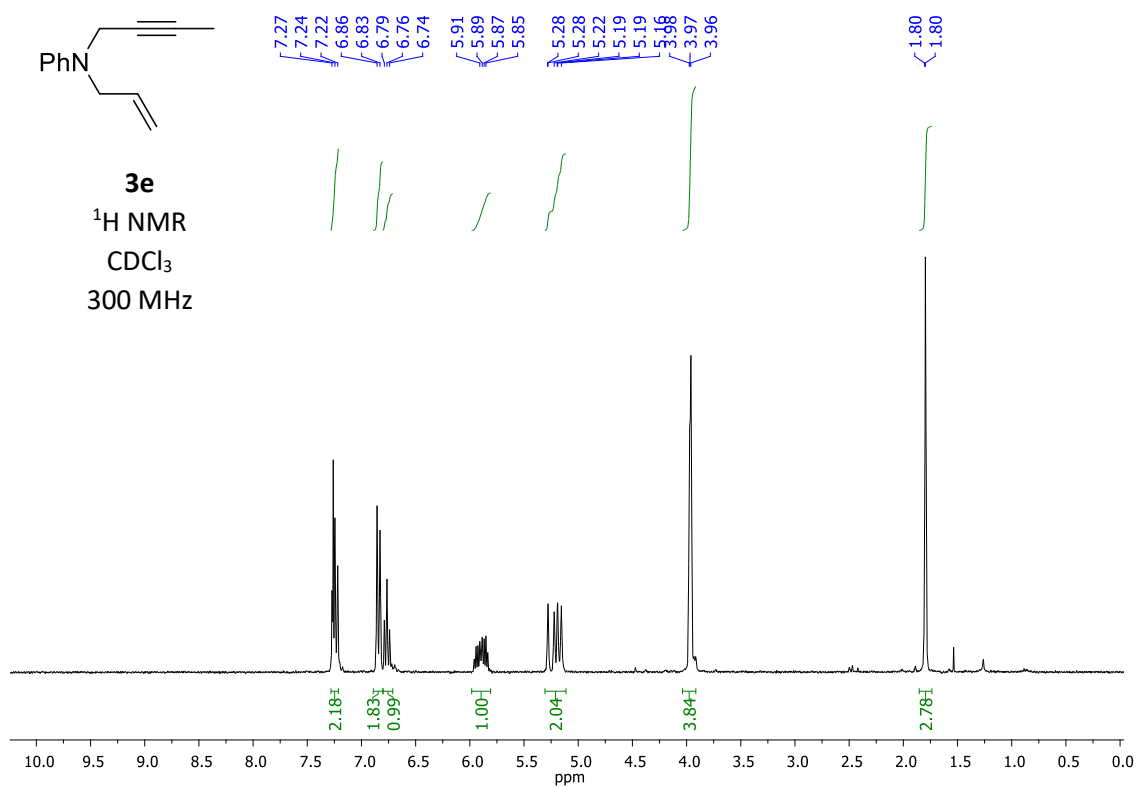


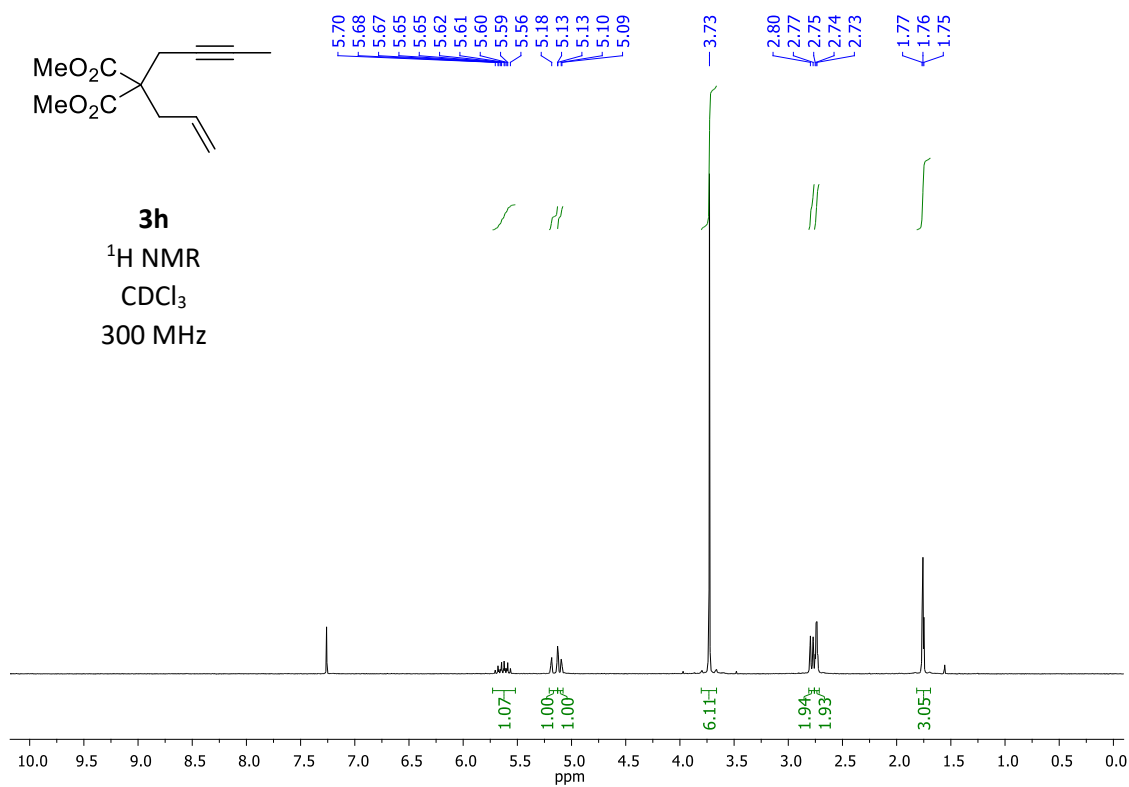
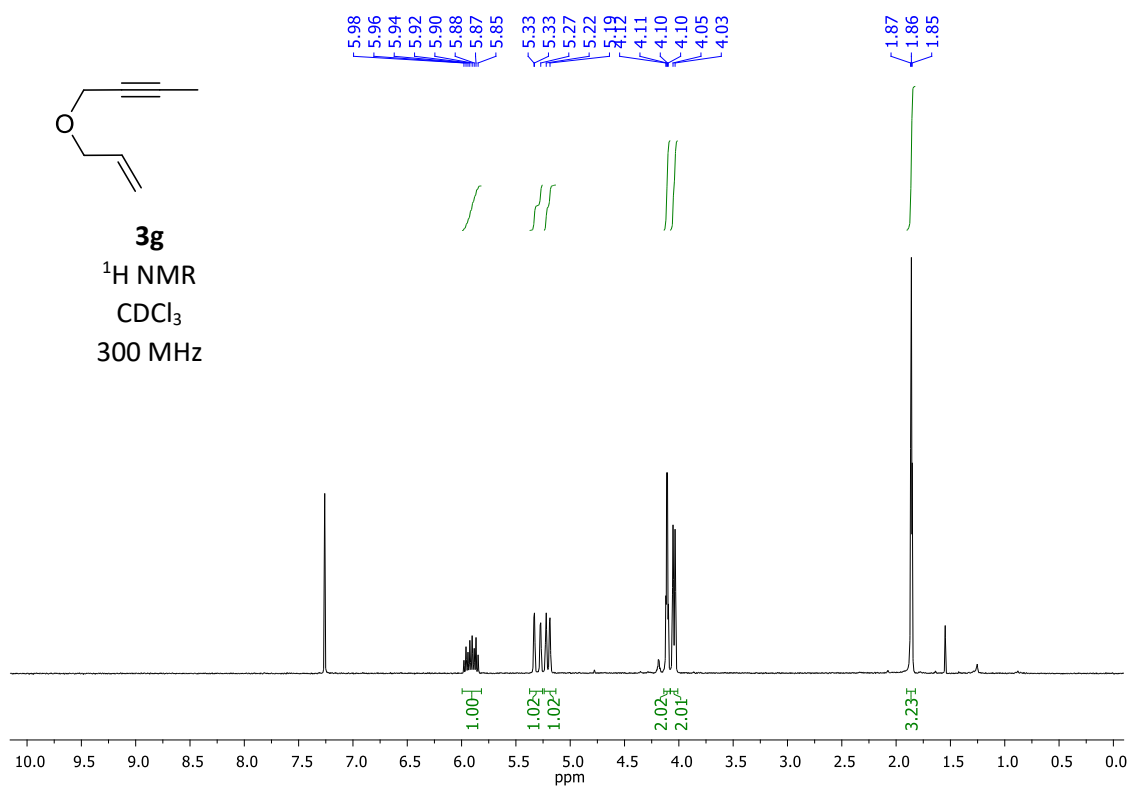


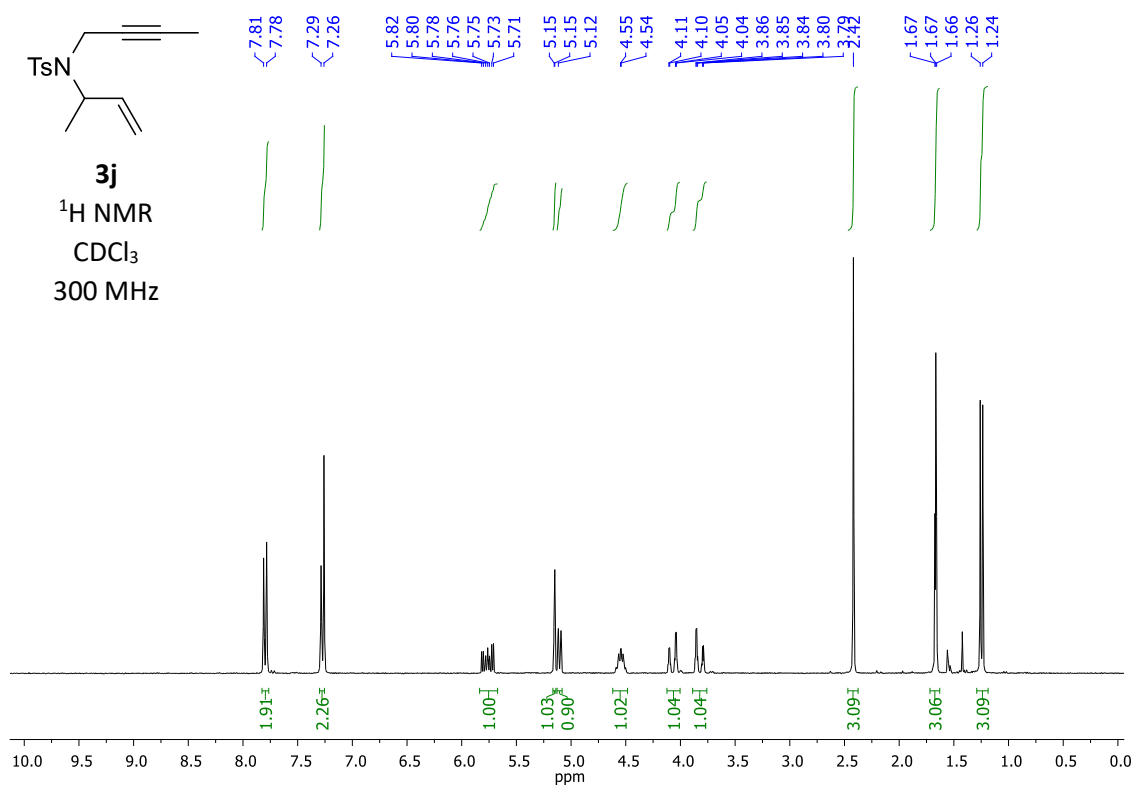
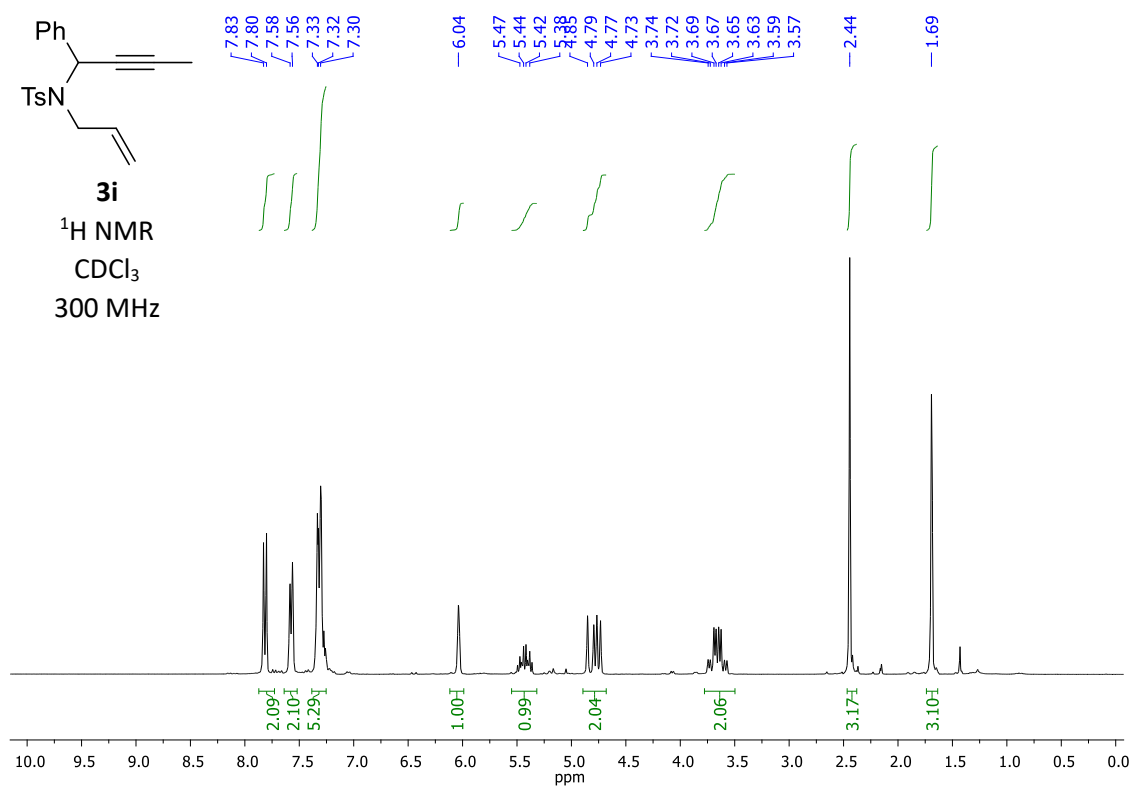




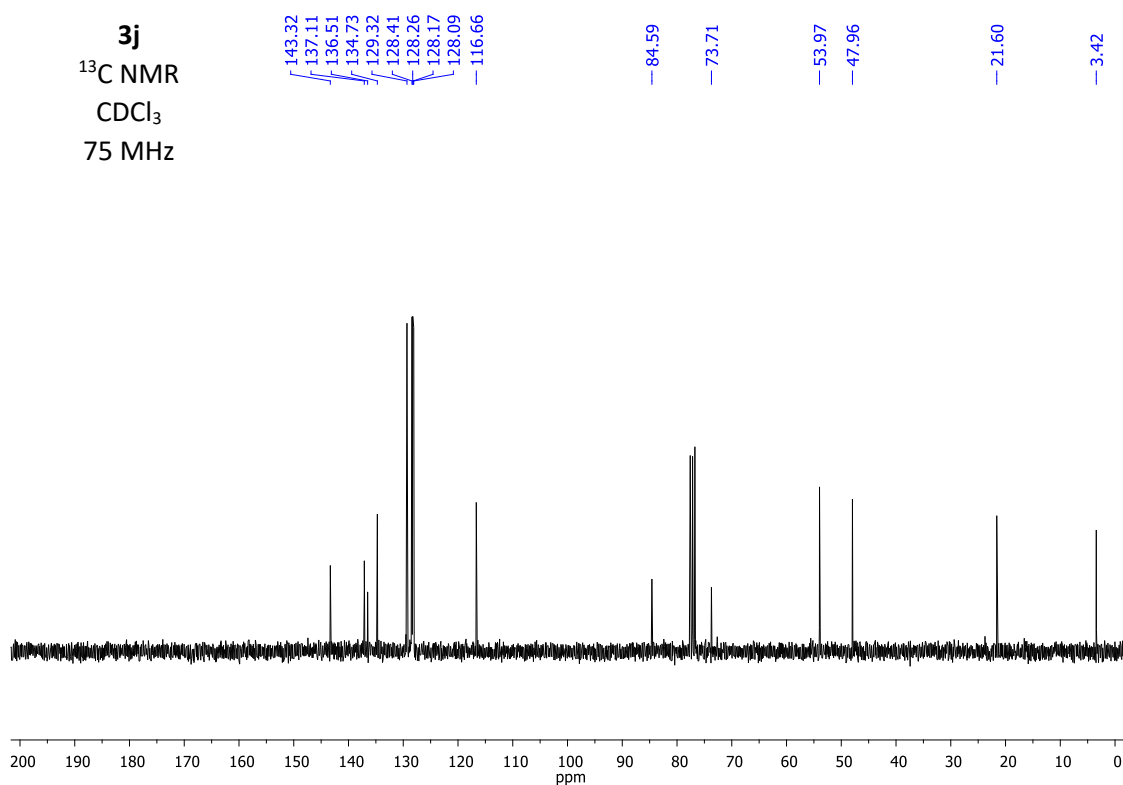




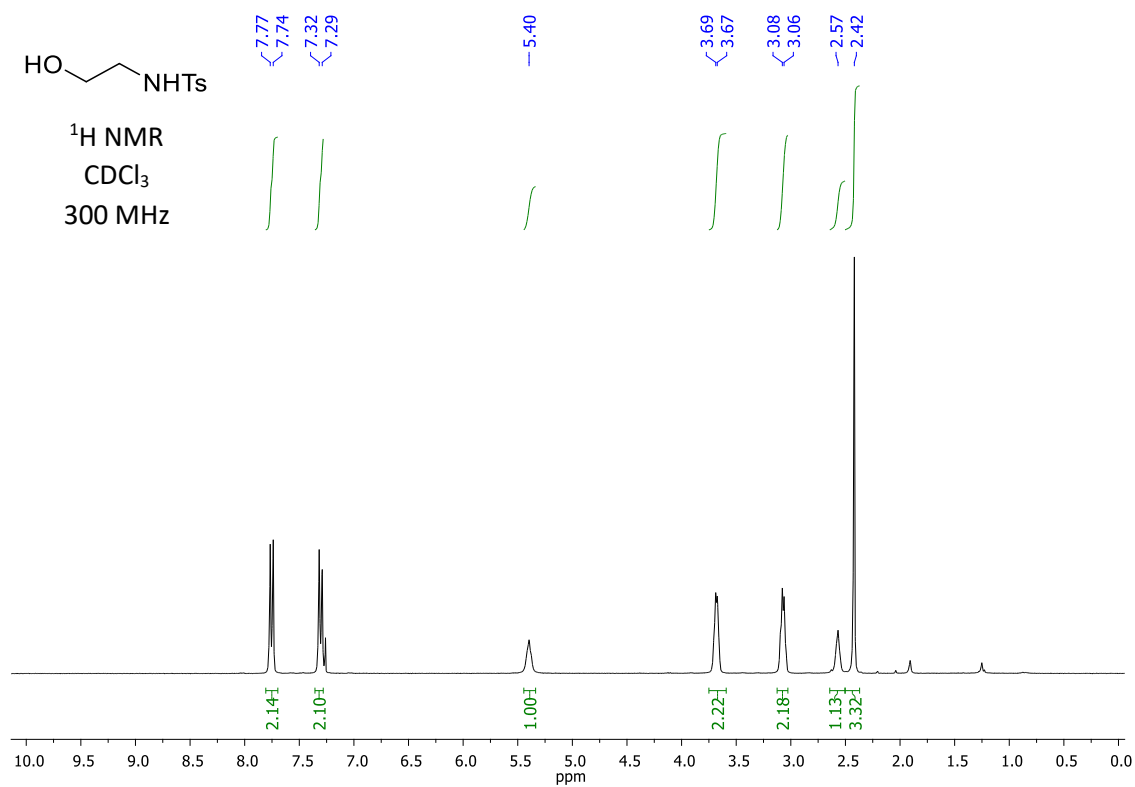


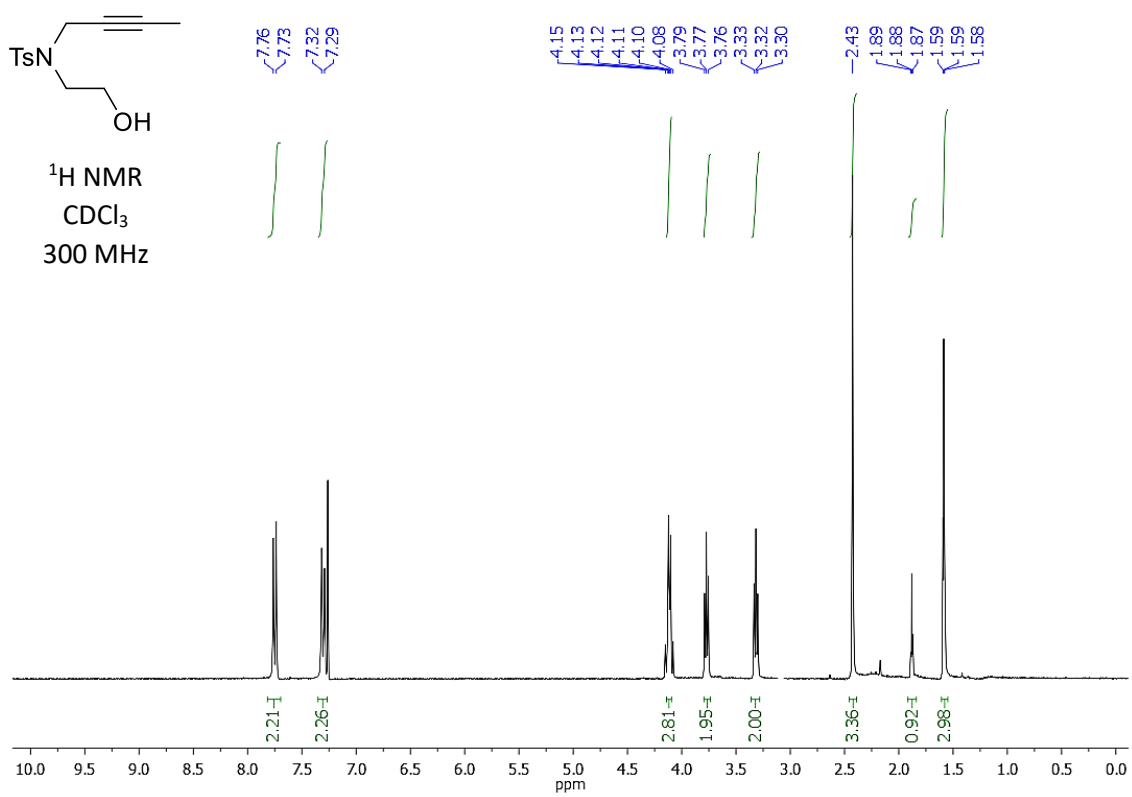
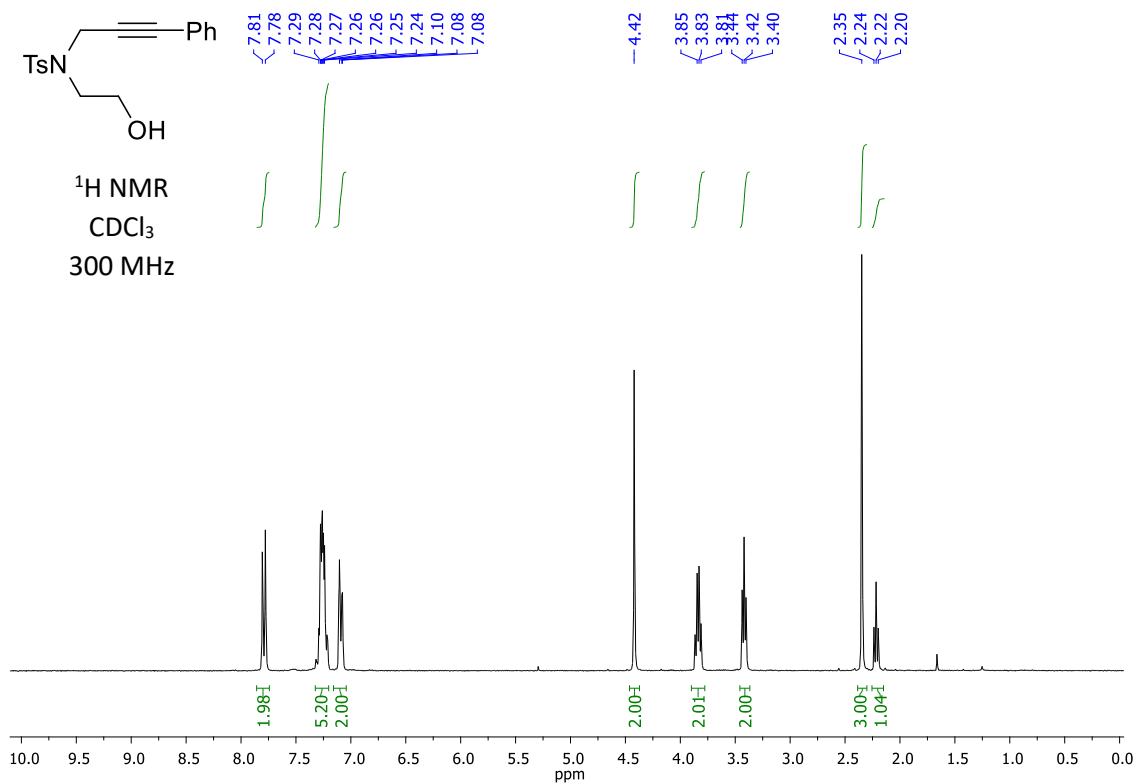


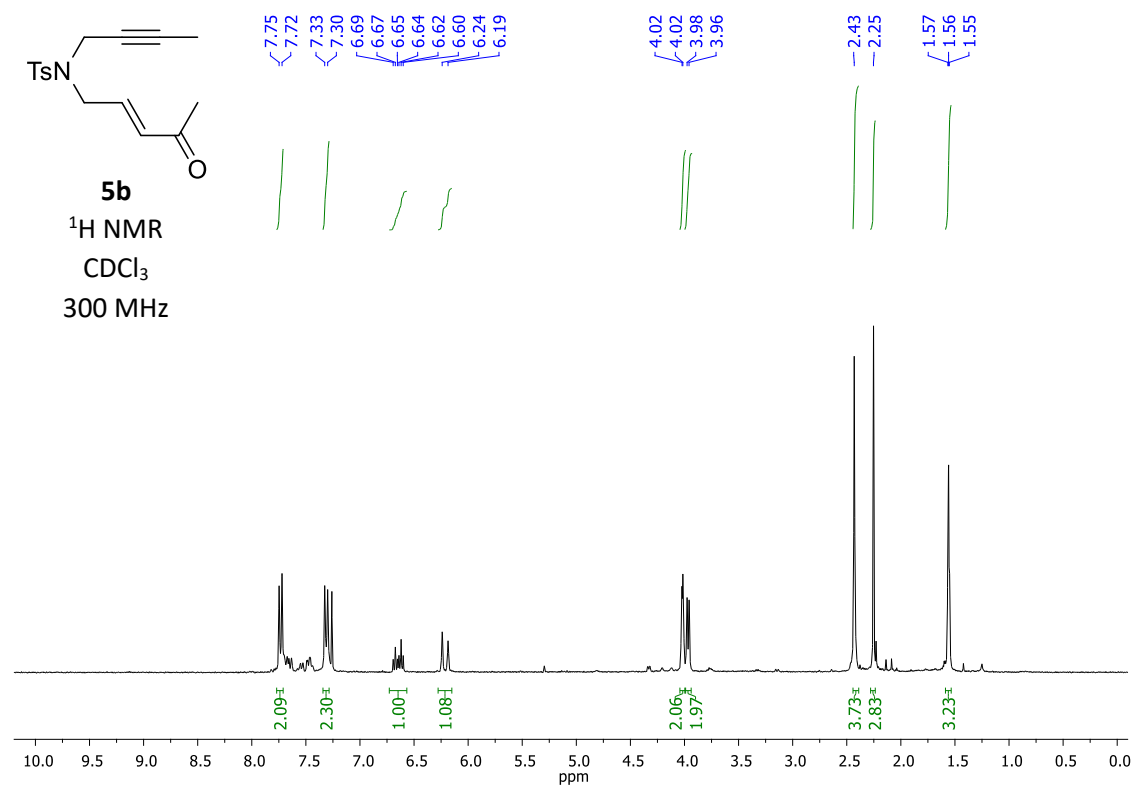
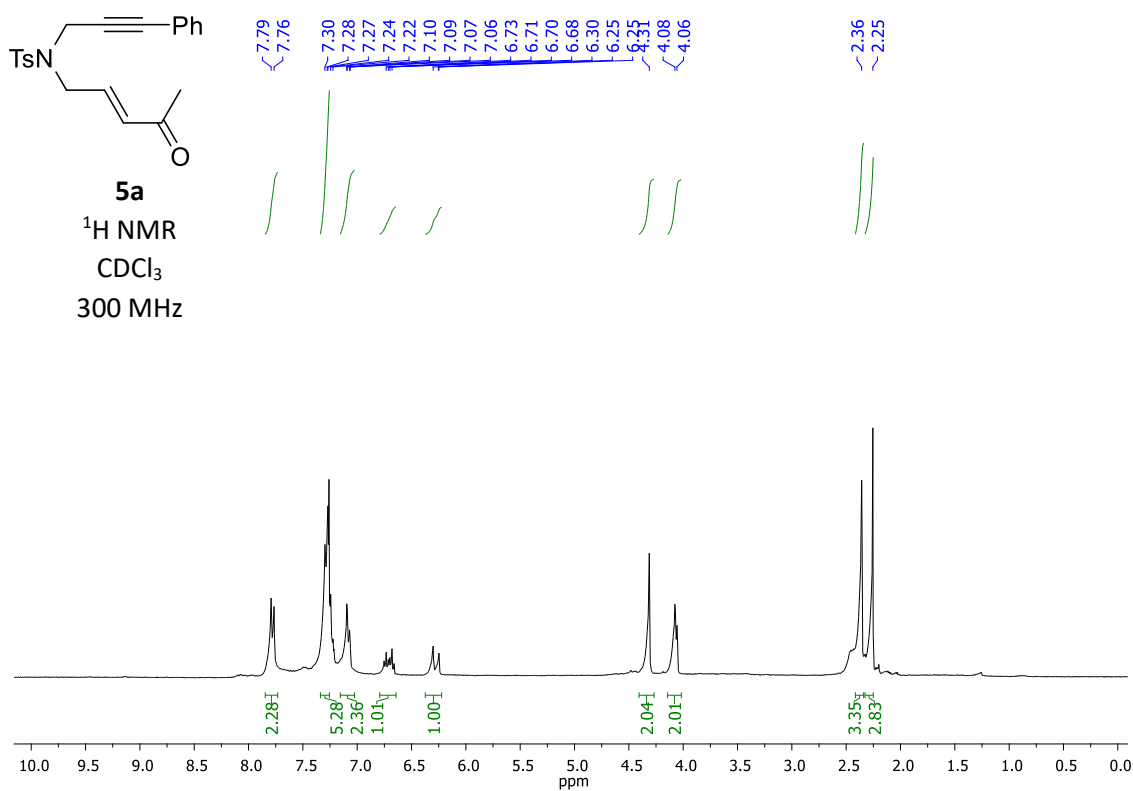
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 CDCl_3
 75 MHz

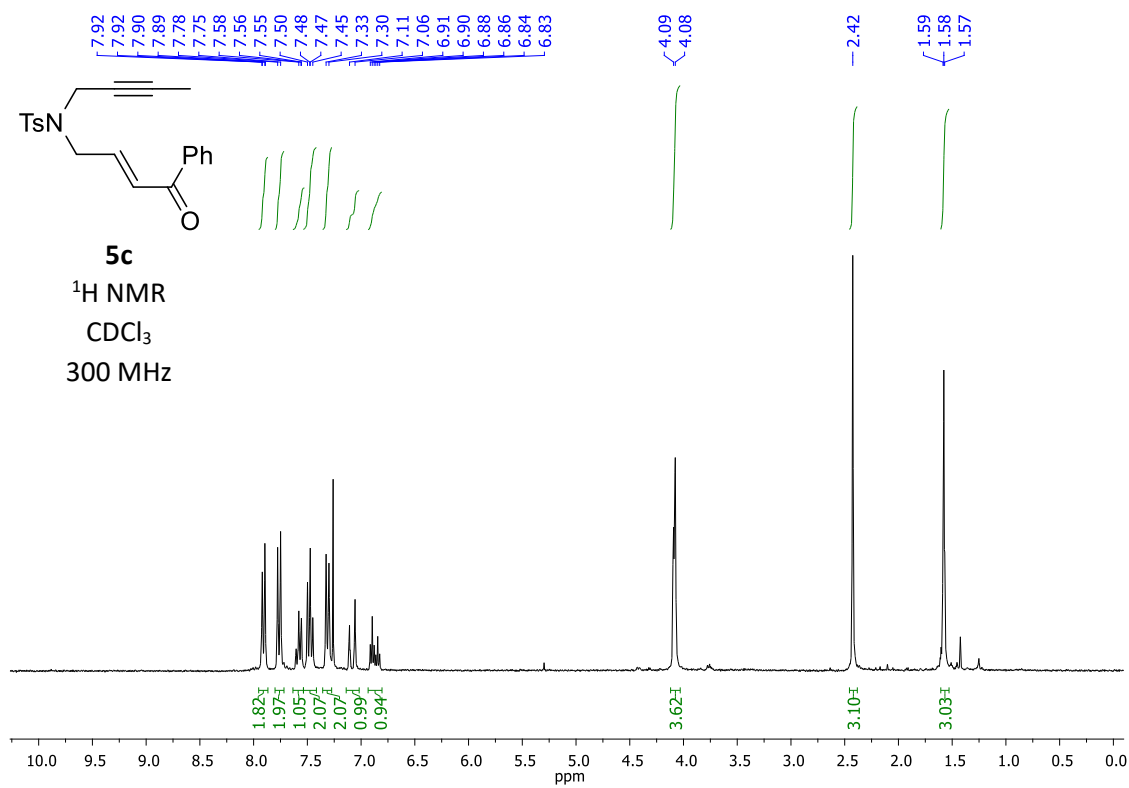
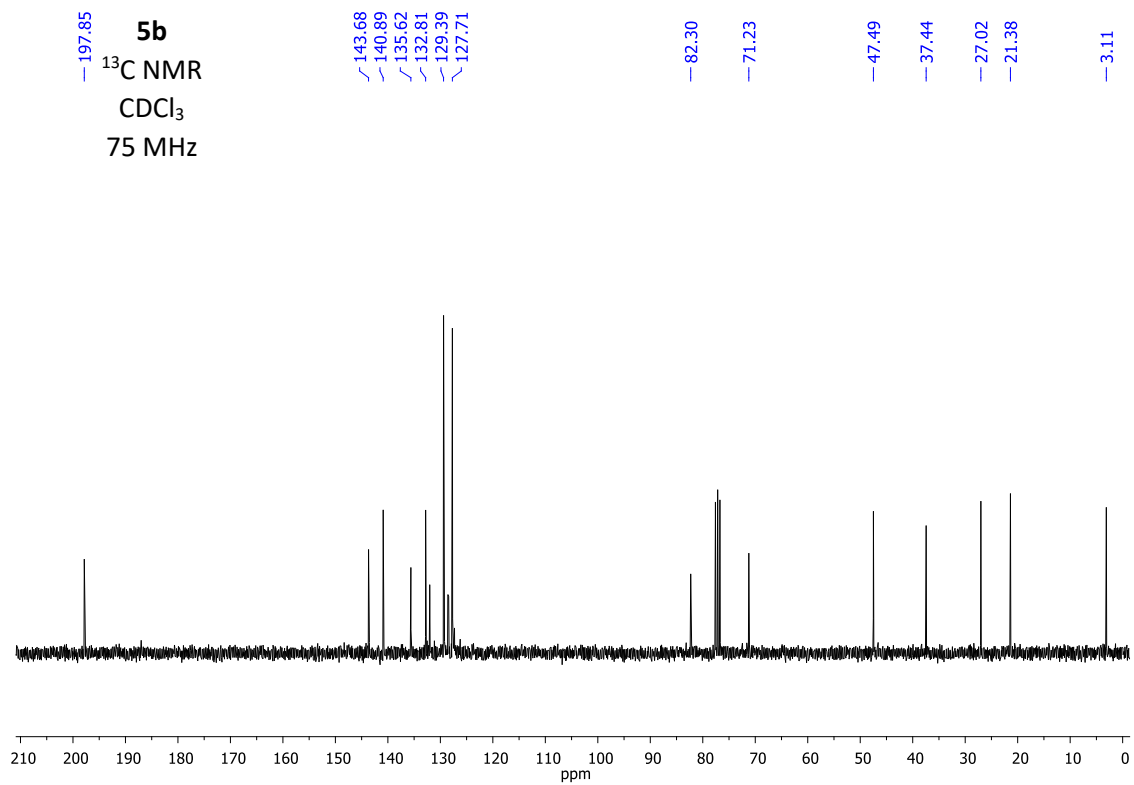


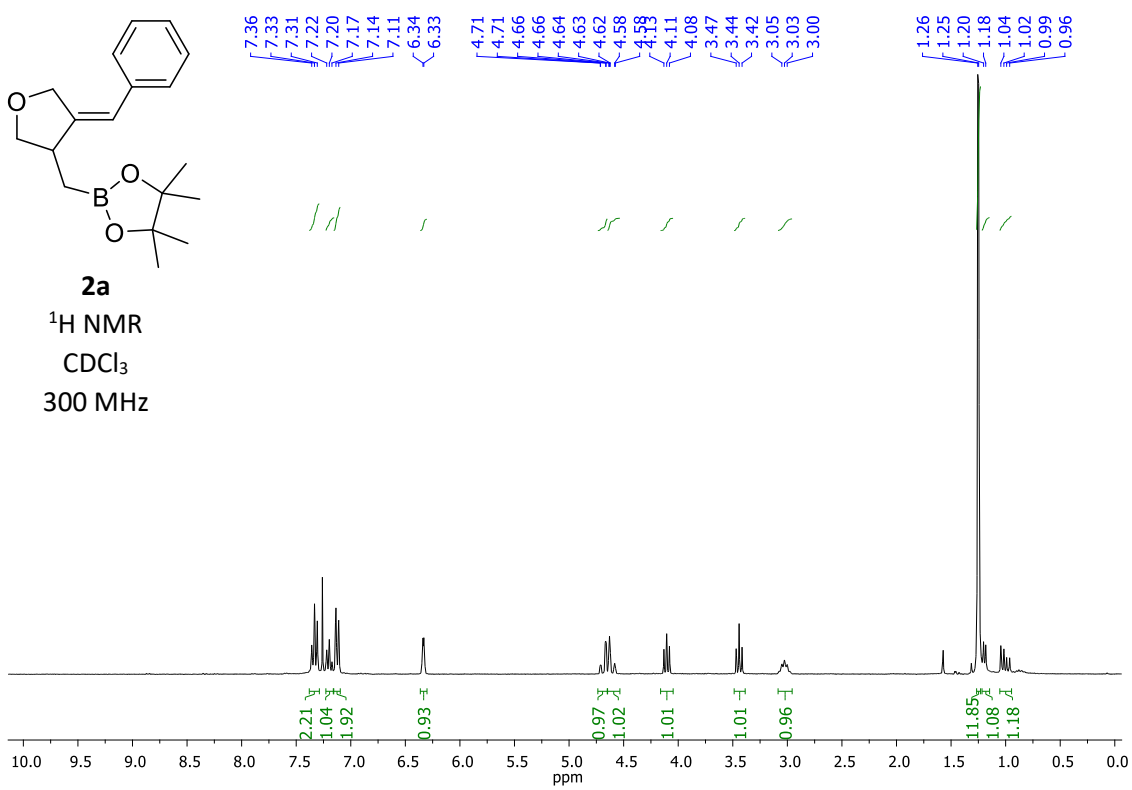
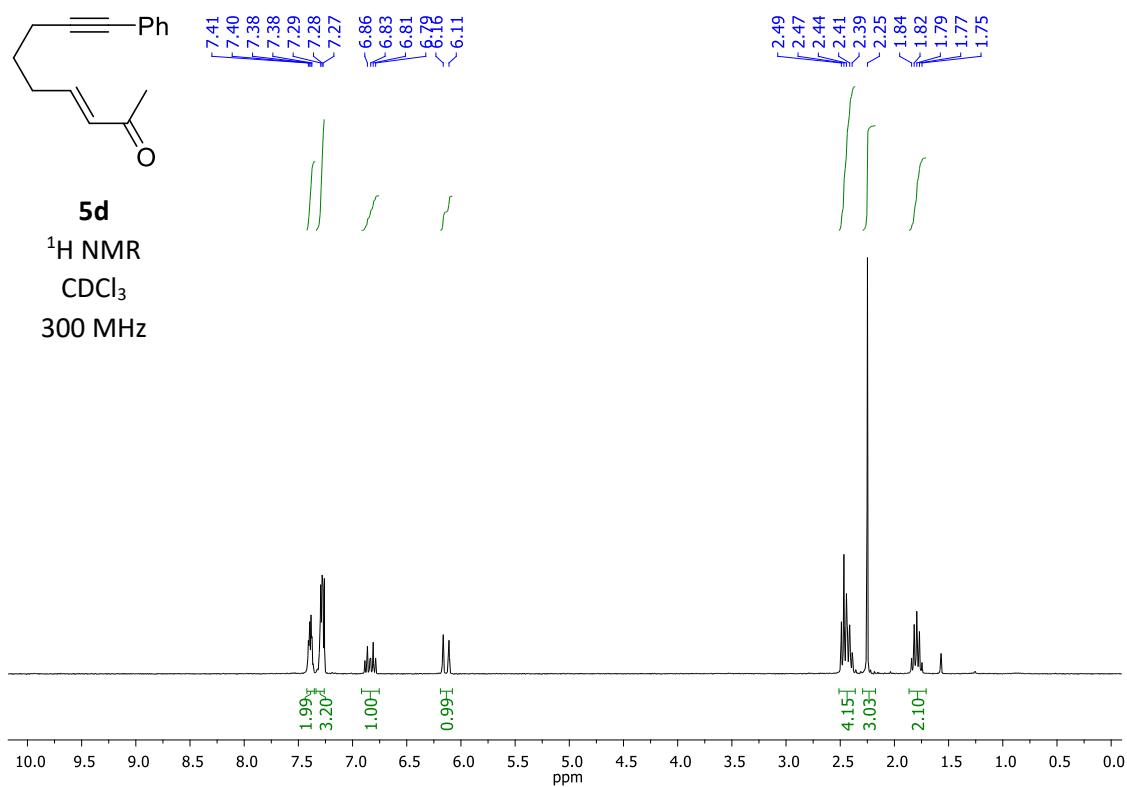
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 ^1H NMR
 CDCl_3
 300 MHz

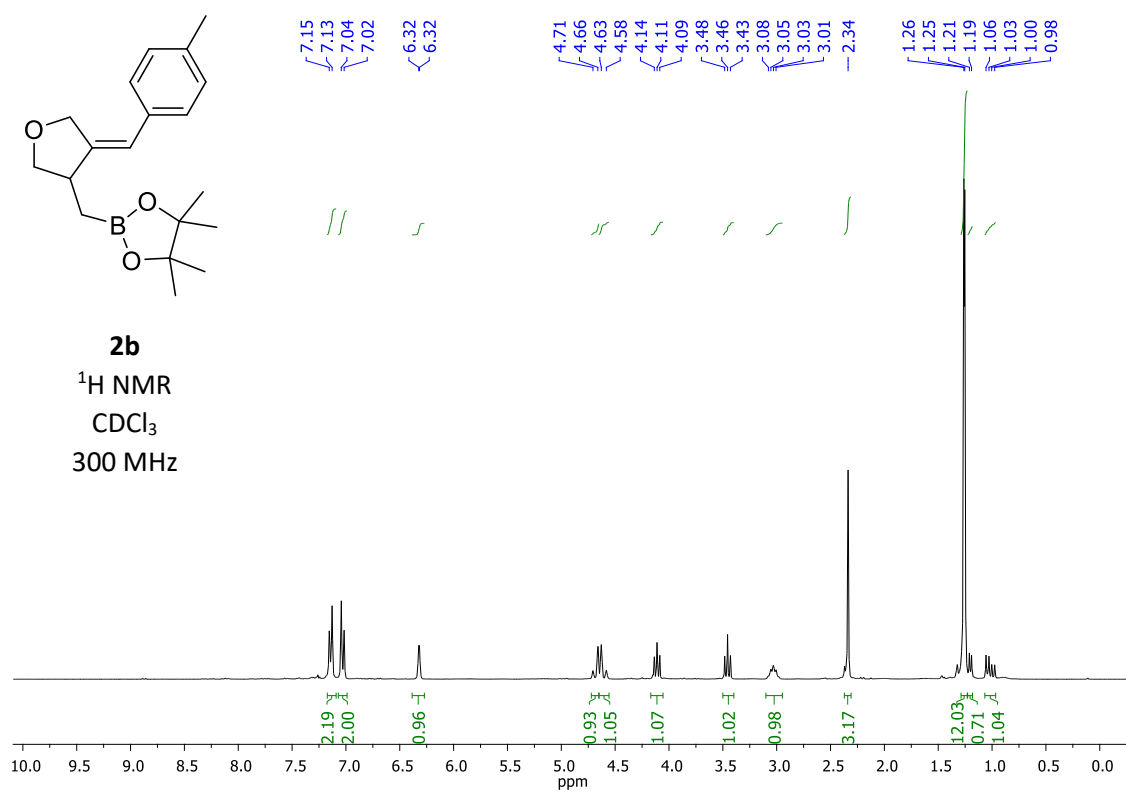
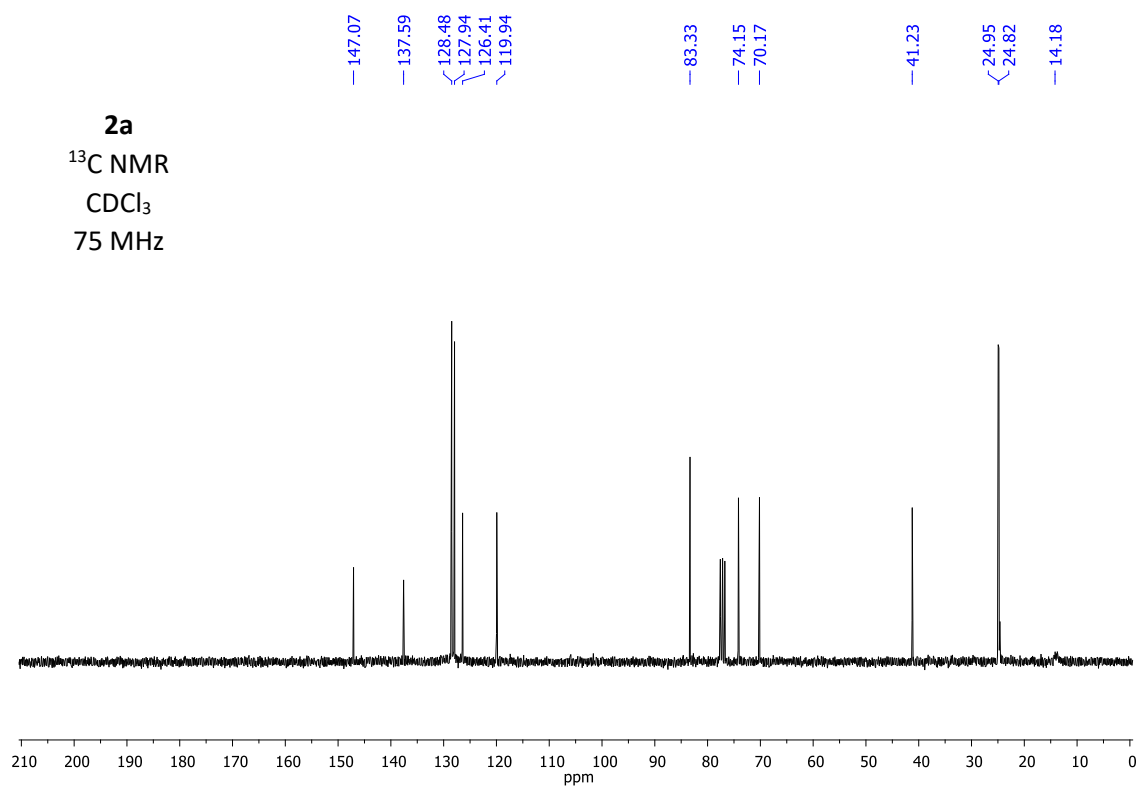


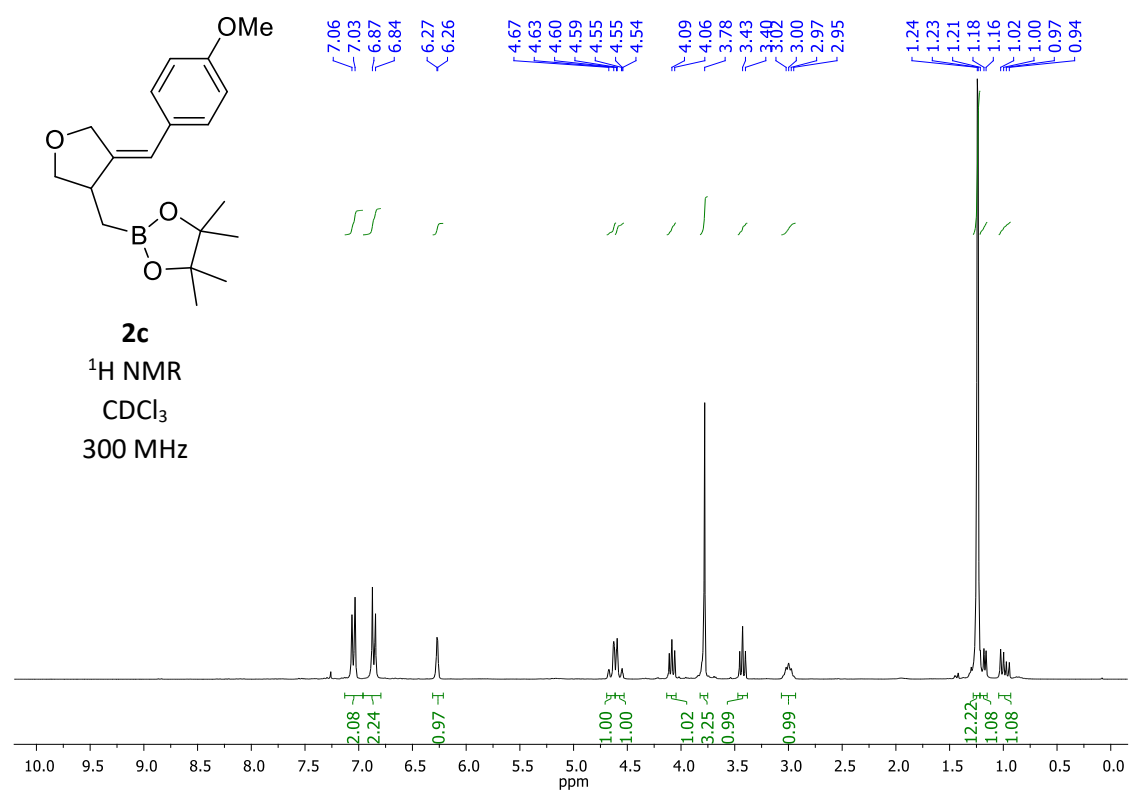
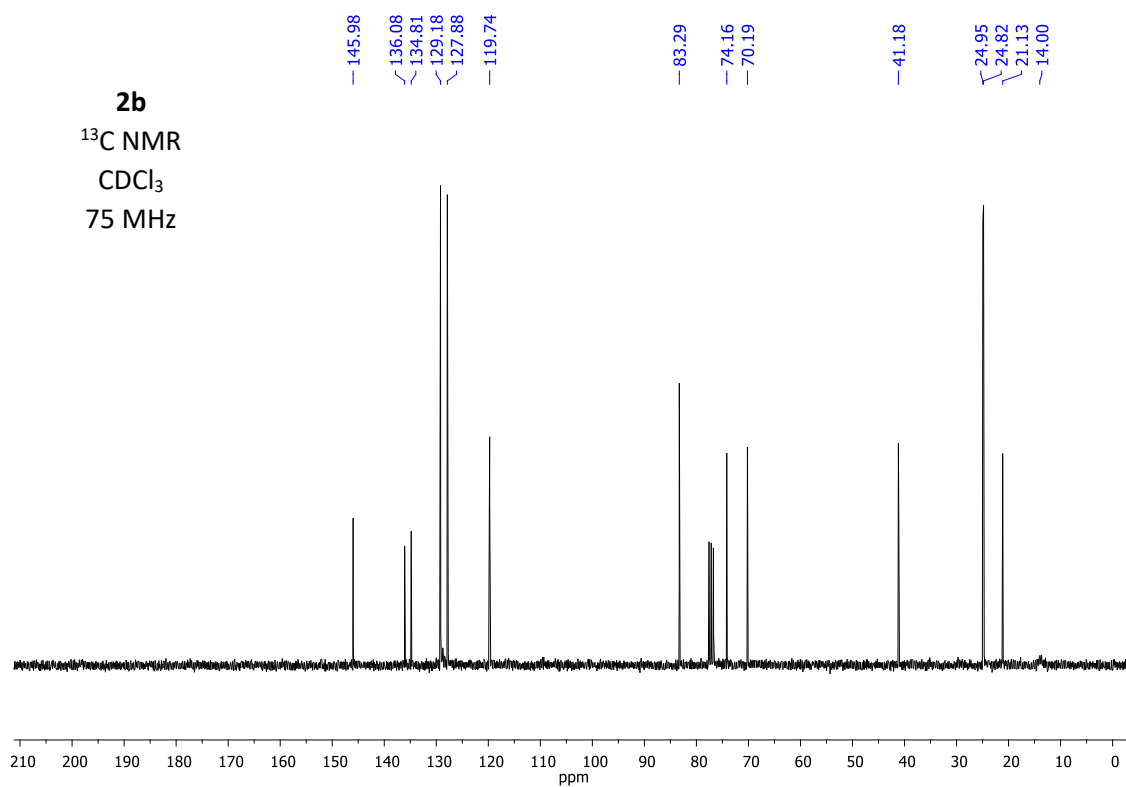


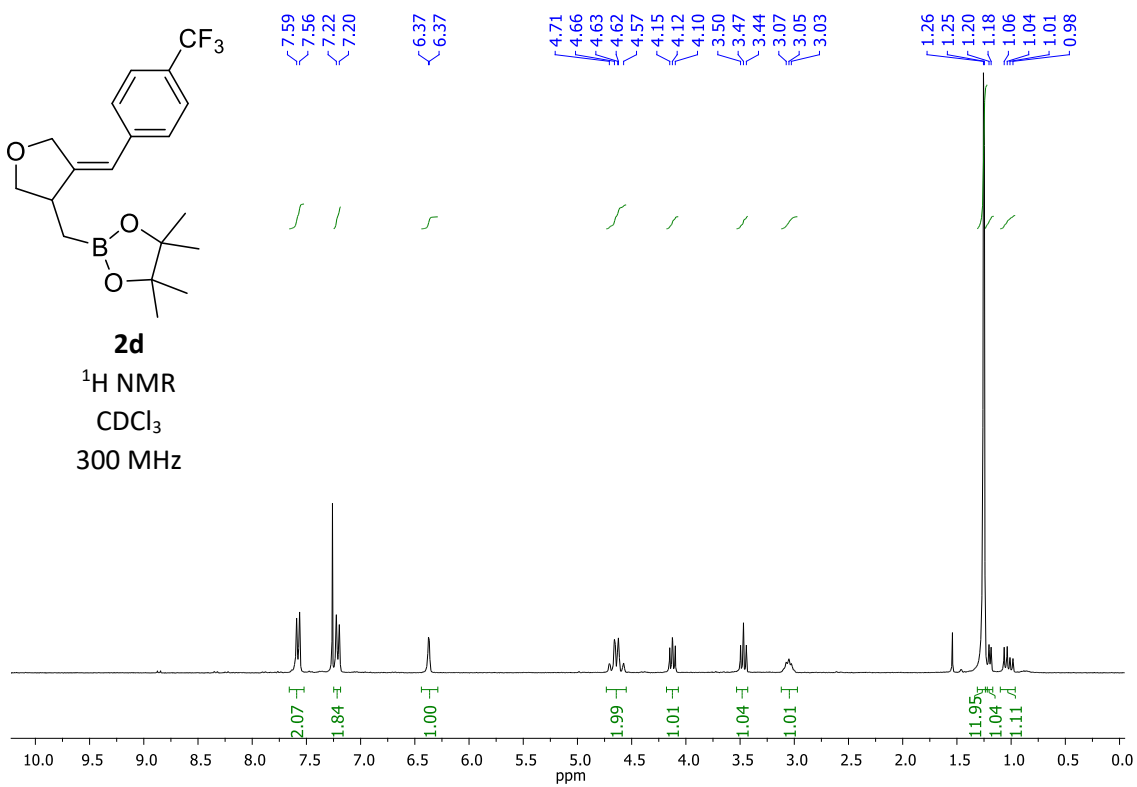
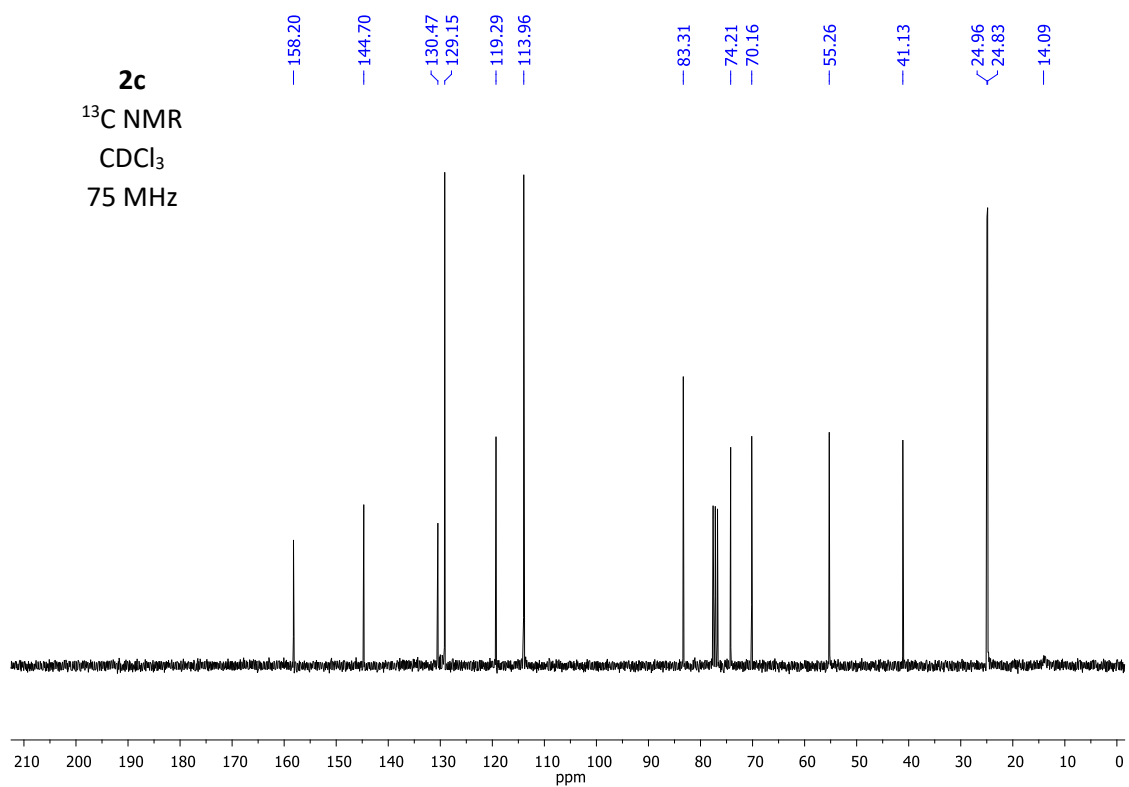


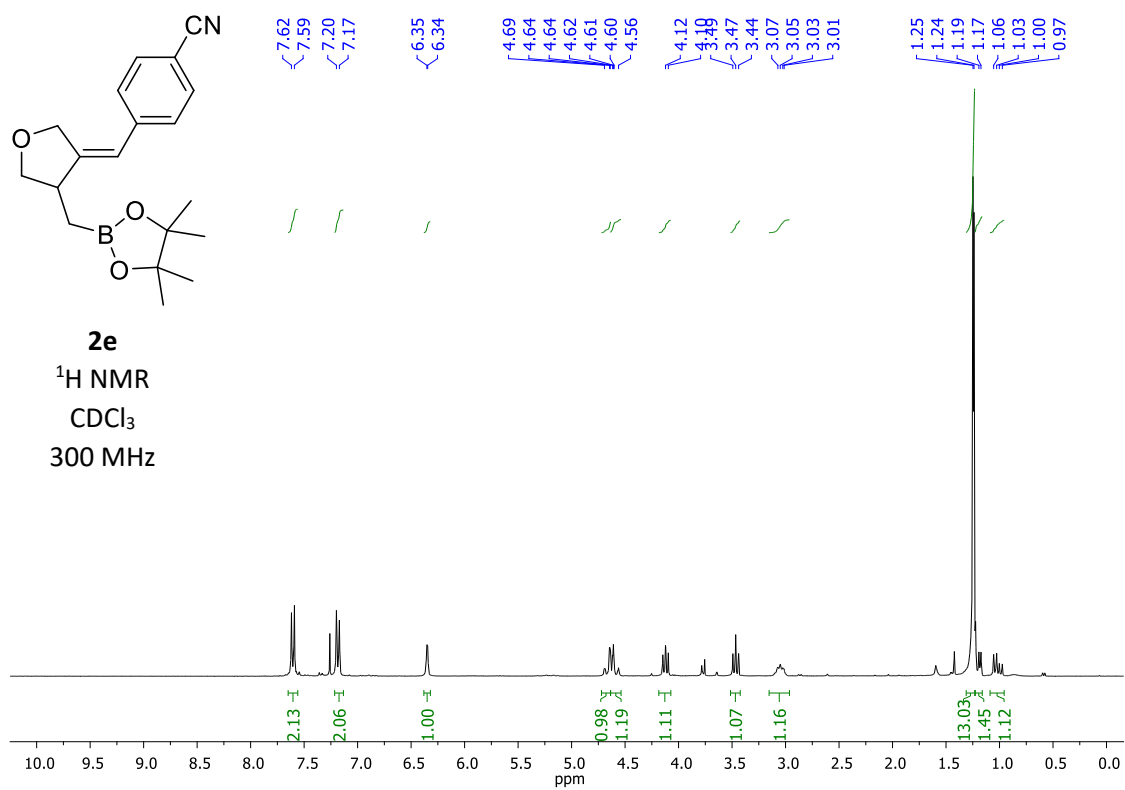
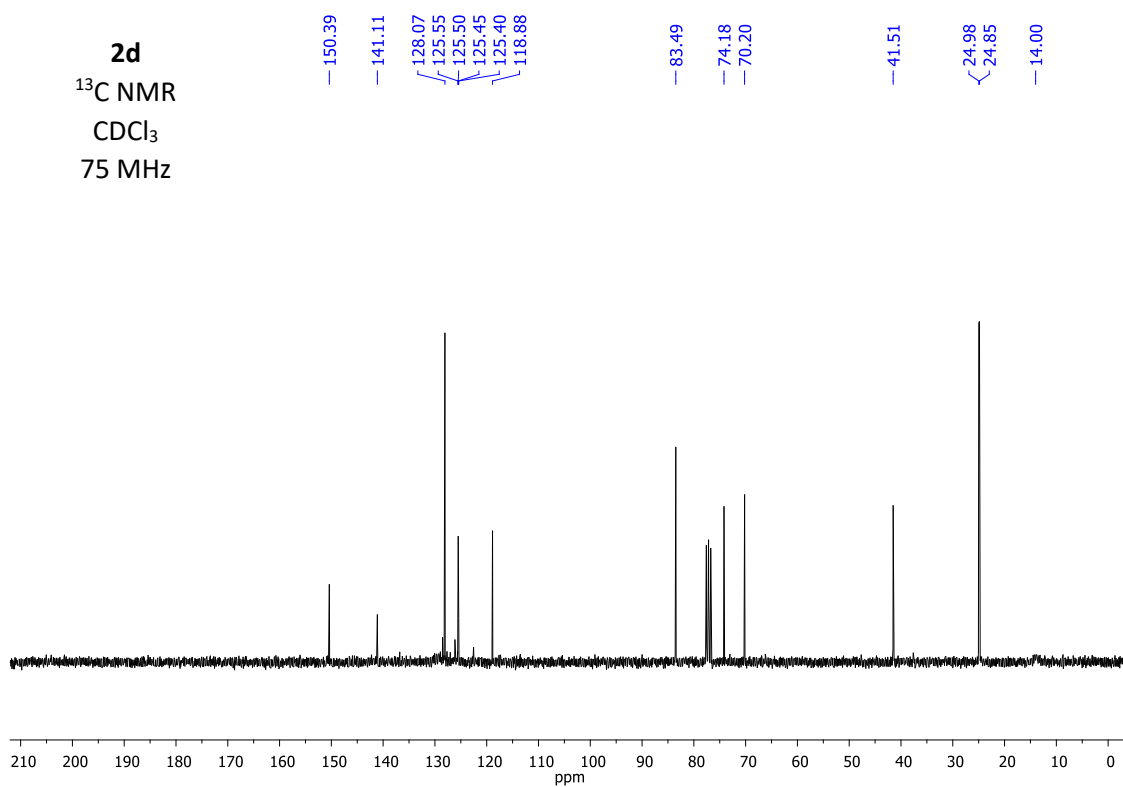


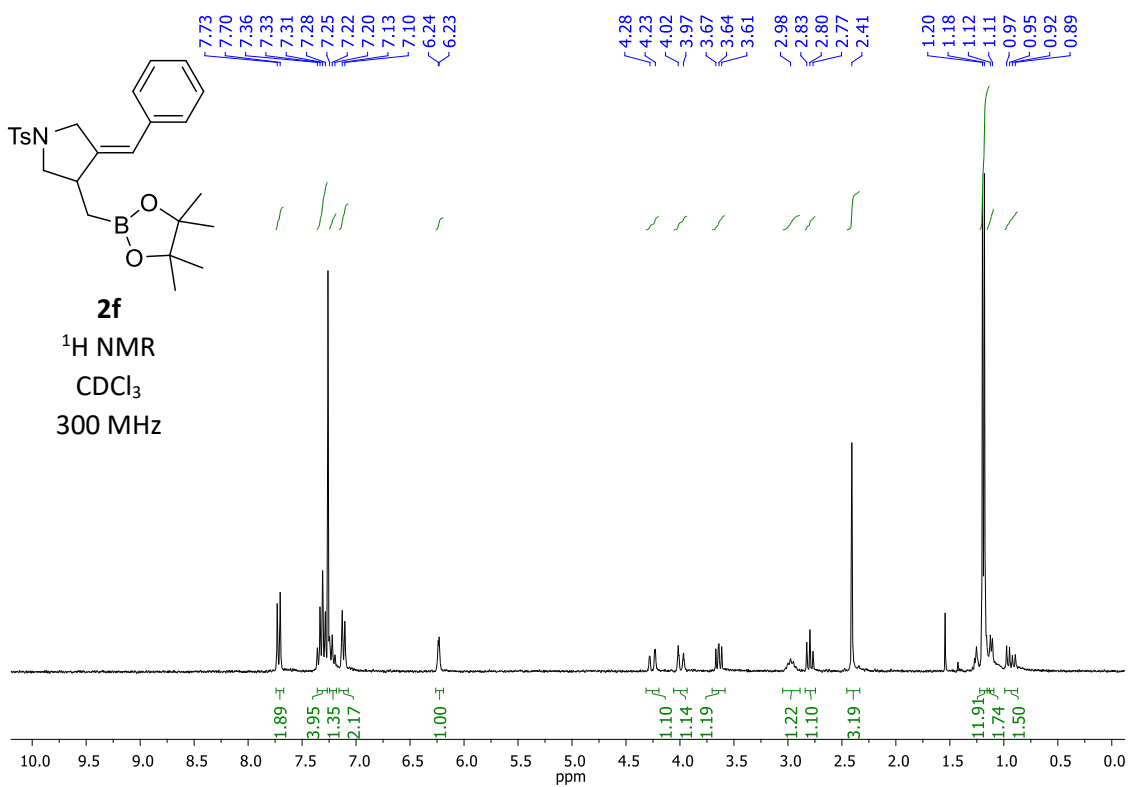
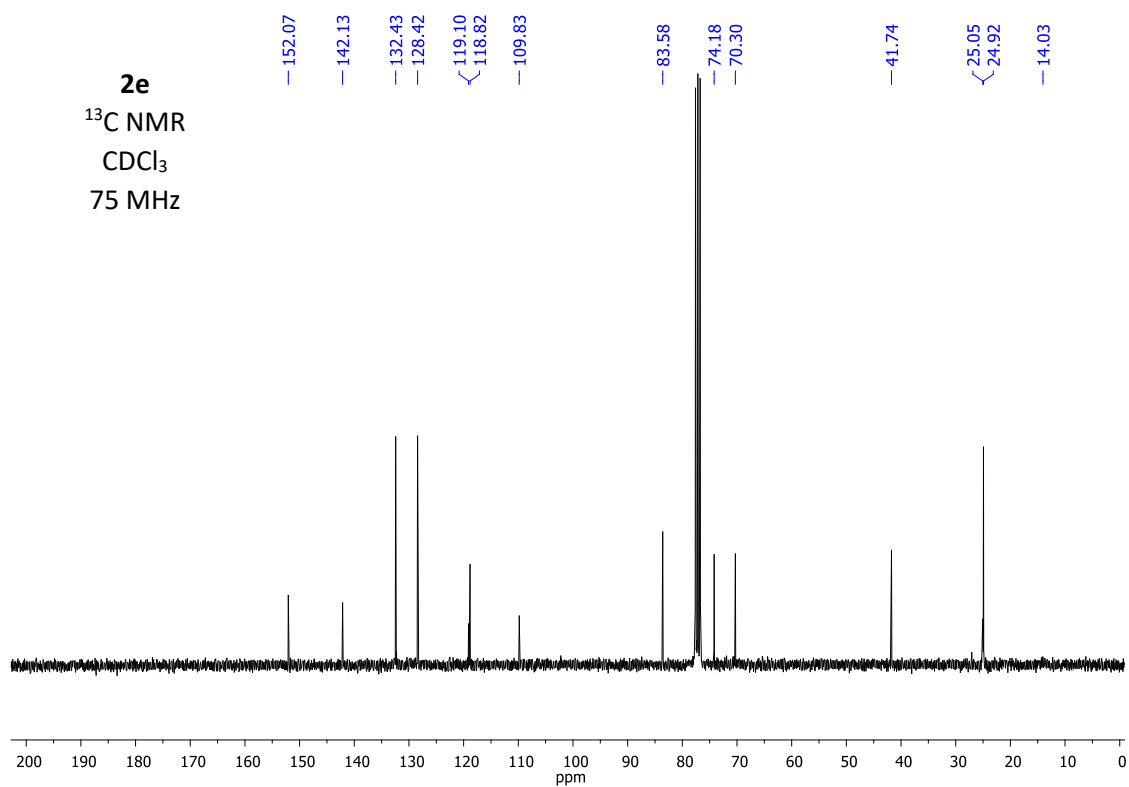


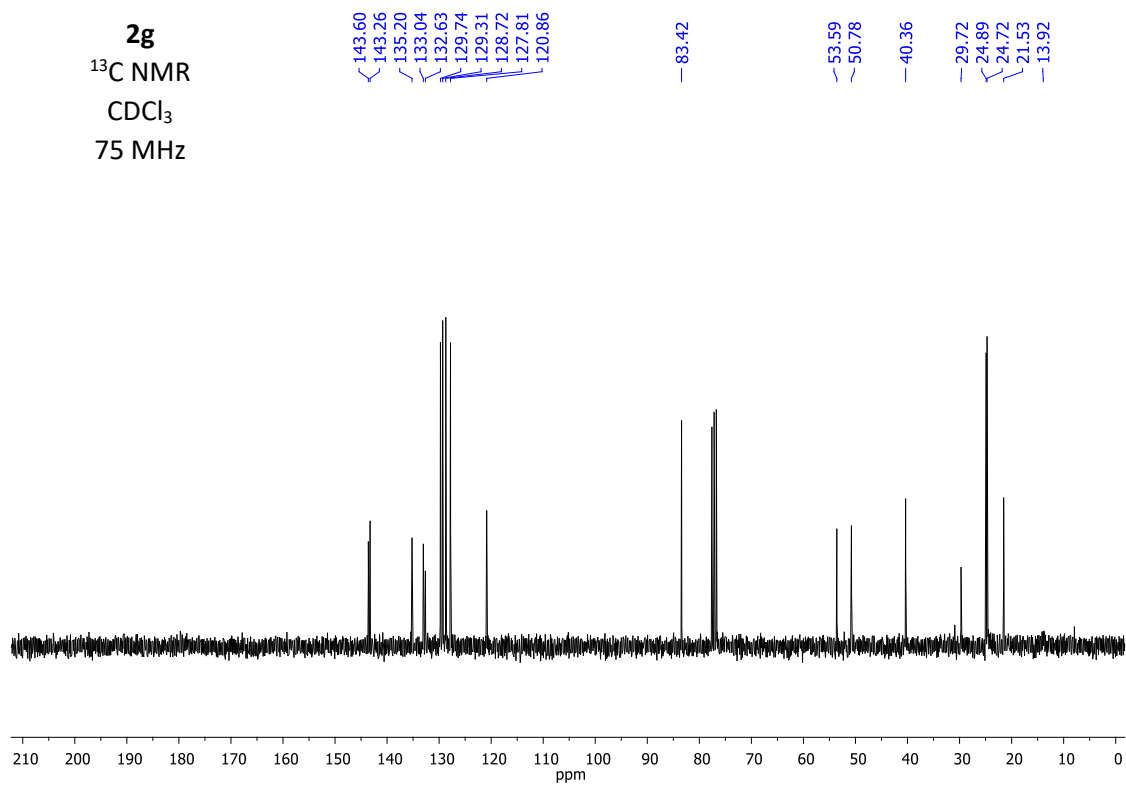
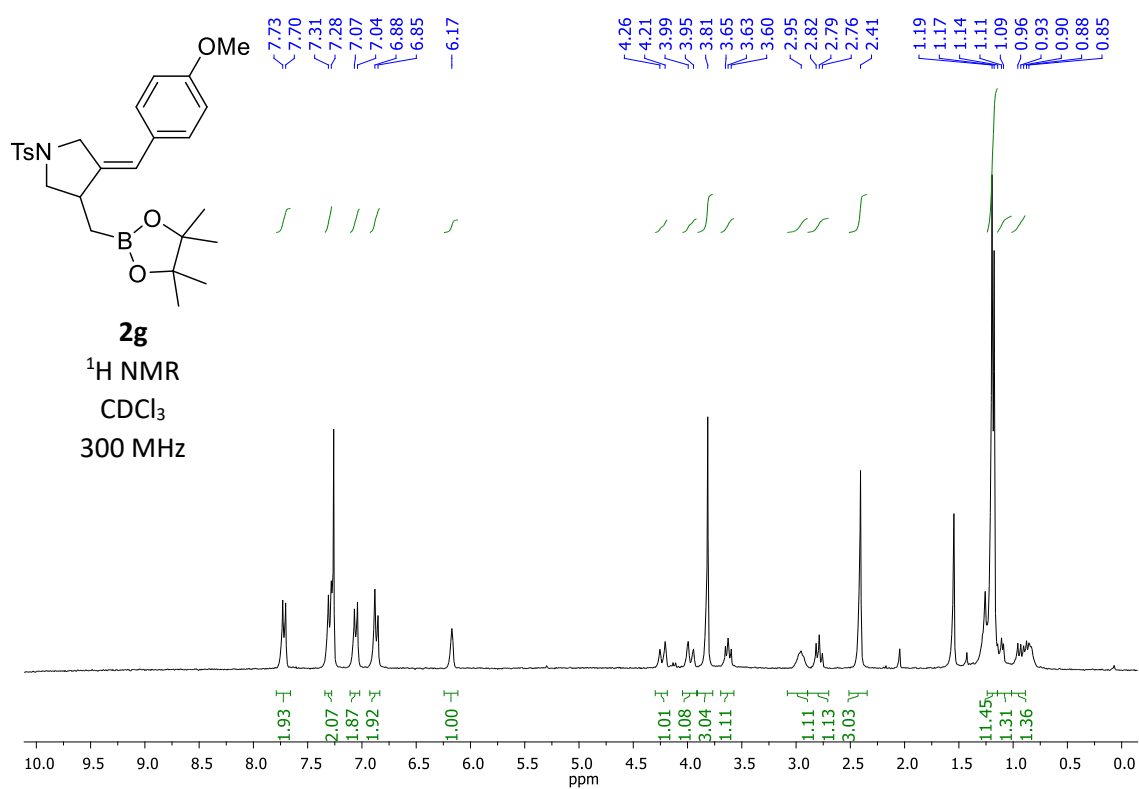


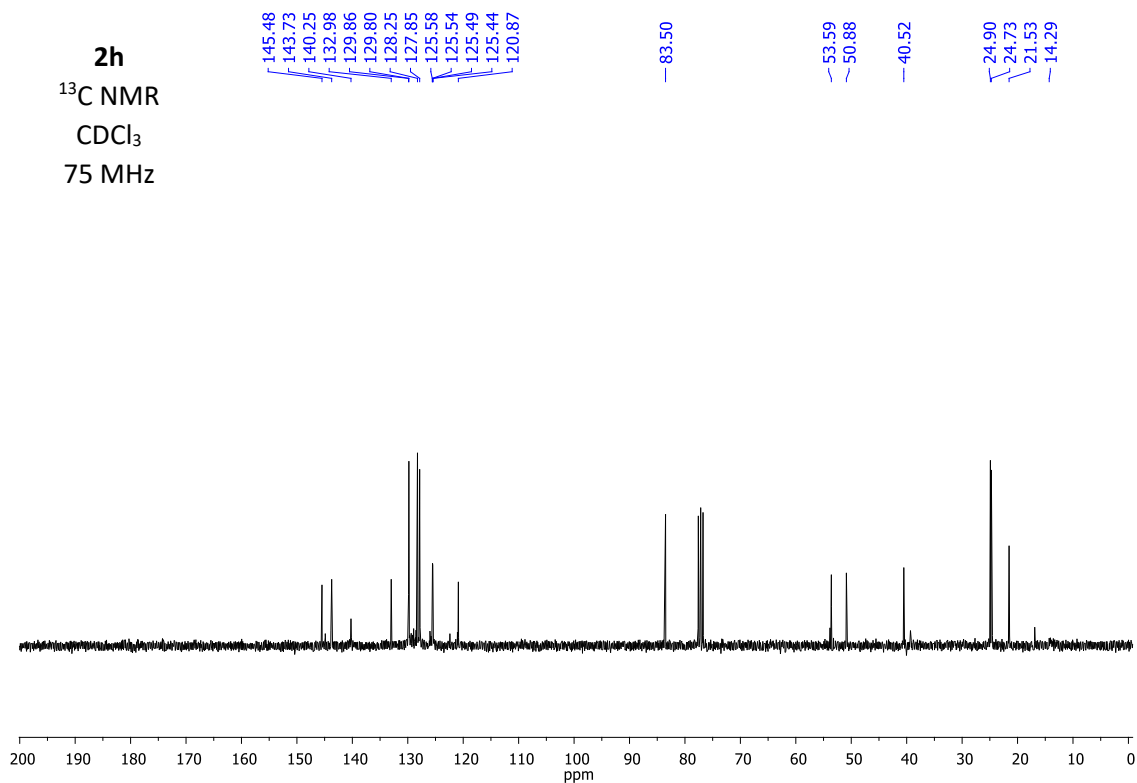
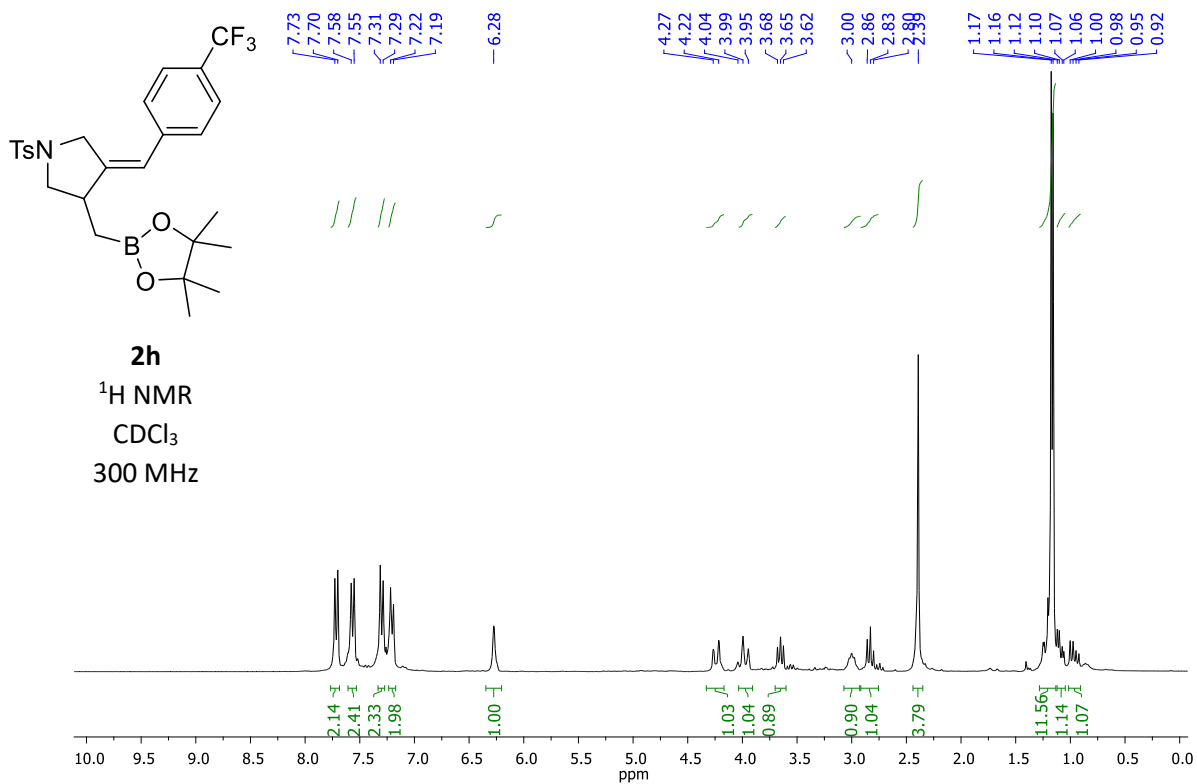


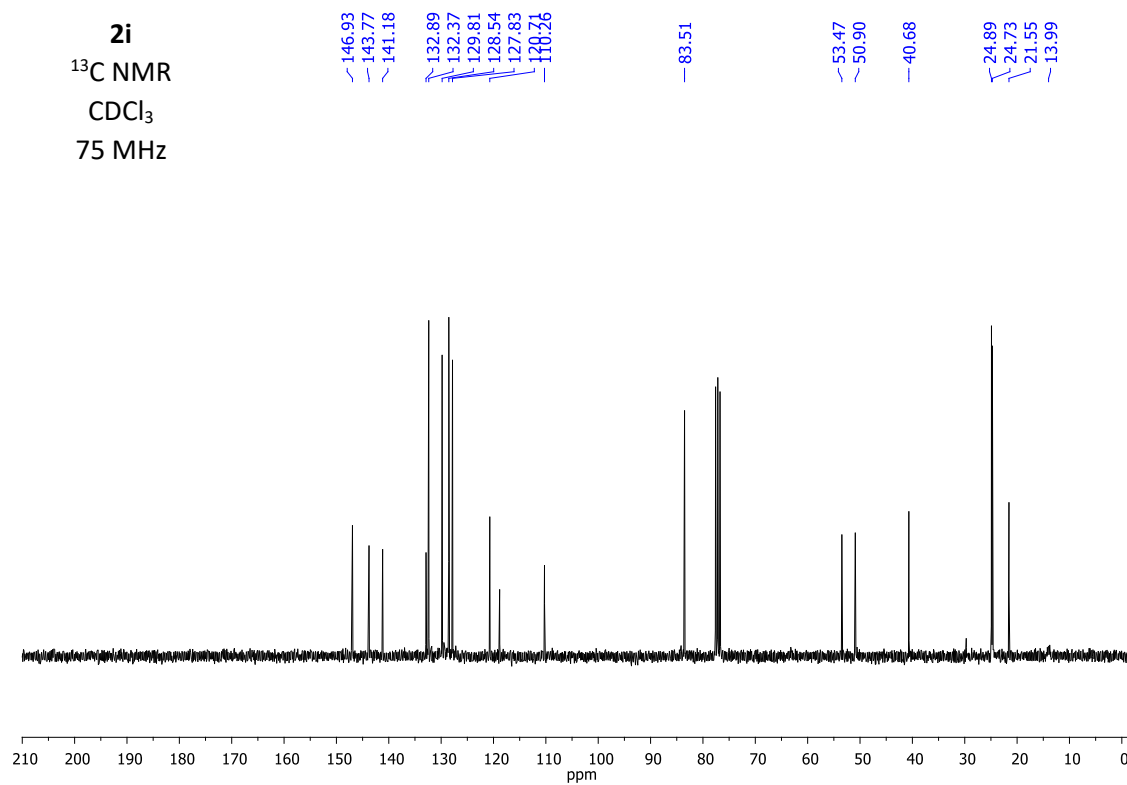
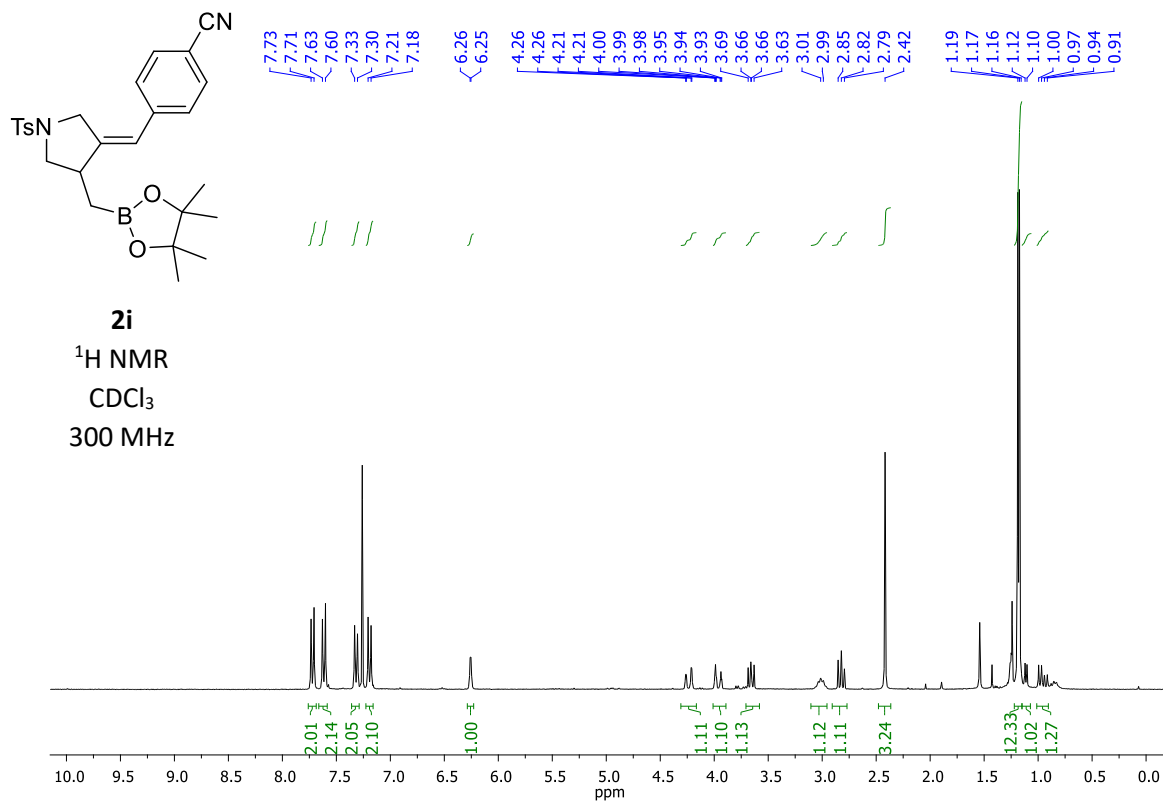


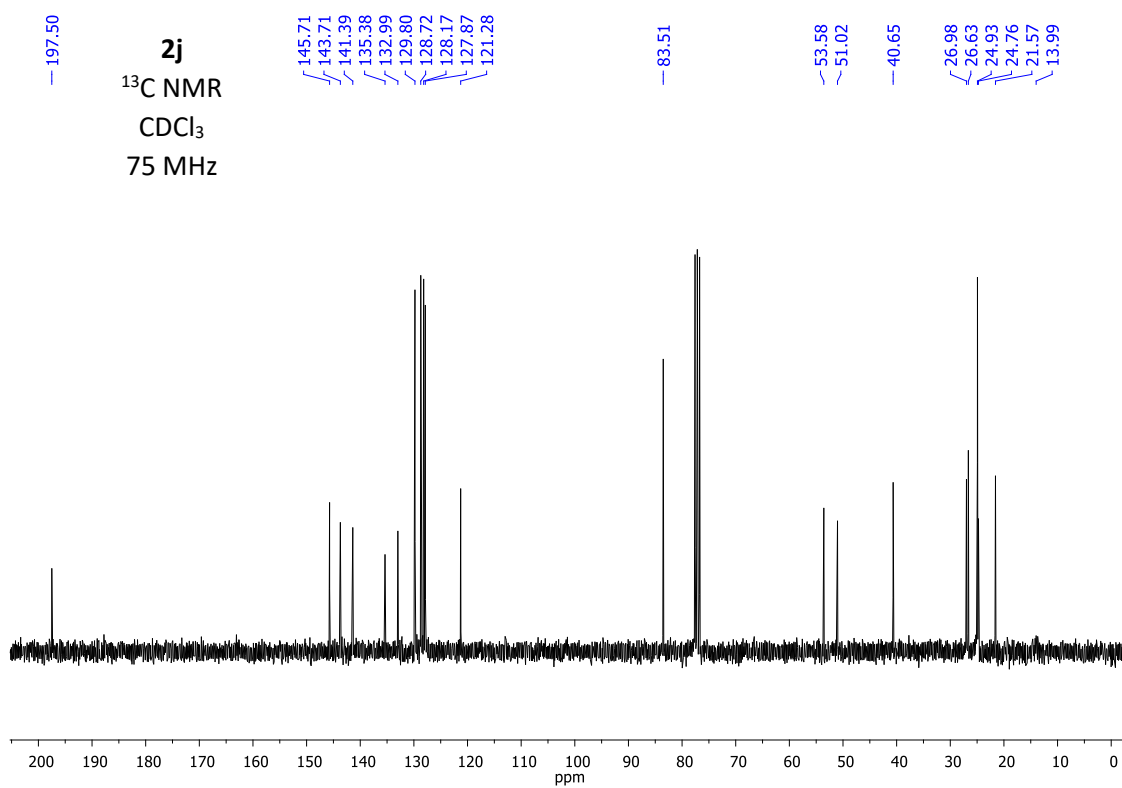
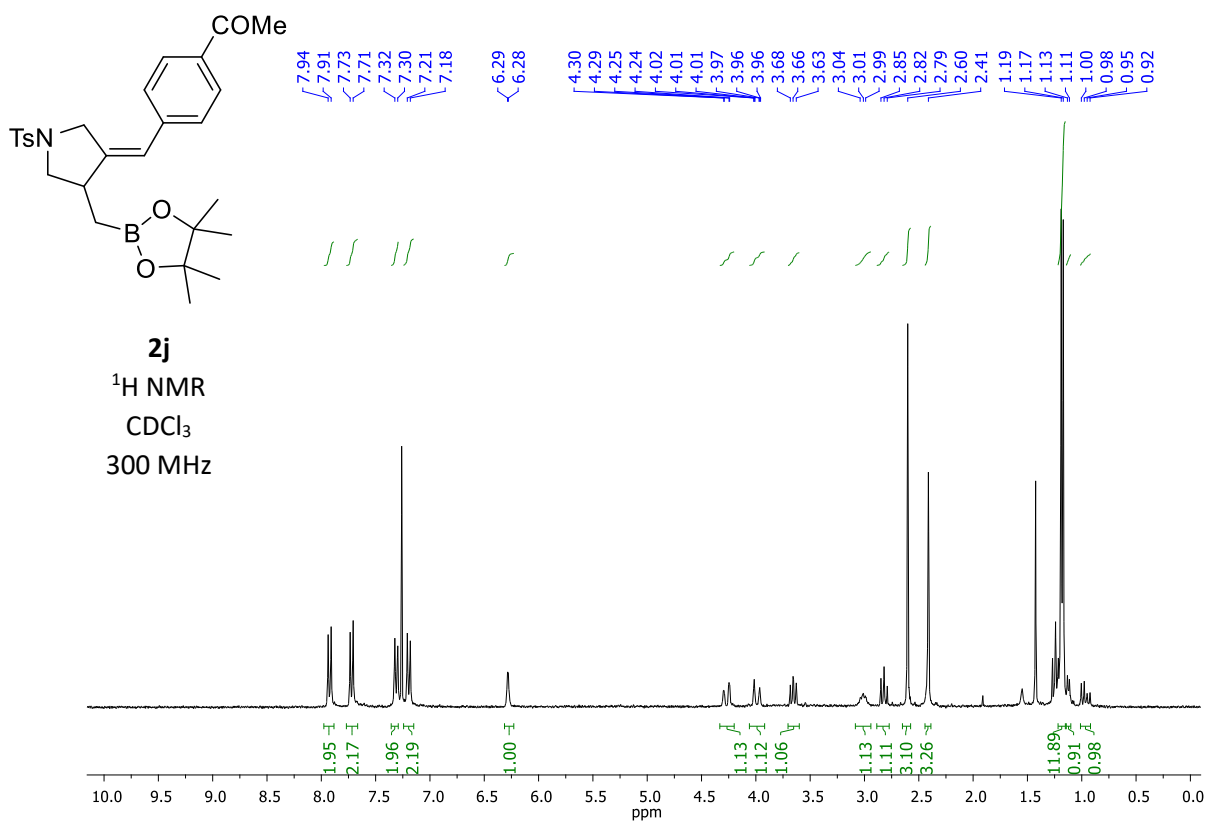


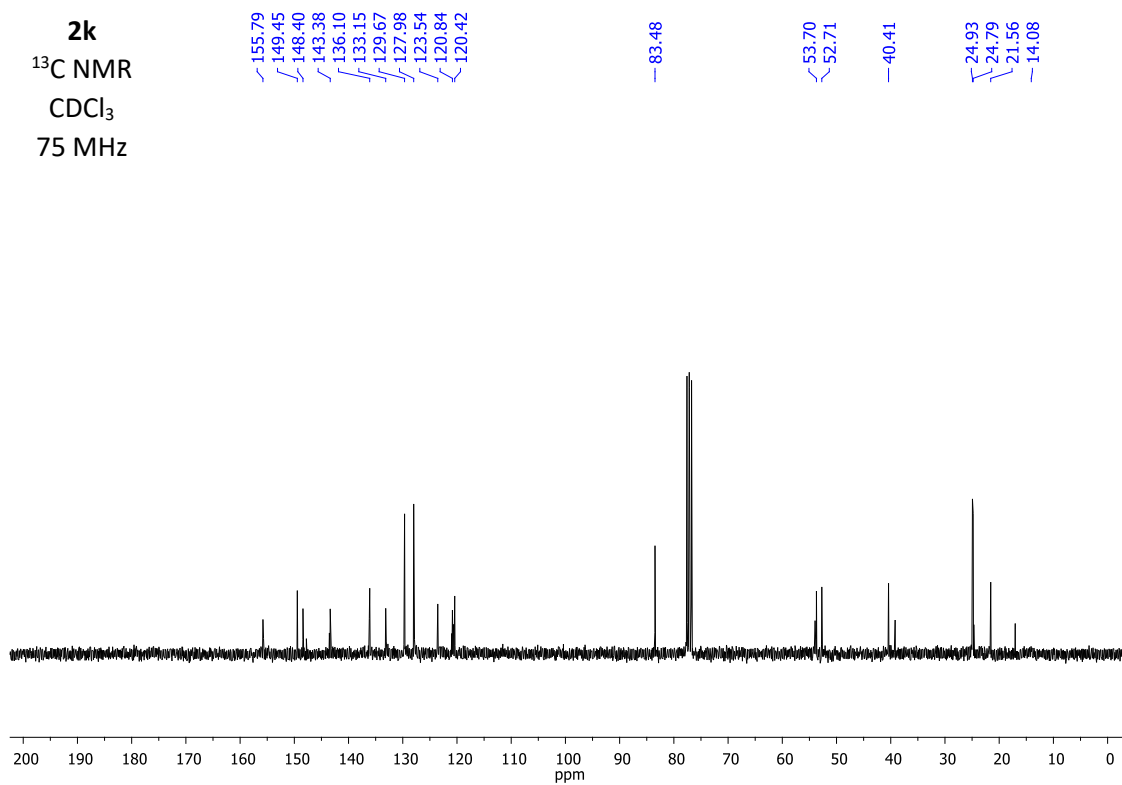
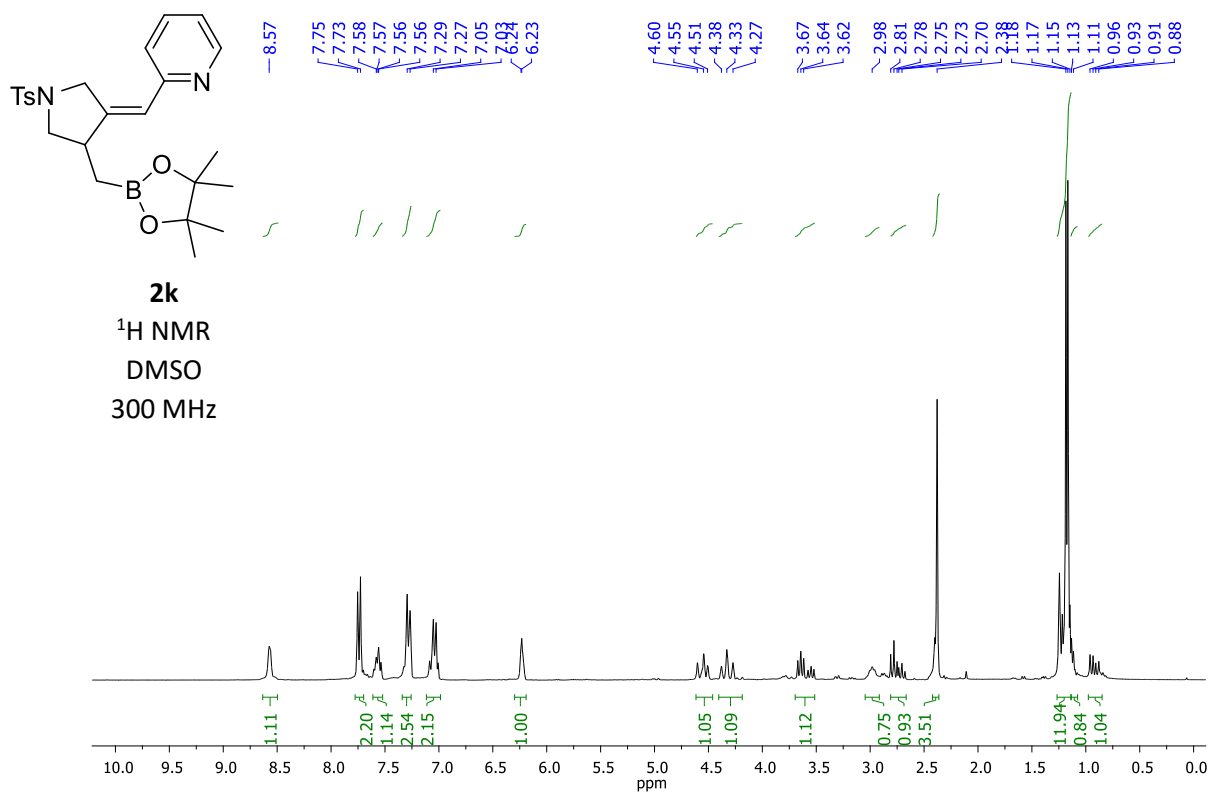


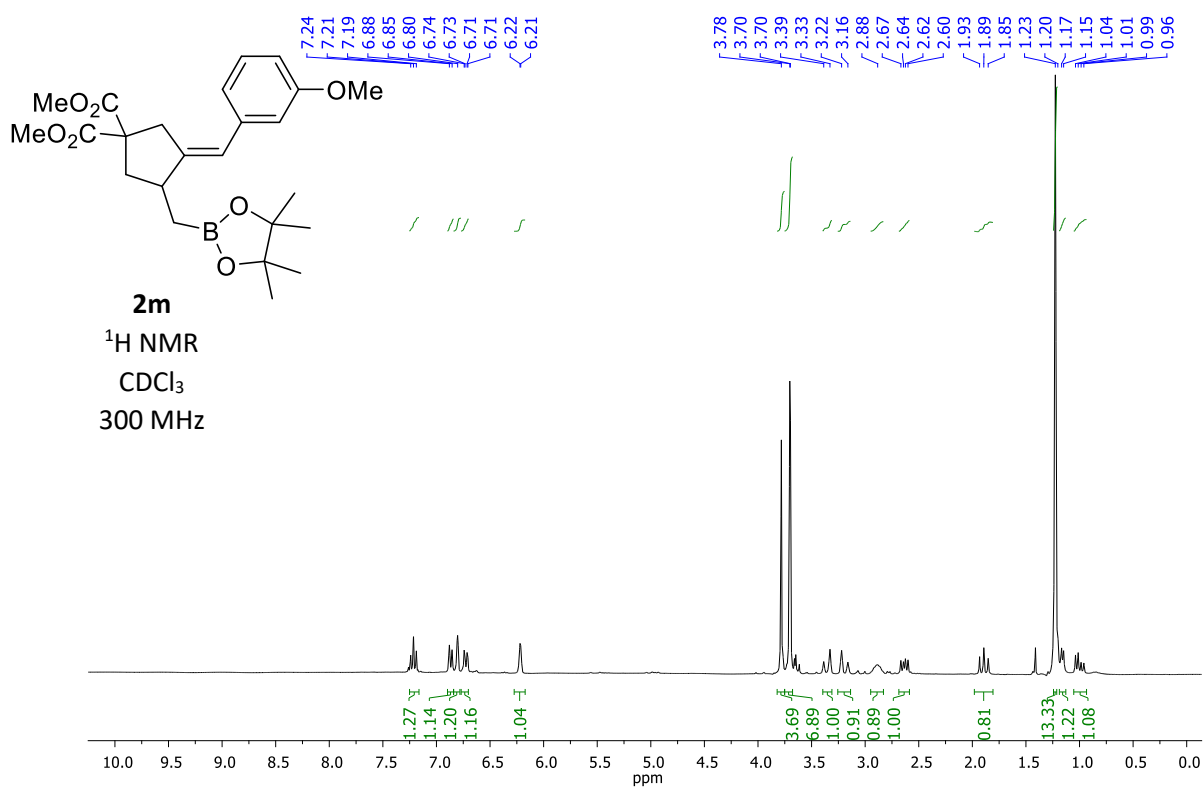
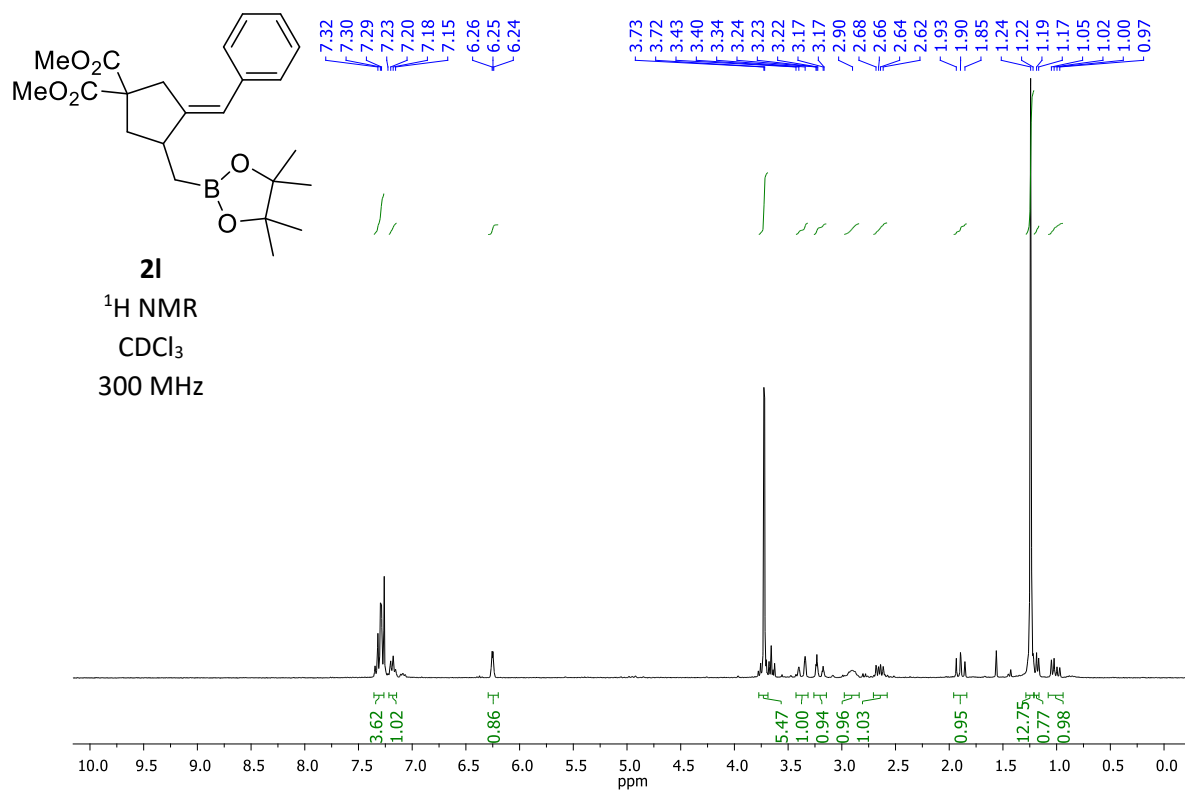




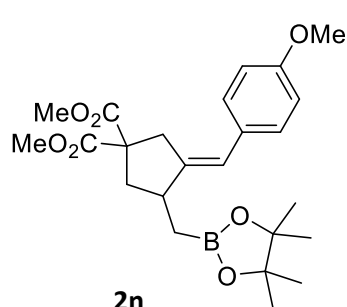
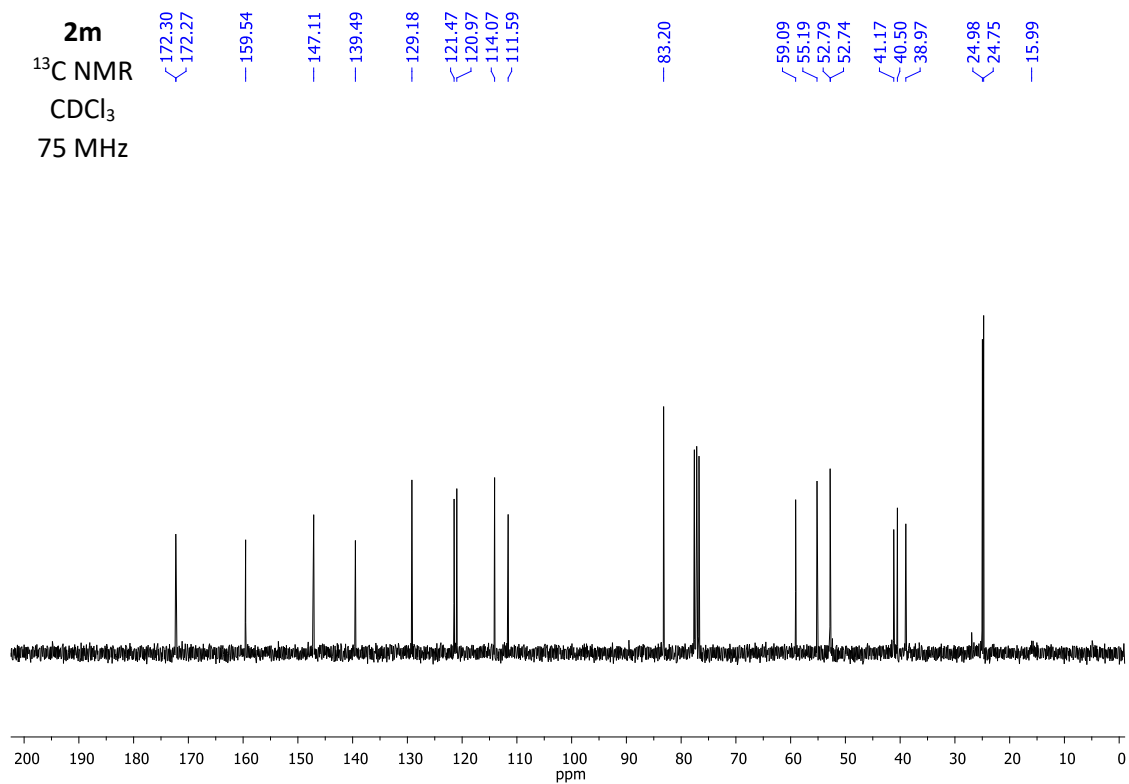




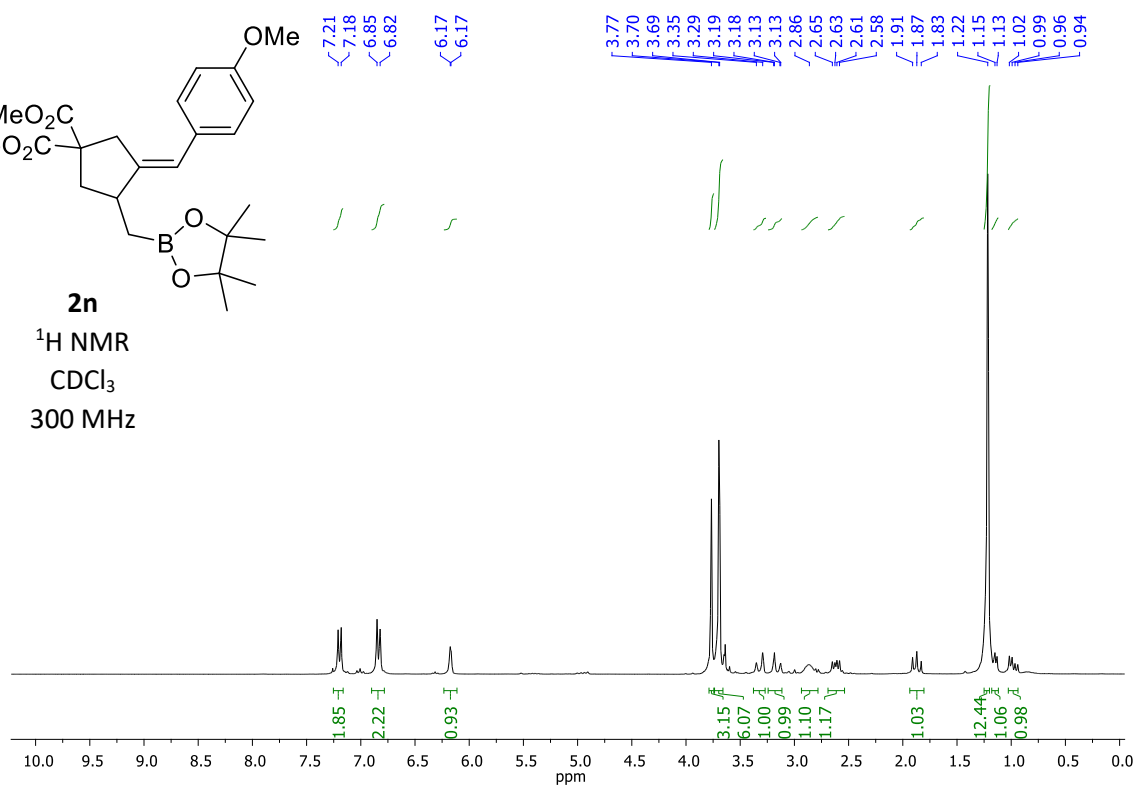


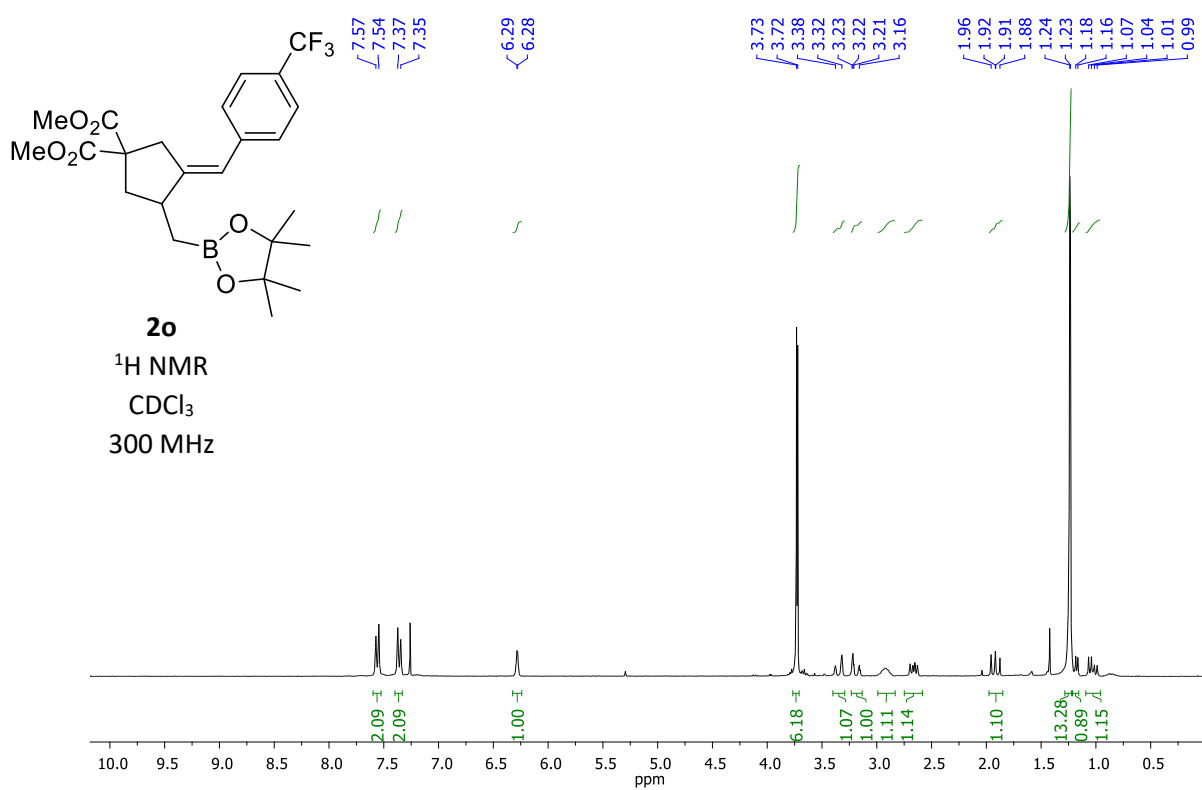
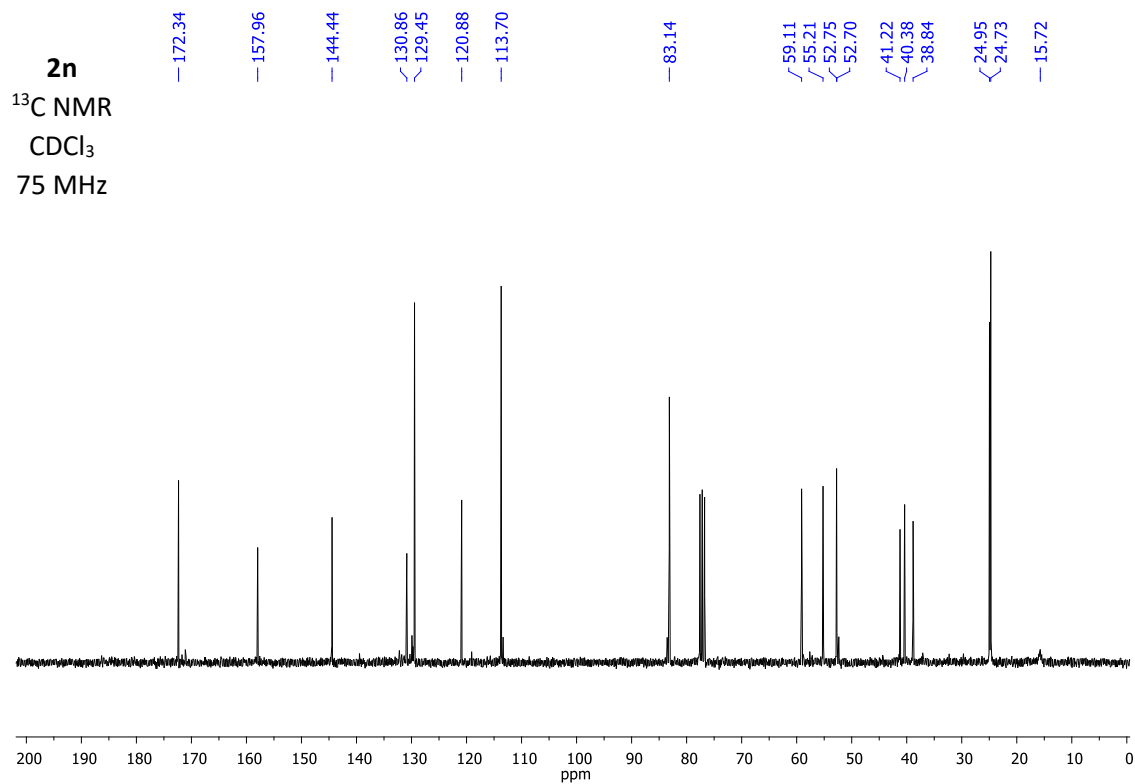


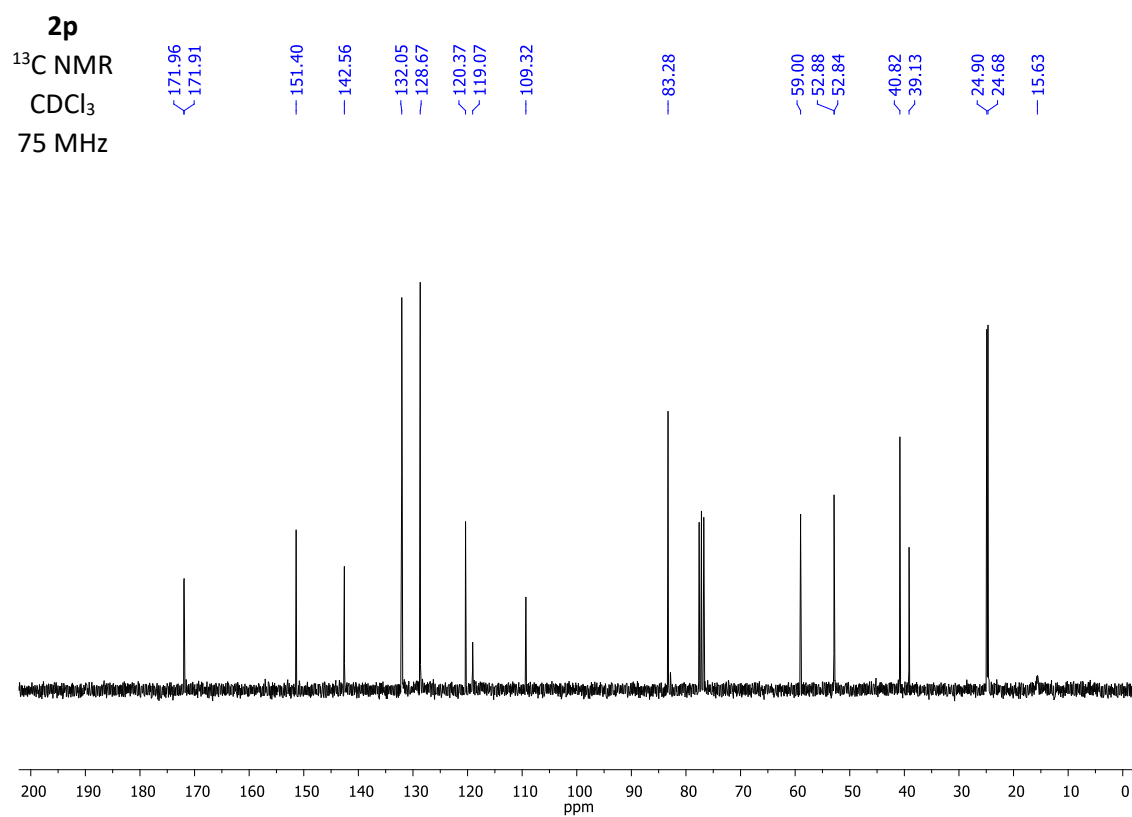
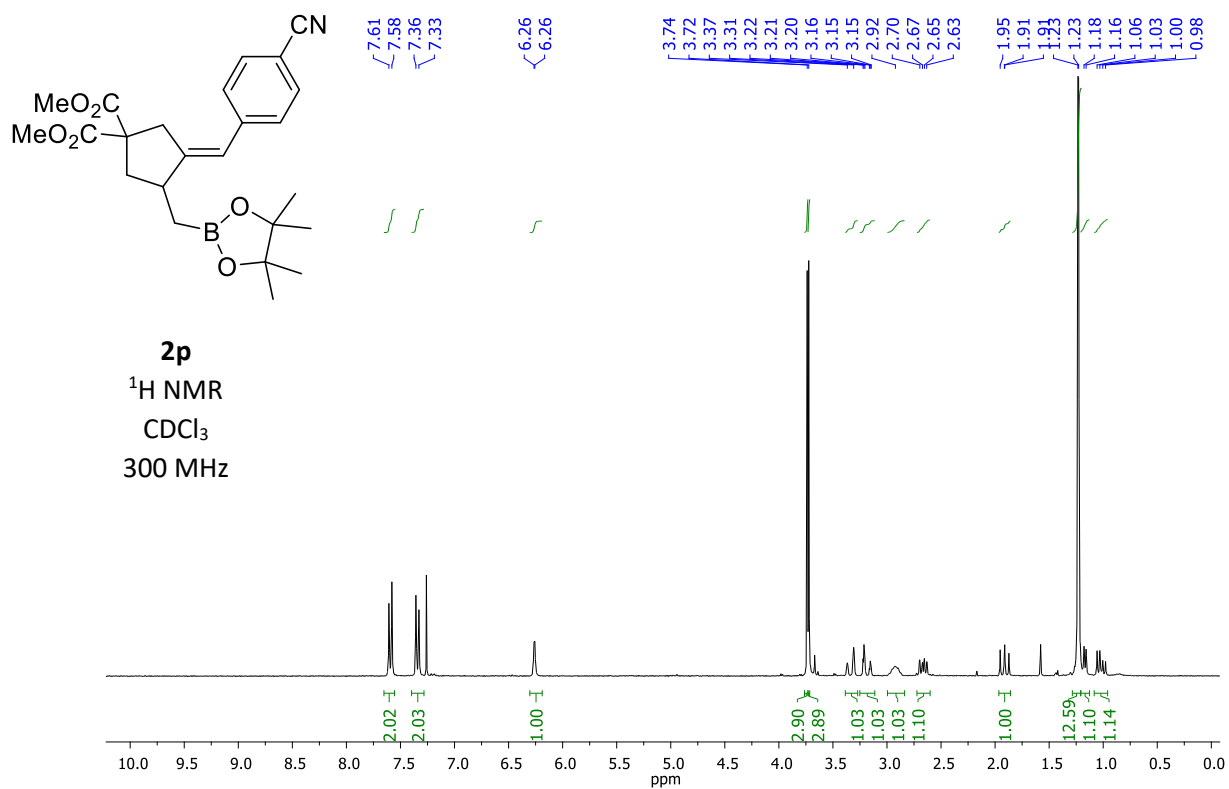
2m
¹³C NMR
 CDCl₃
 75 MHz

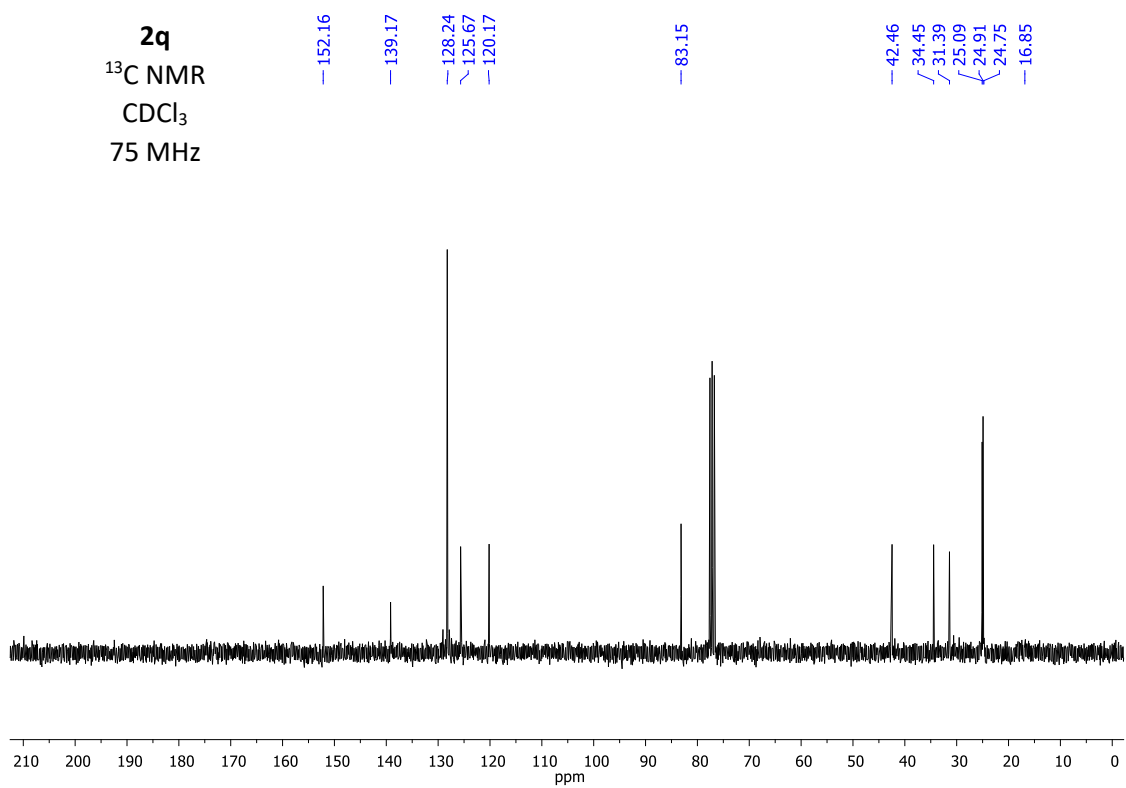
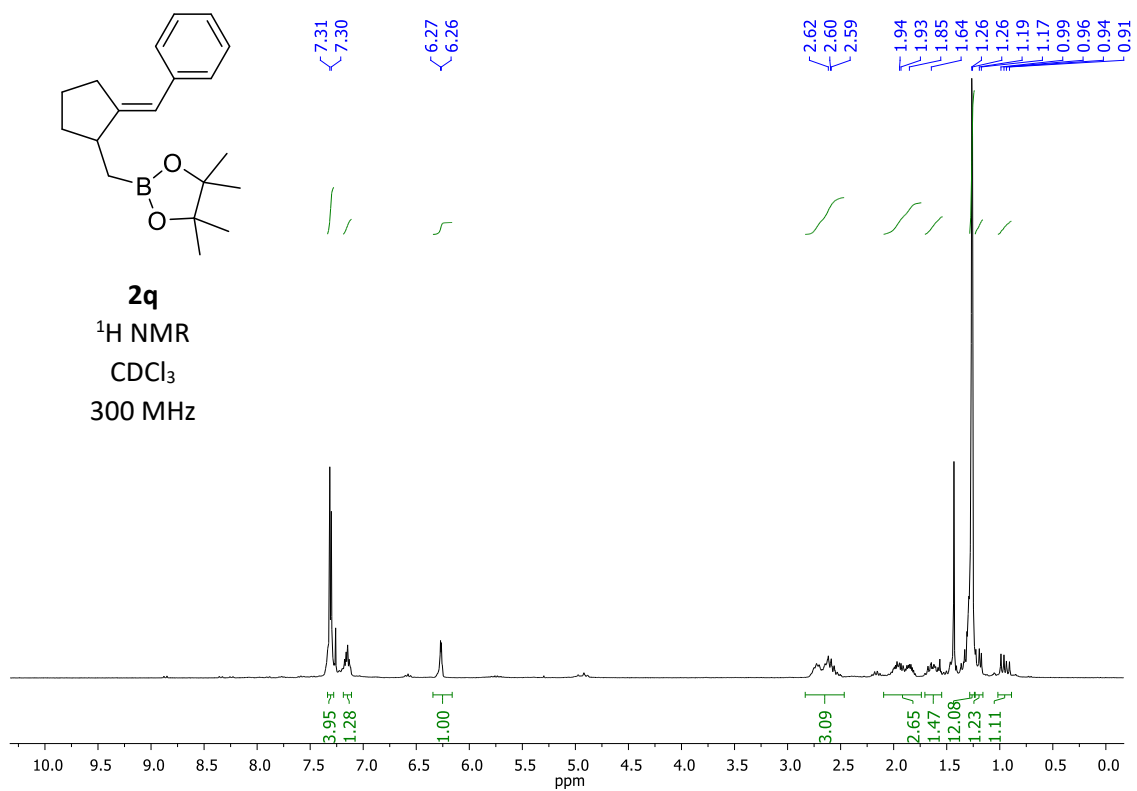


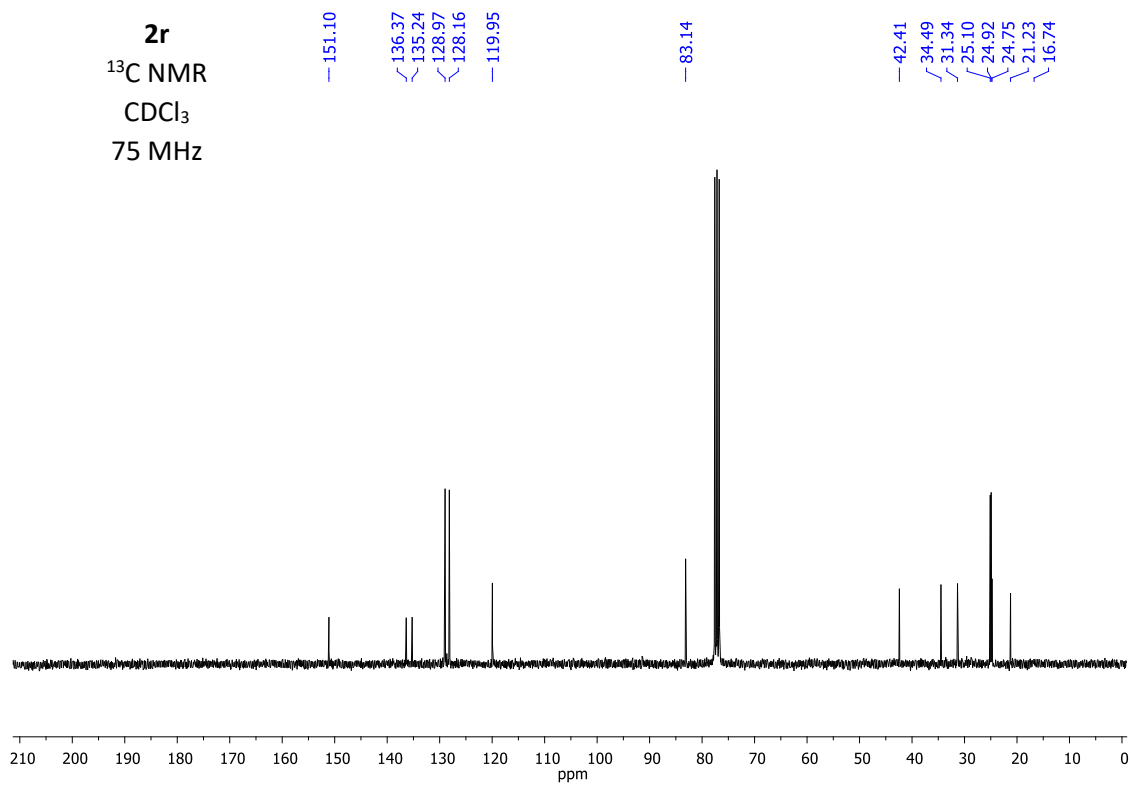
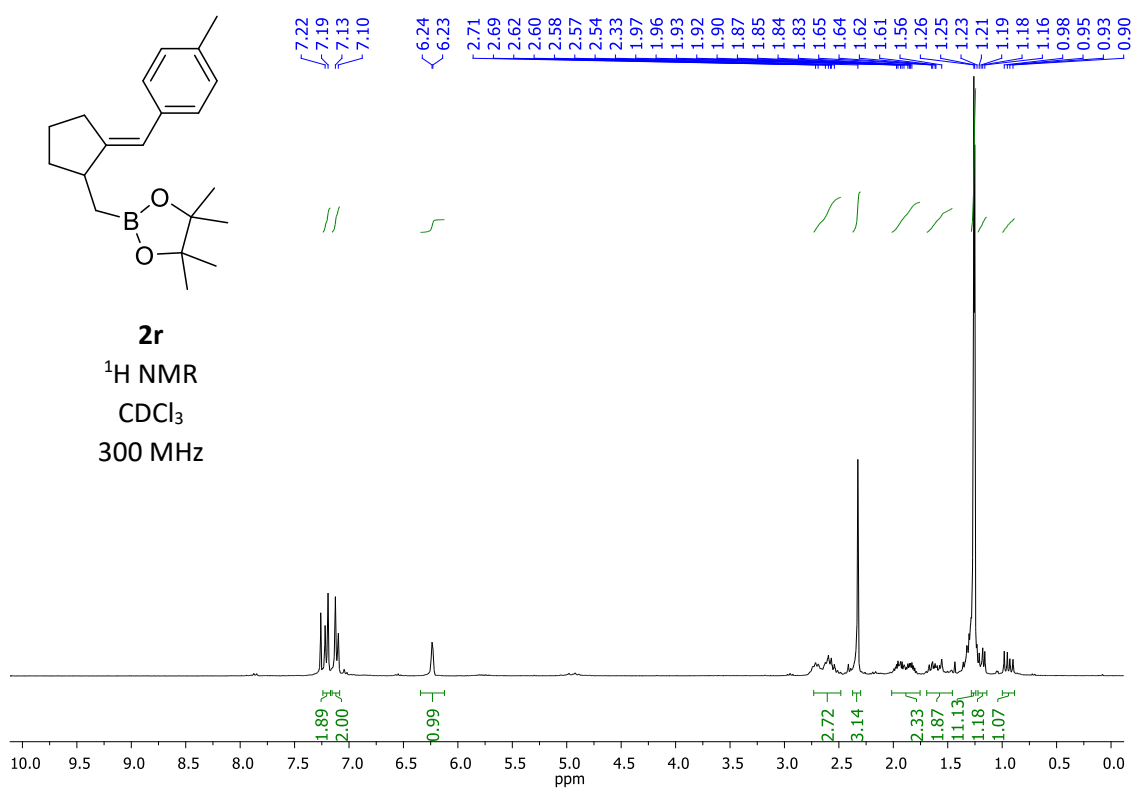
2n
¹H NMR
 CDCl₃
 300 MHz

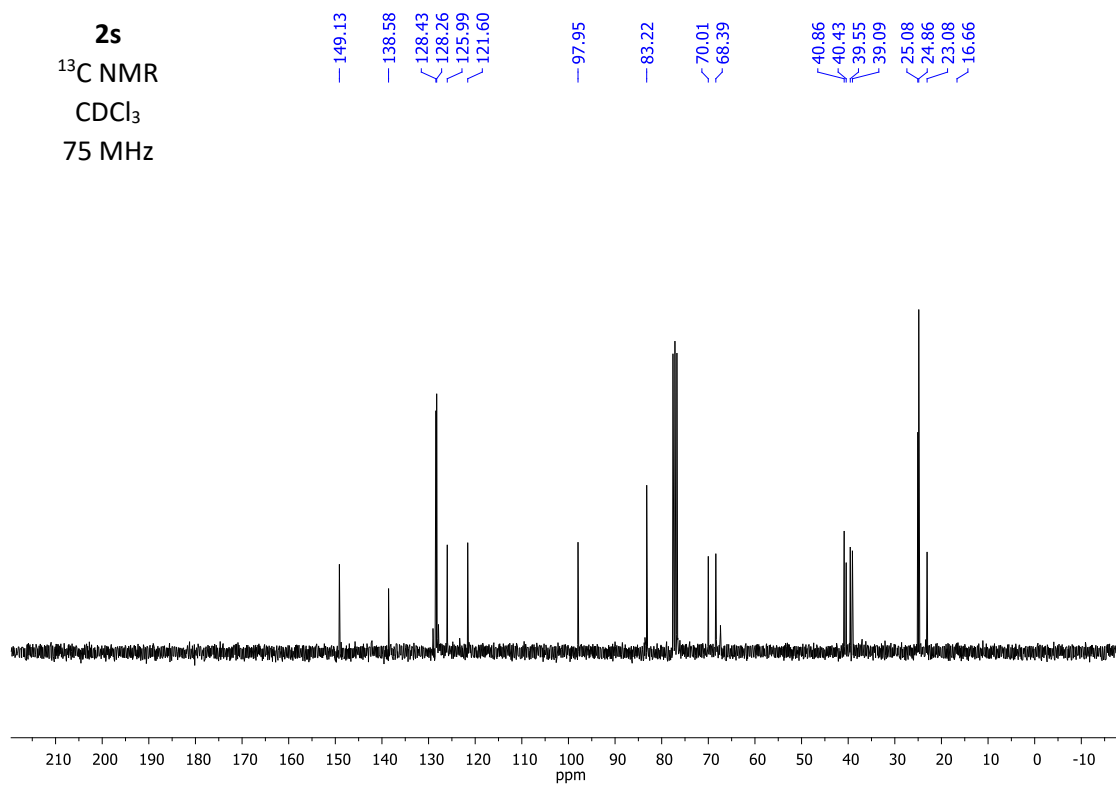
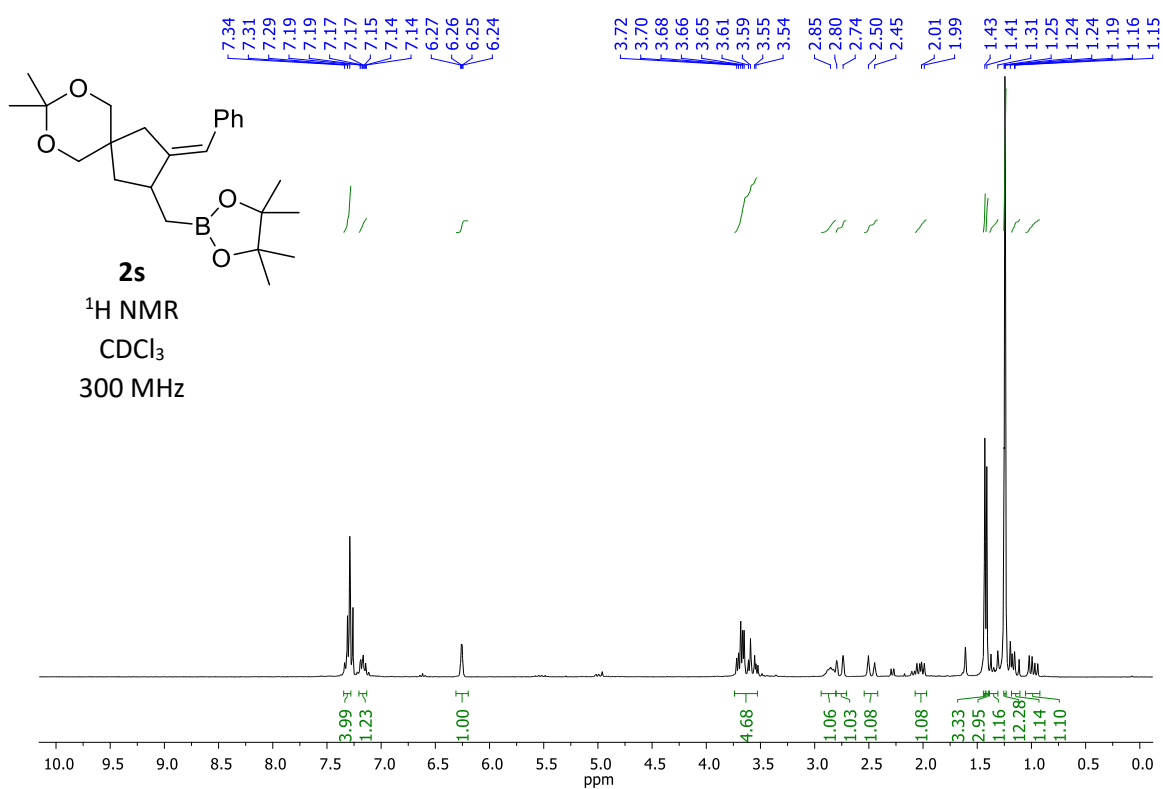


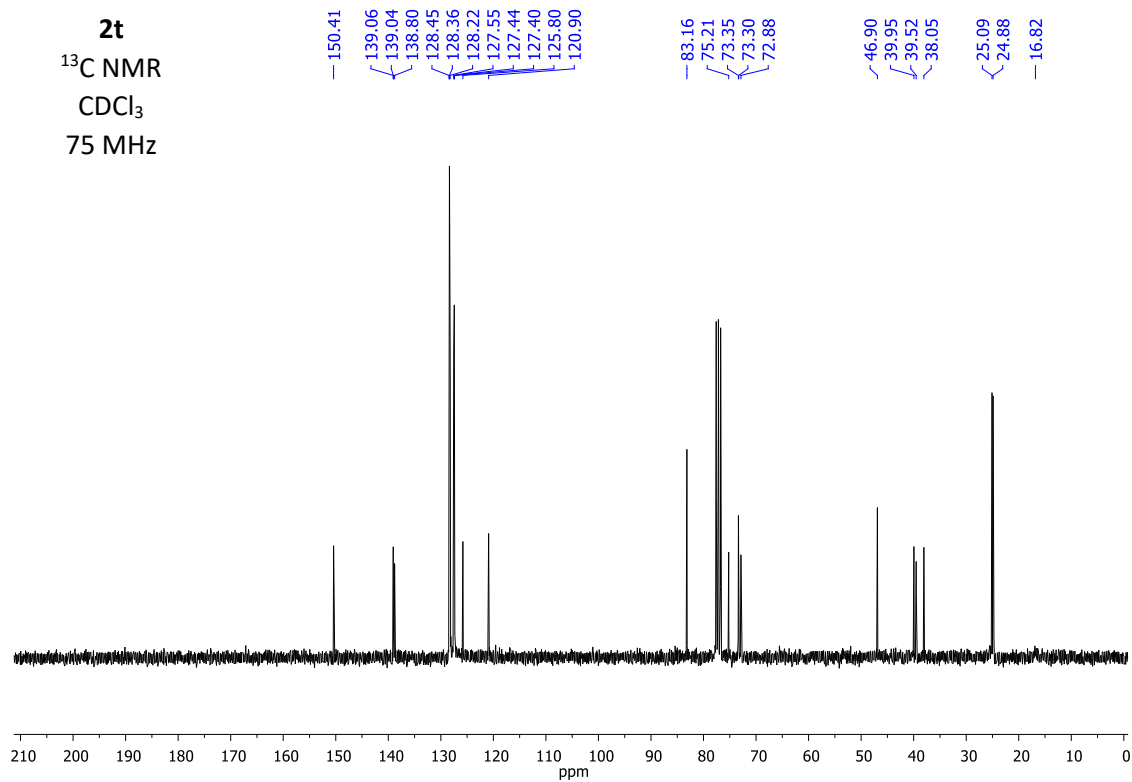
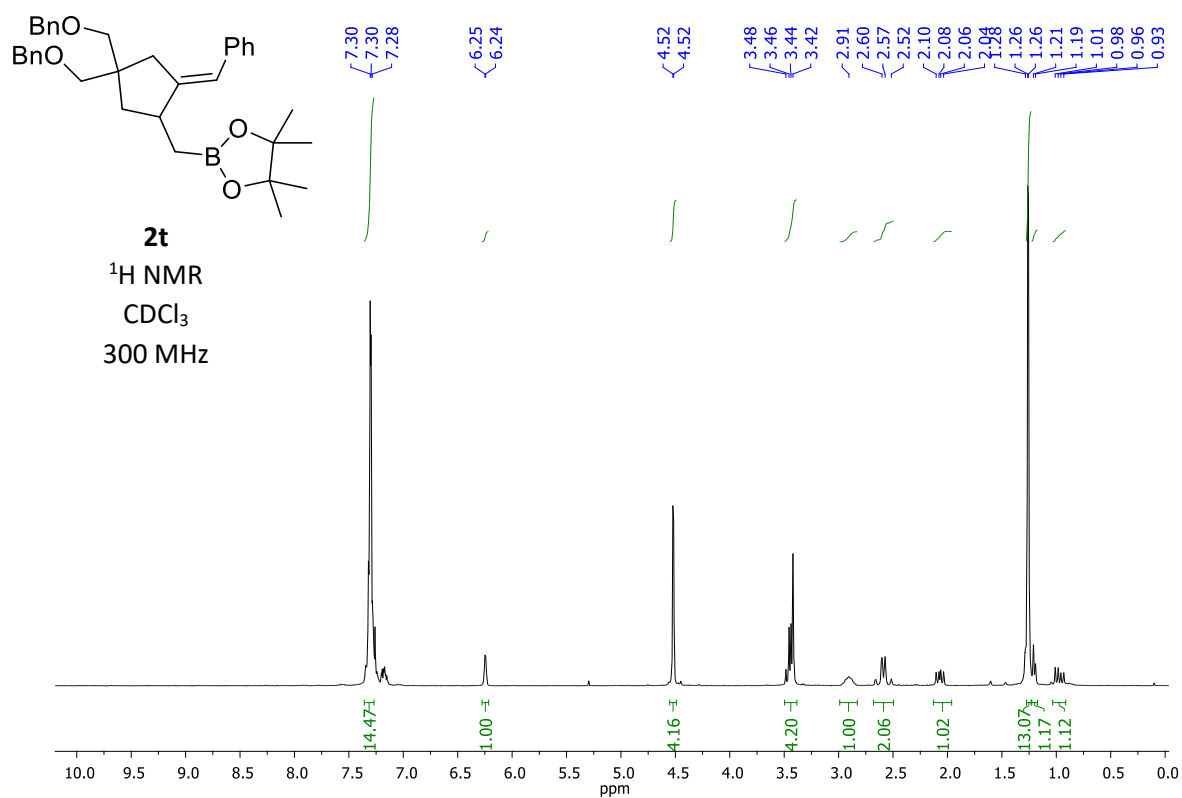


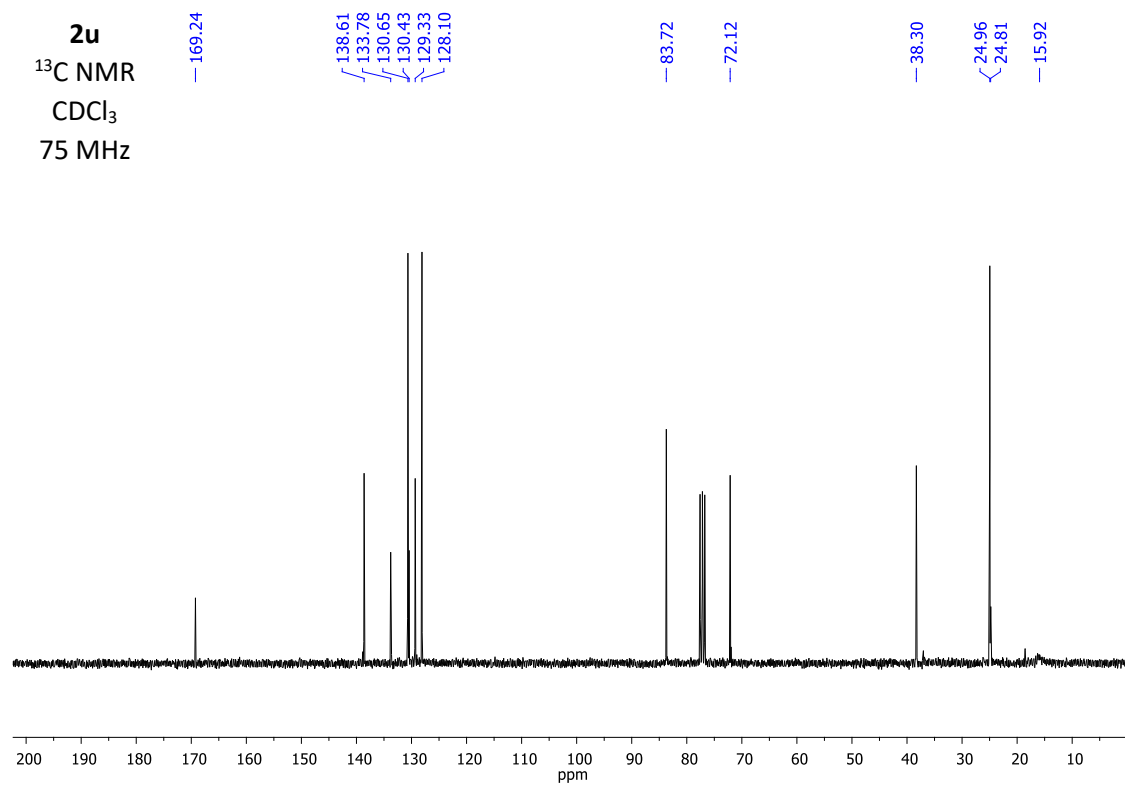
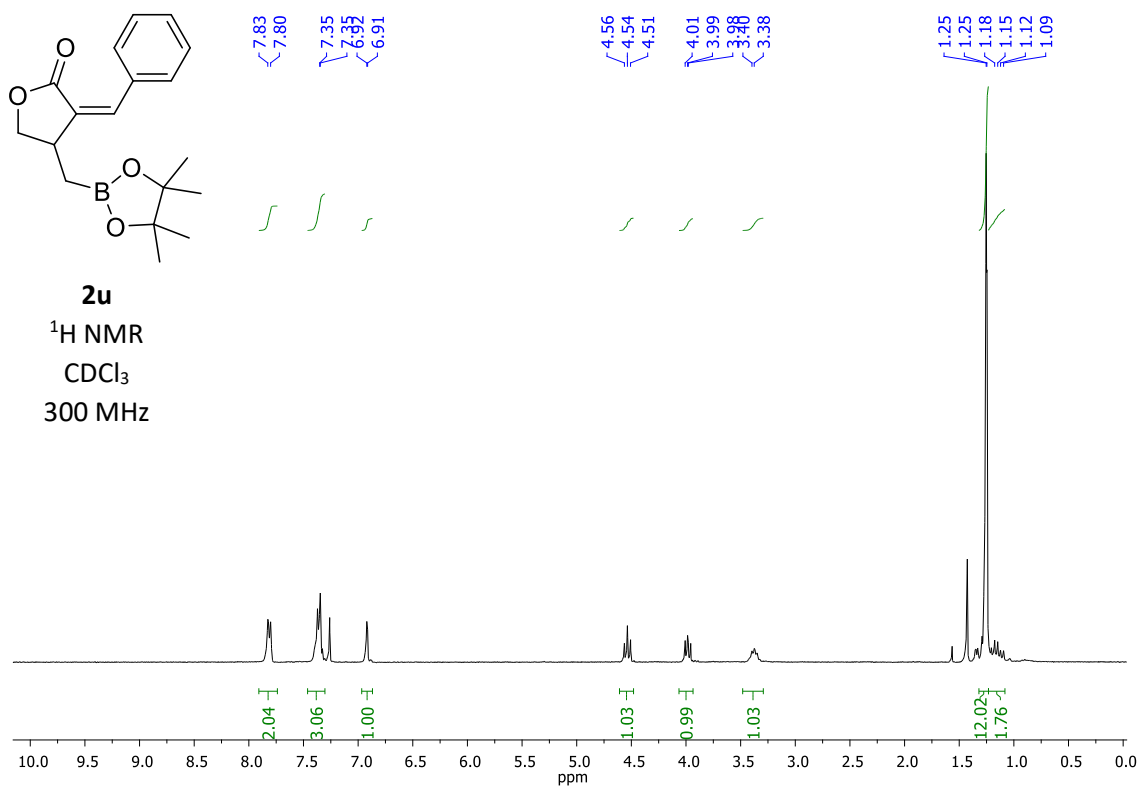


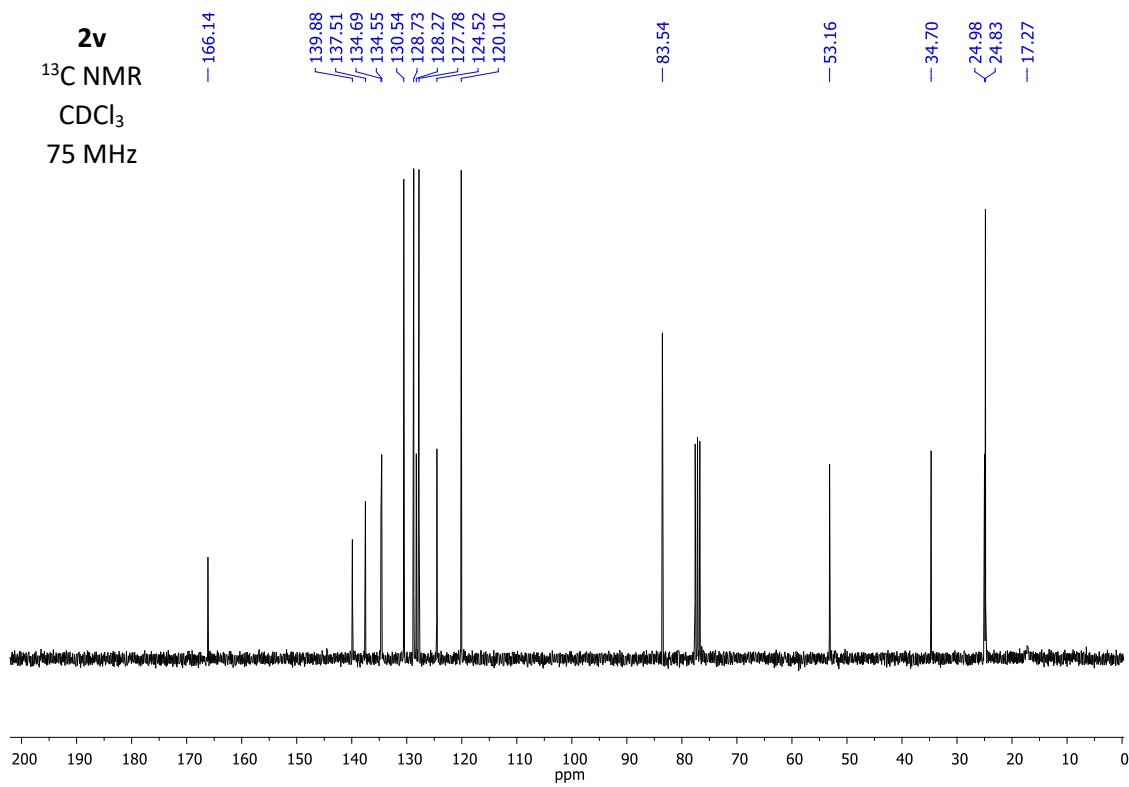
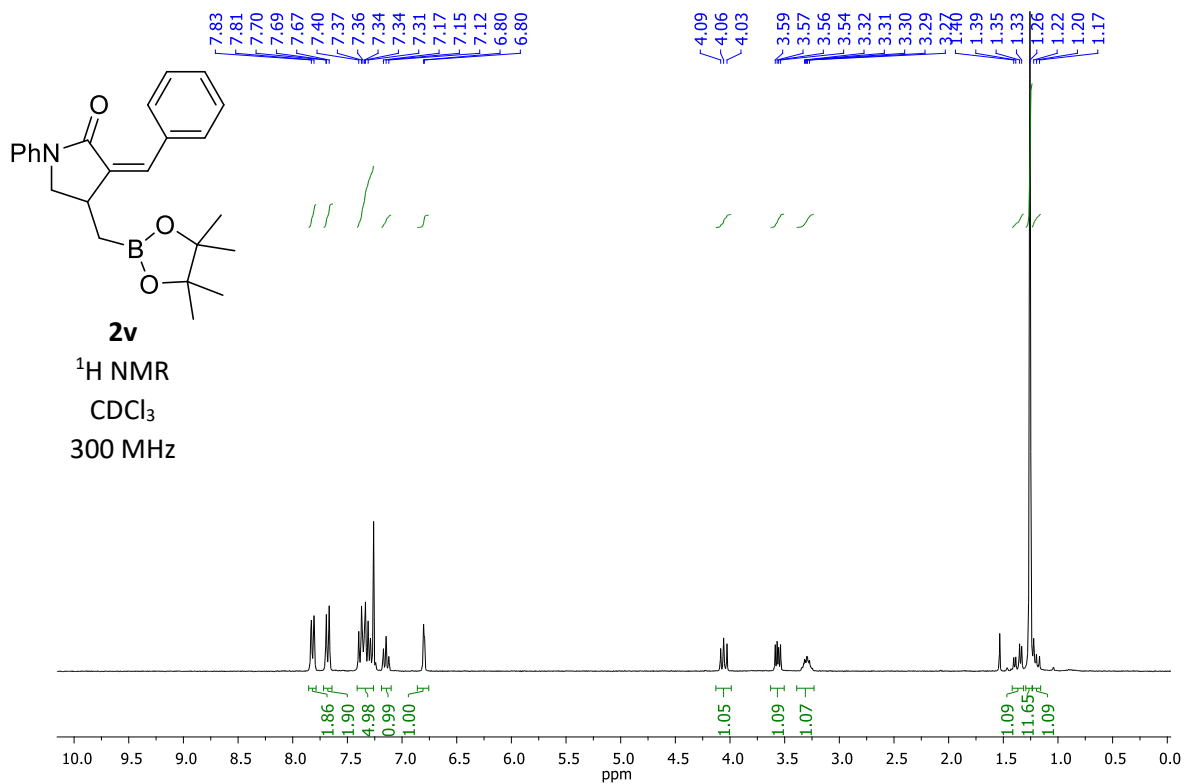


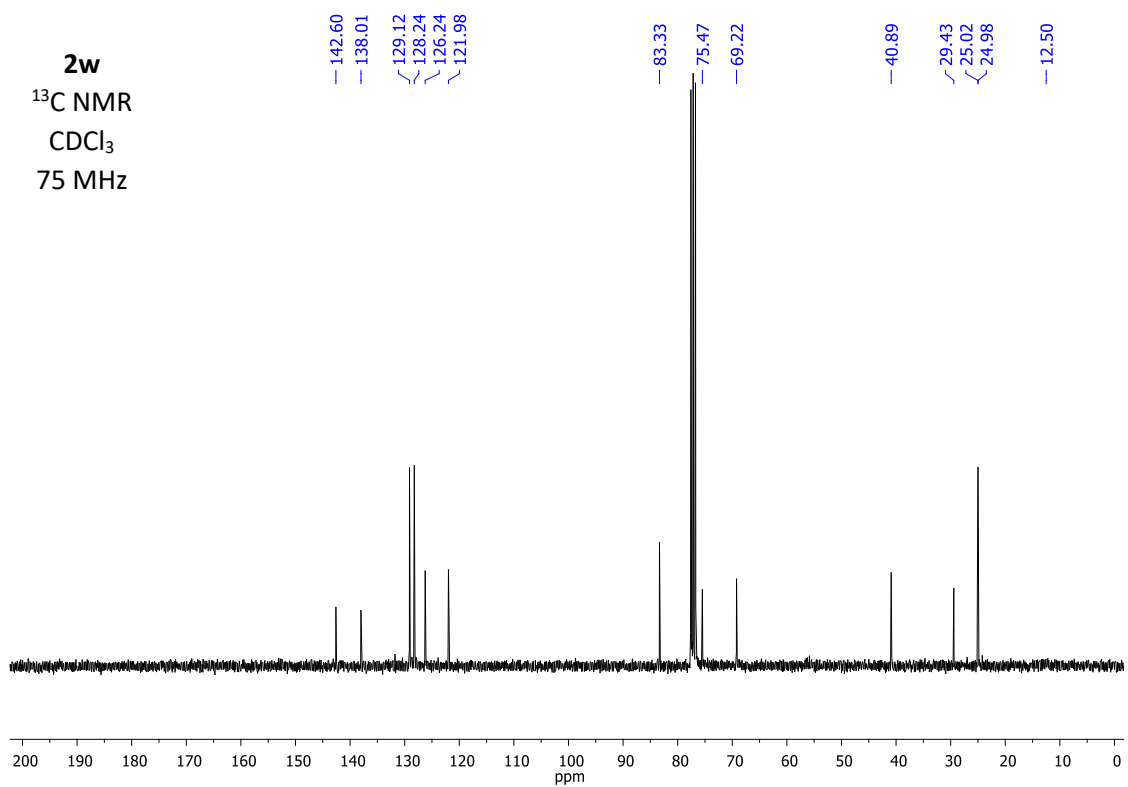
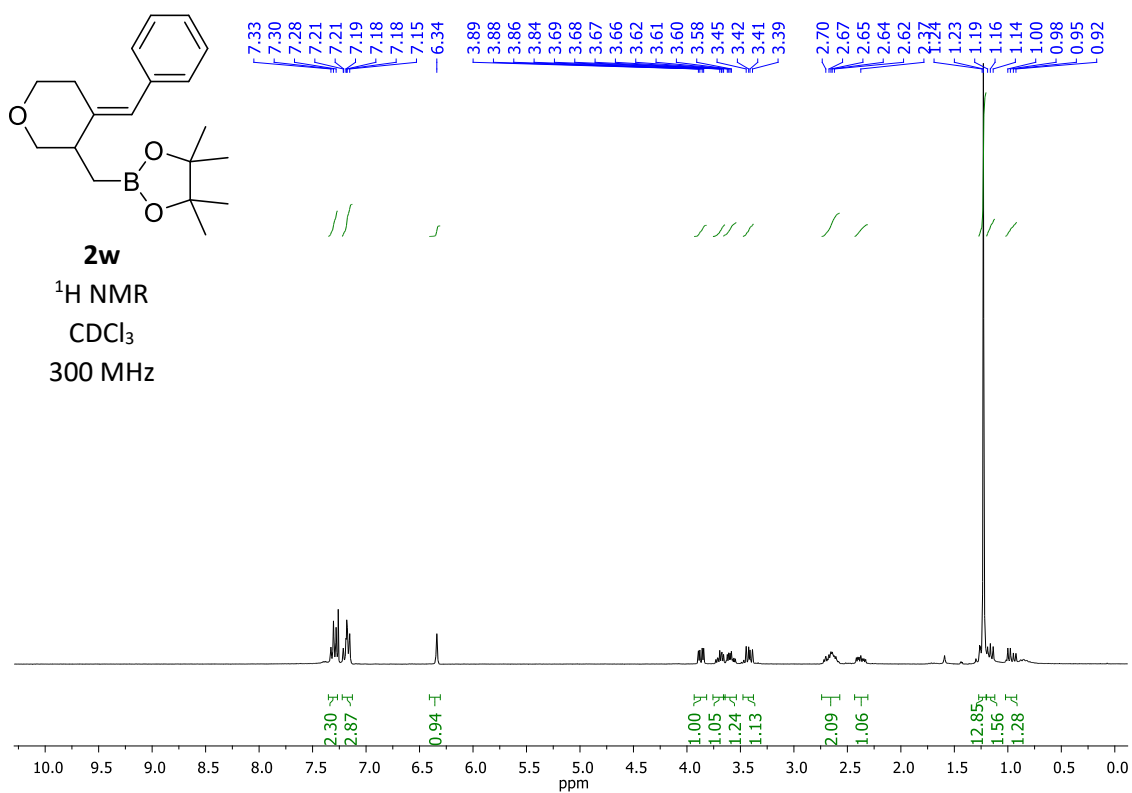


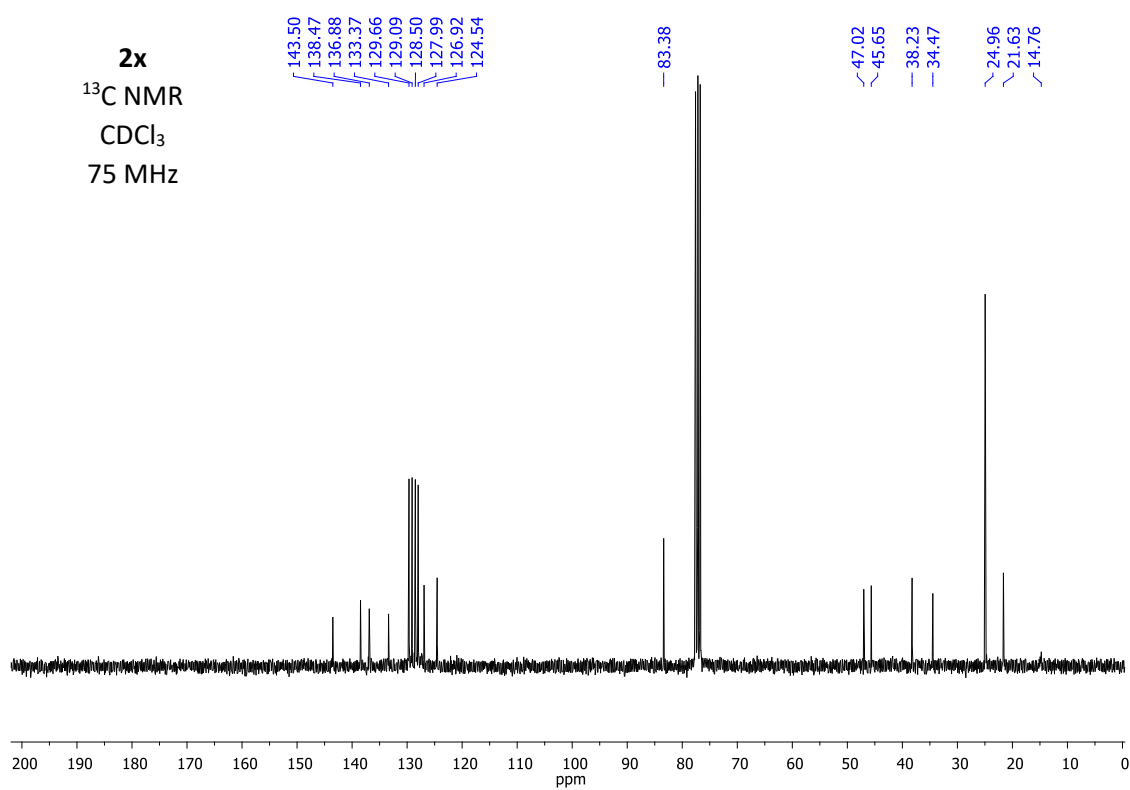
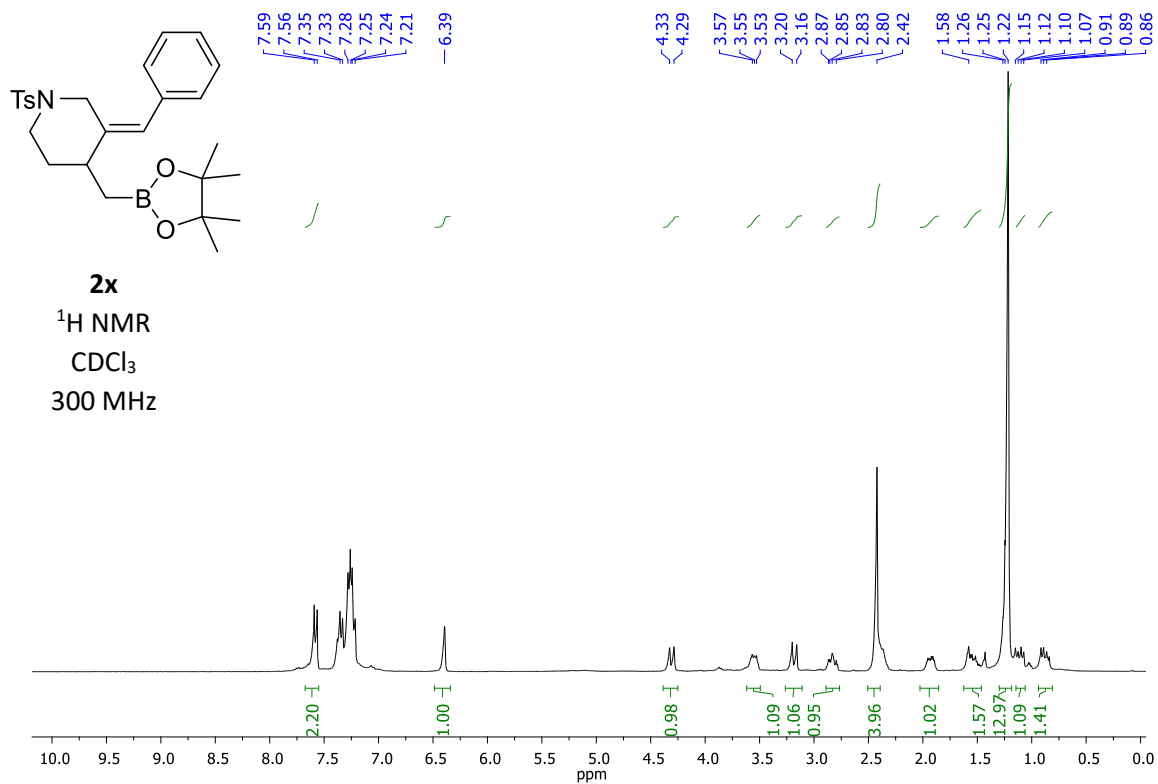


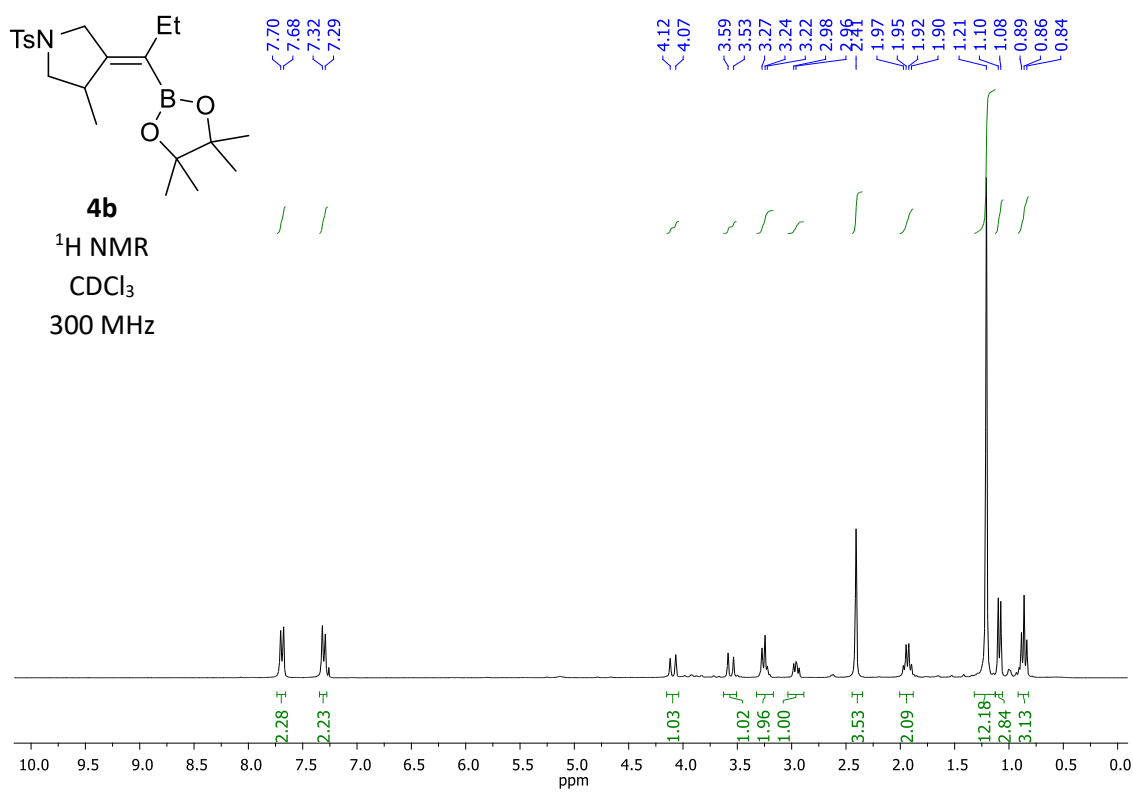
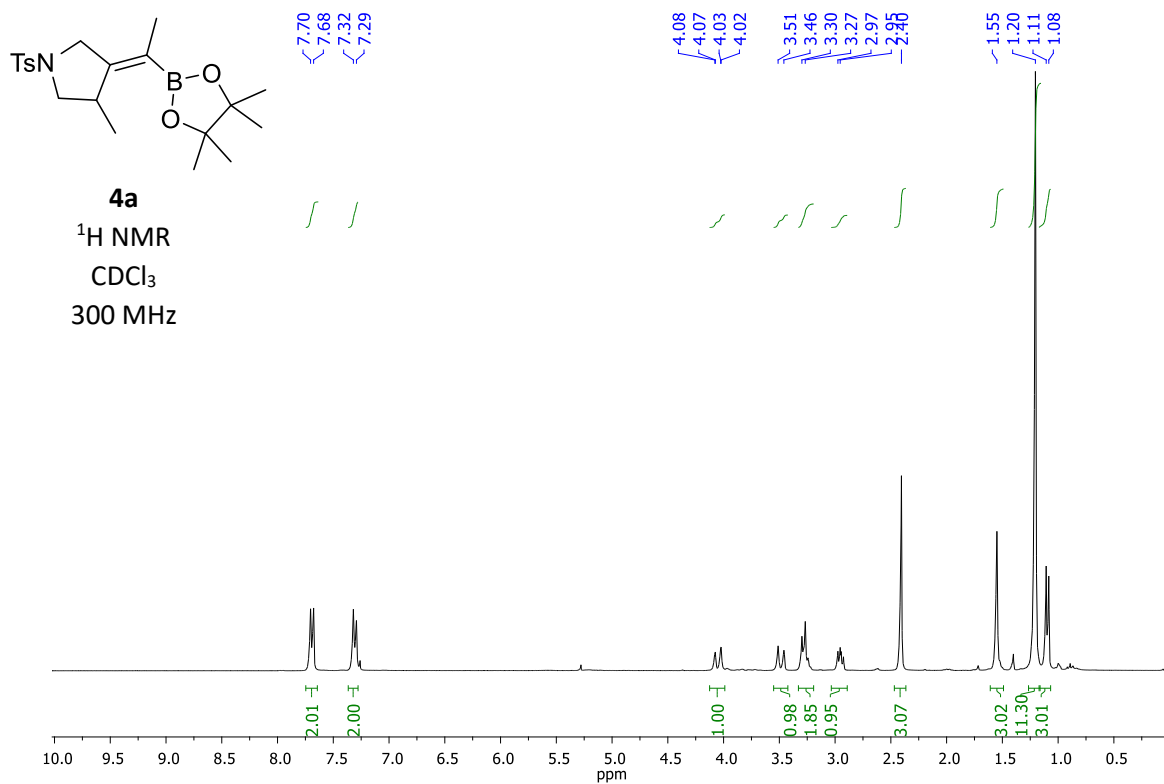




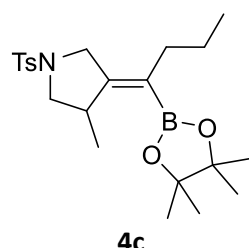
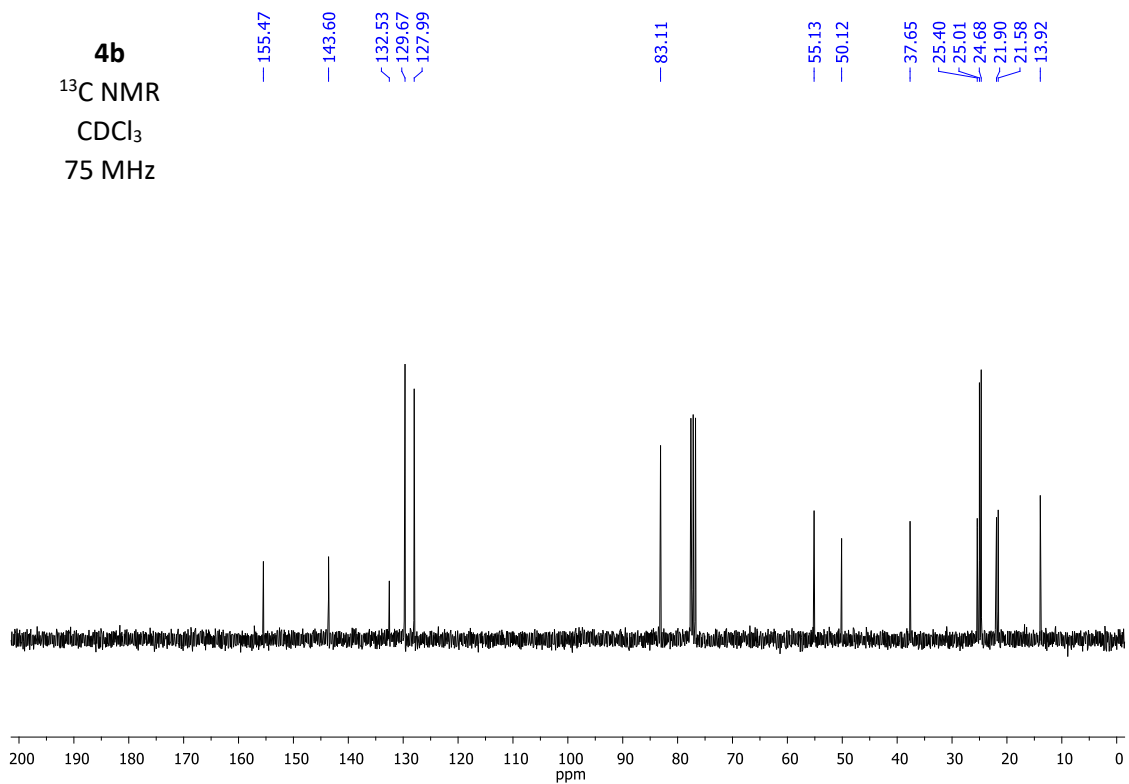




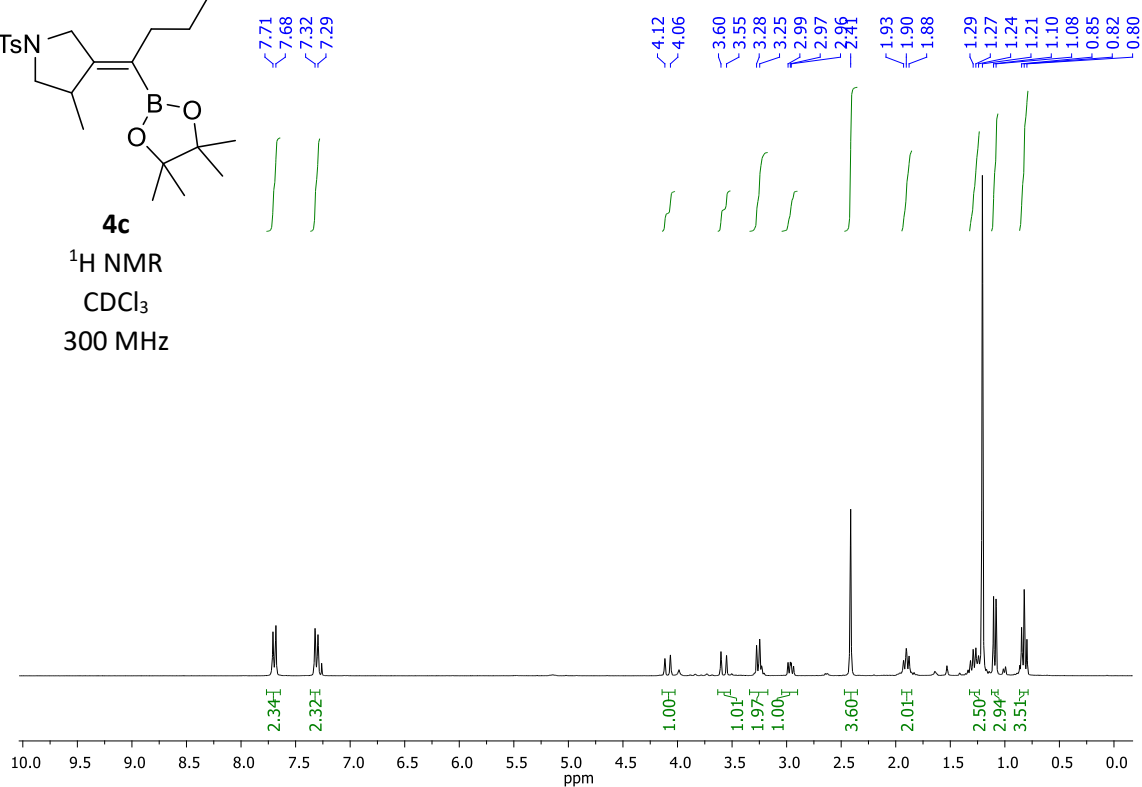


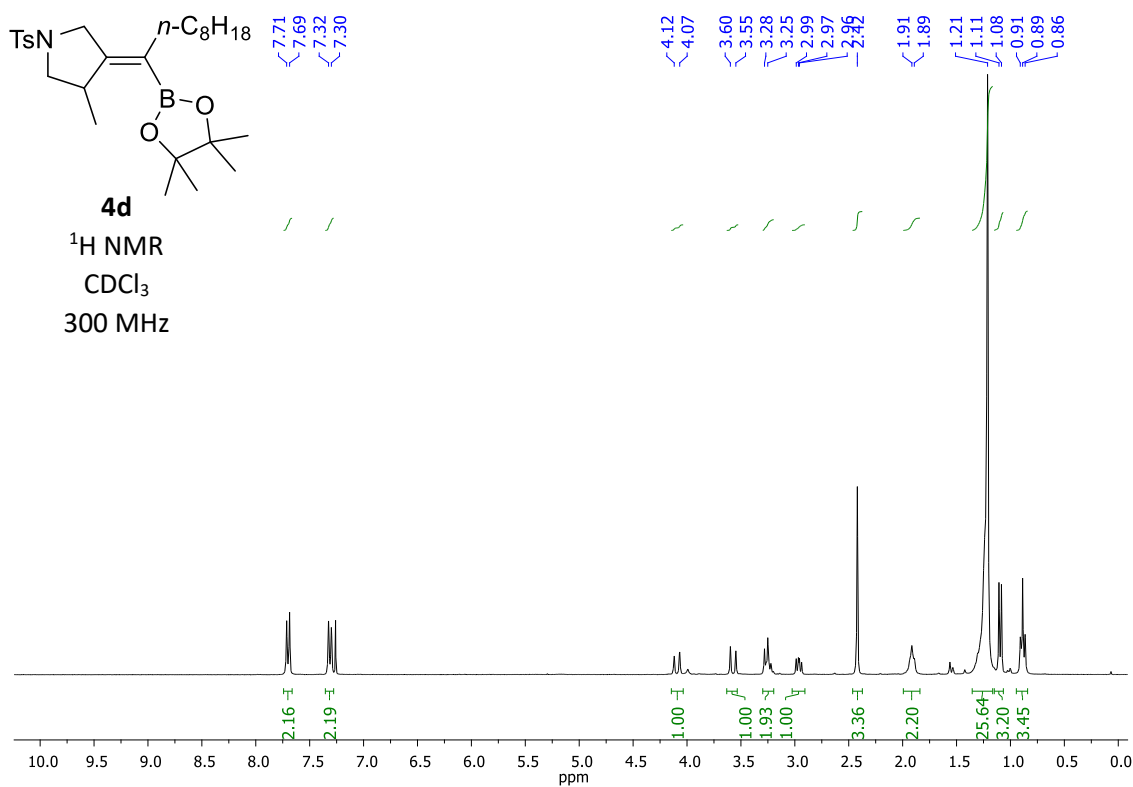
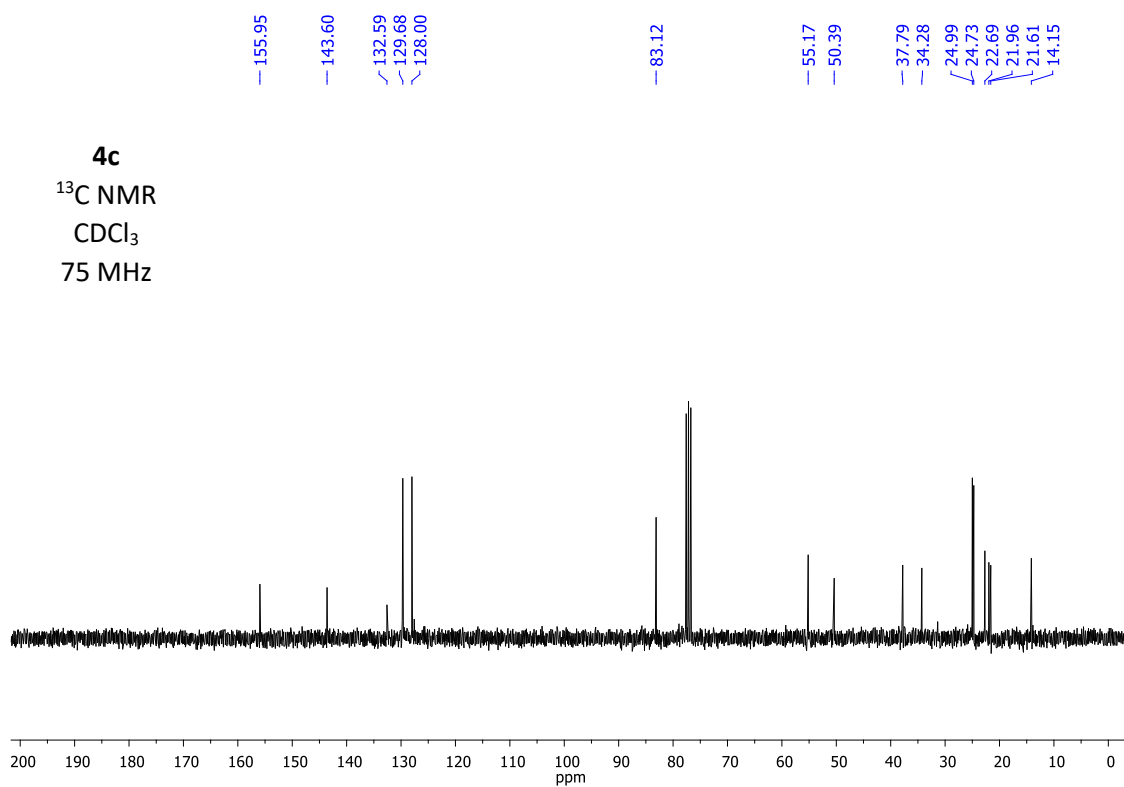


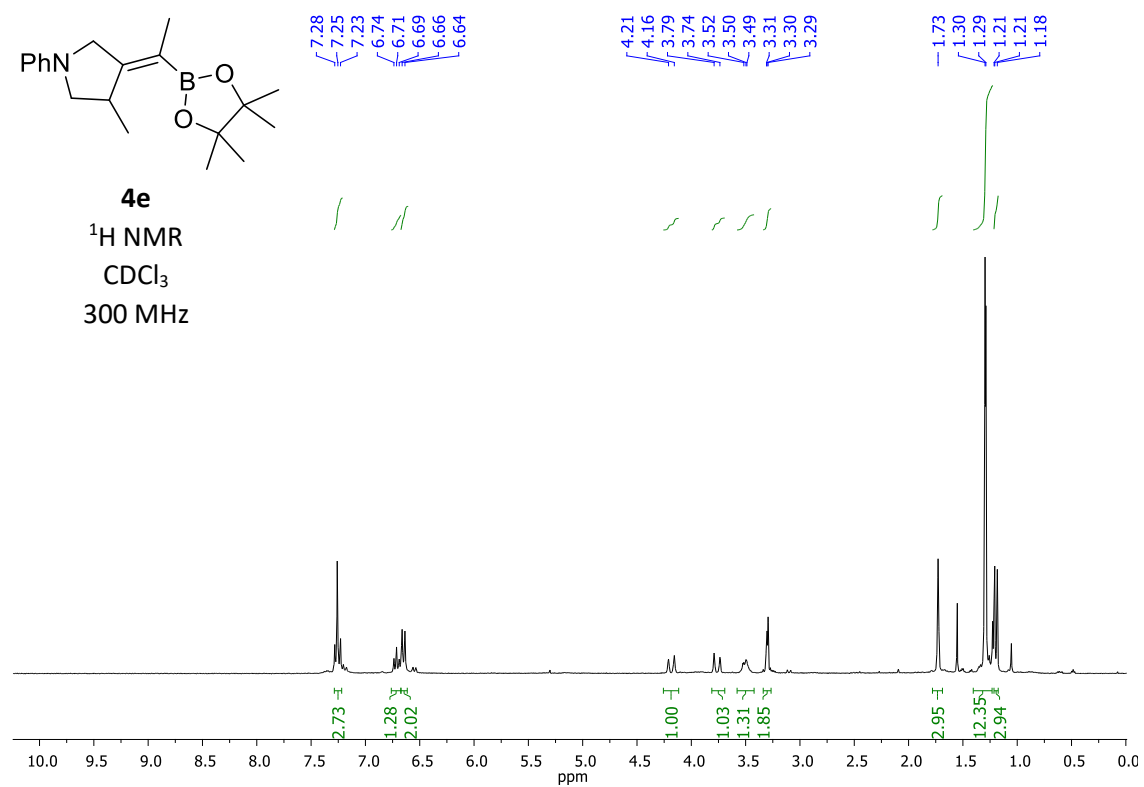
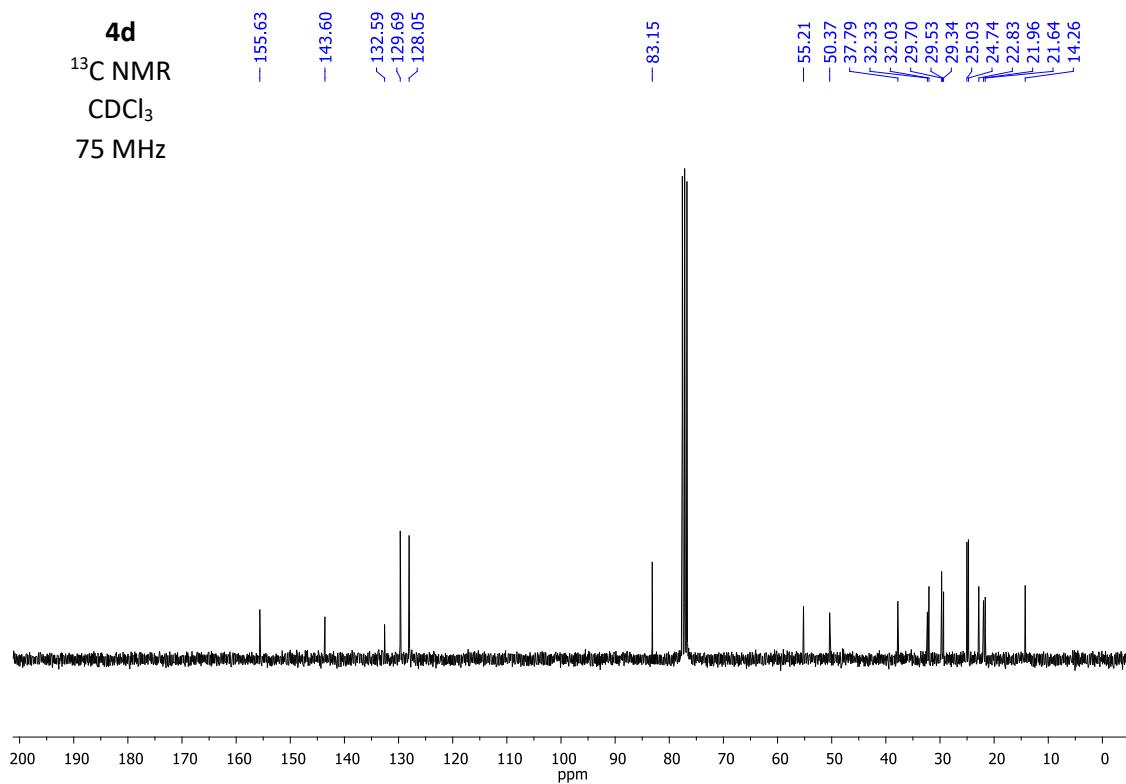
4b
¹³C NMR
 CDCl₃
 75 MHz

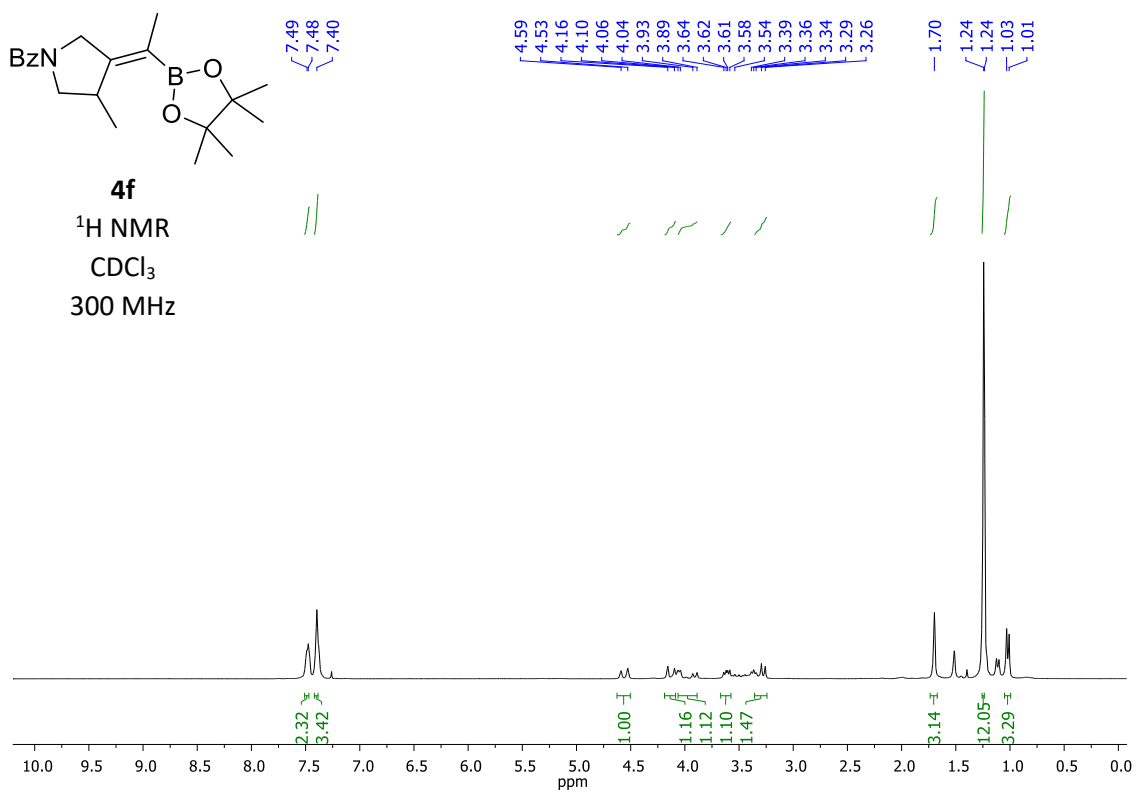
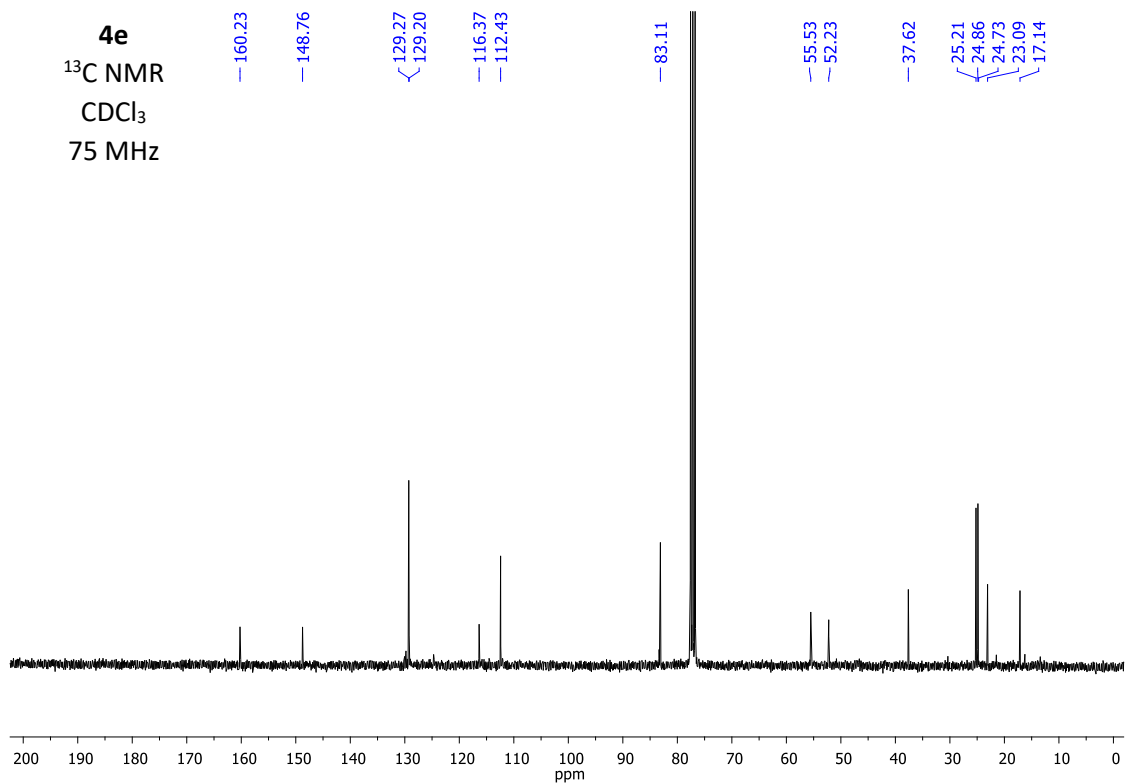


4c
¹H NMR
 CDCl₃
 300 MHz

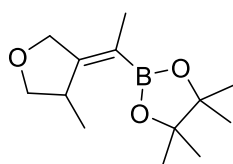
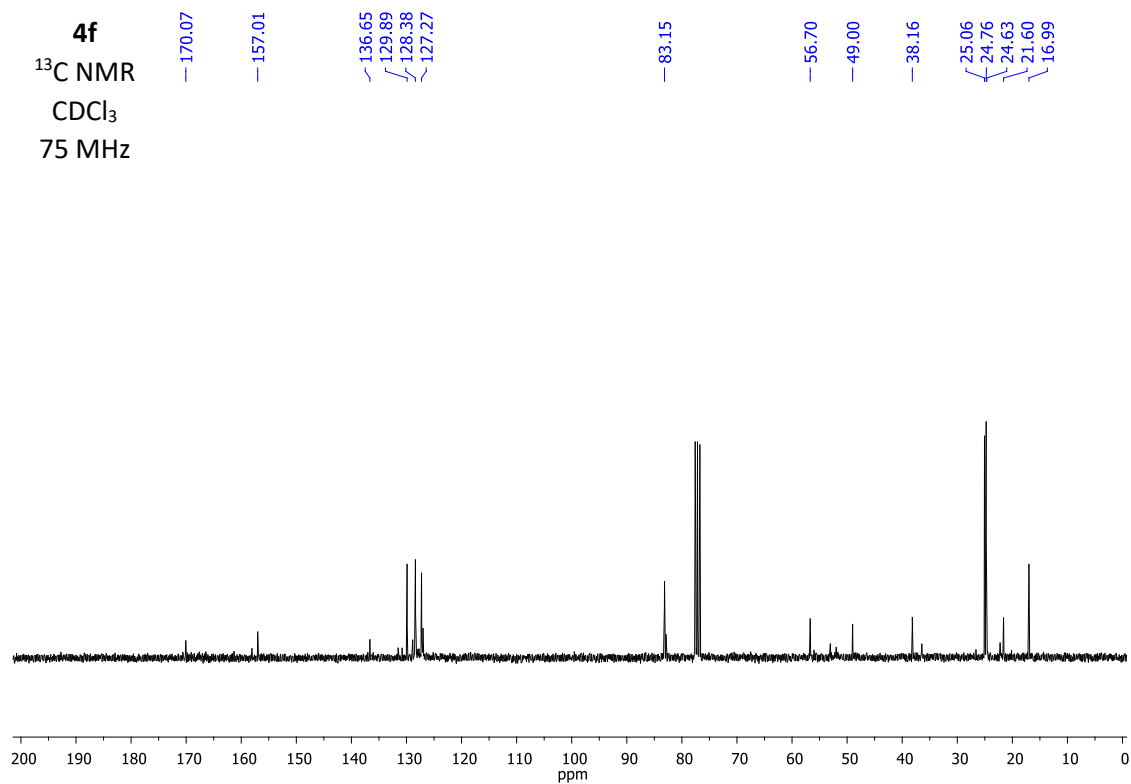




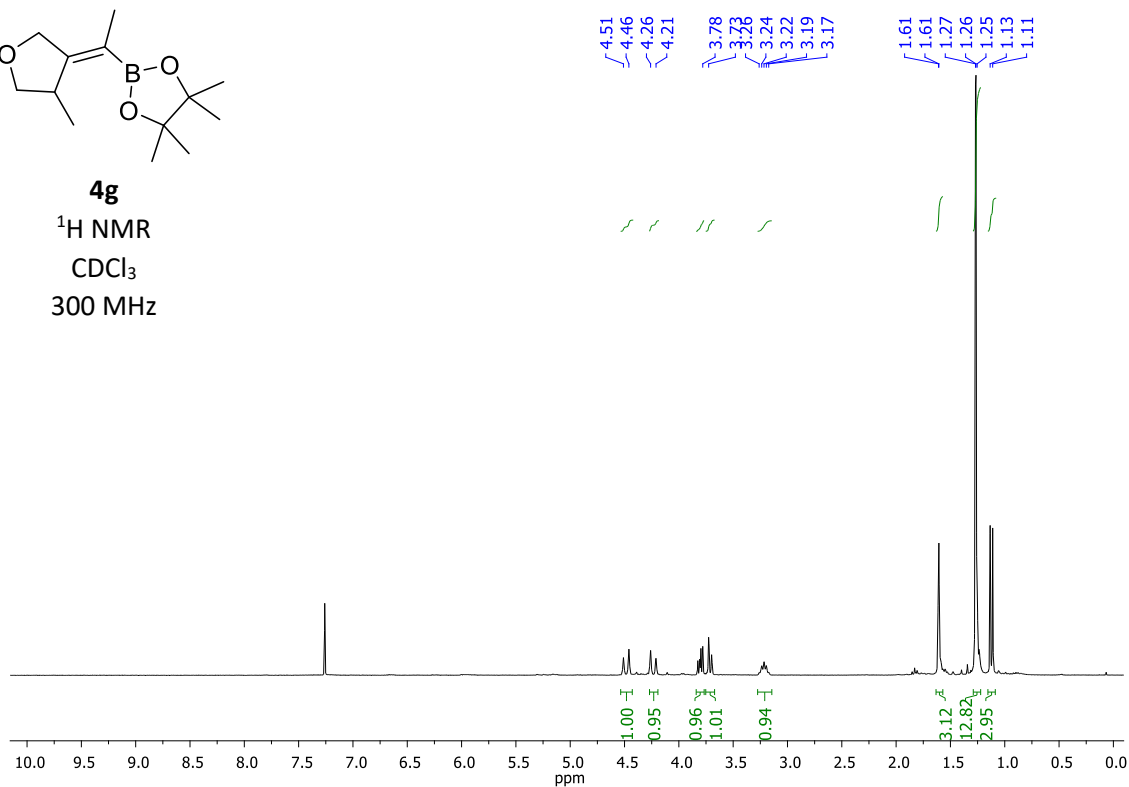


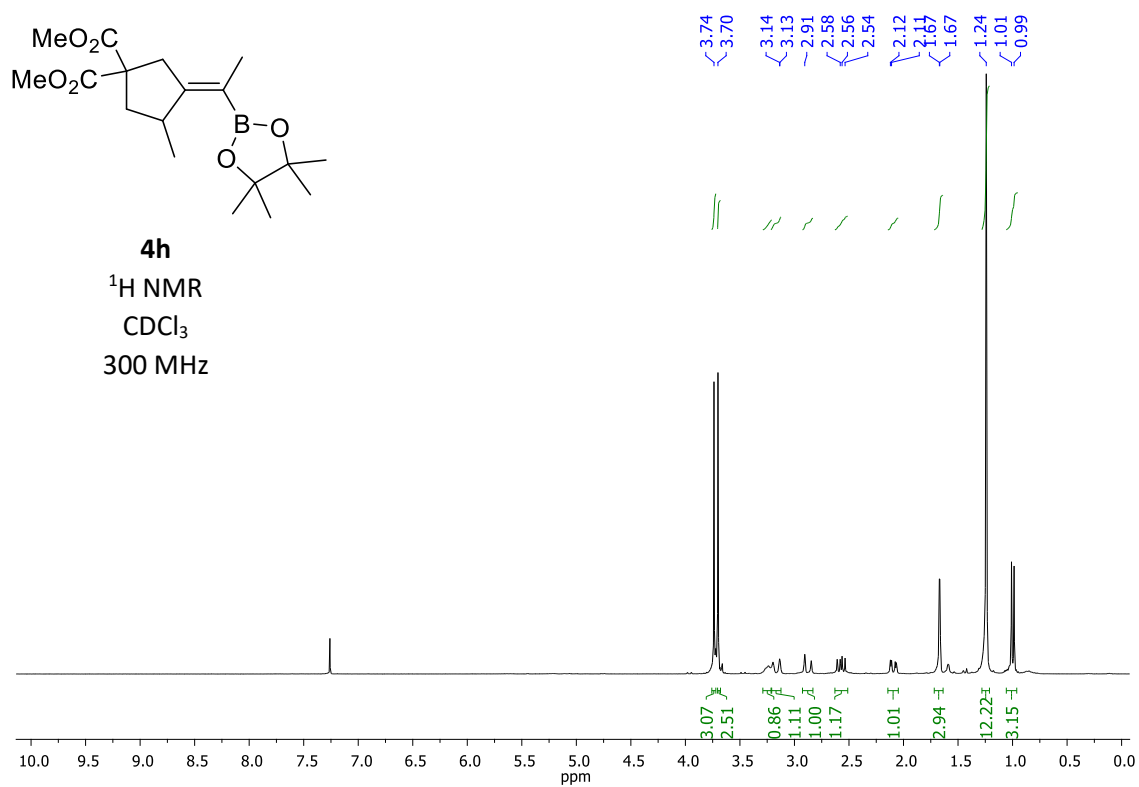
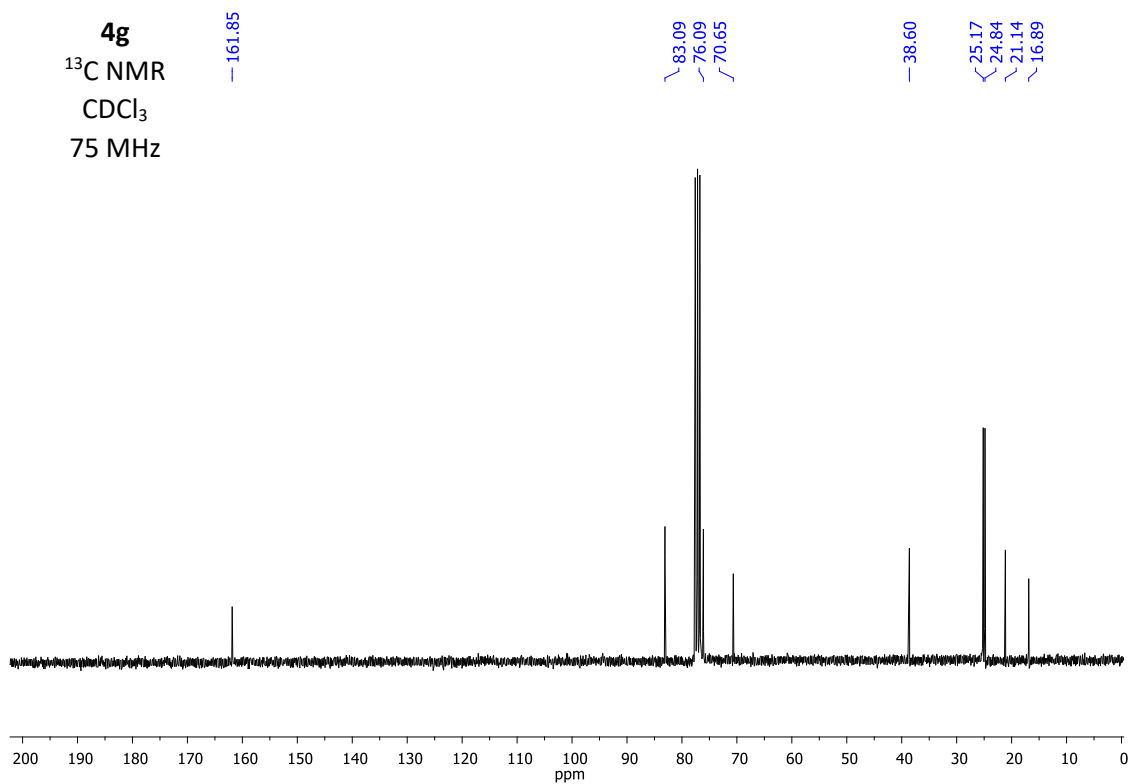


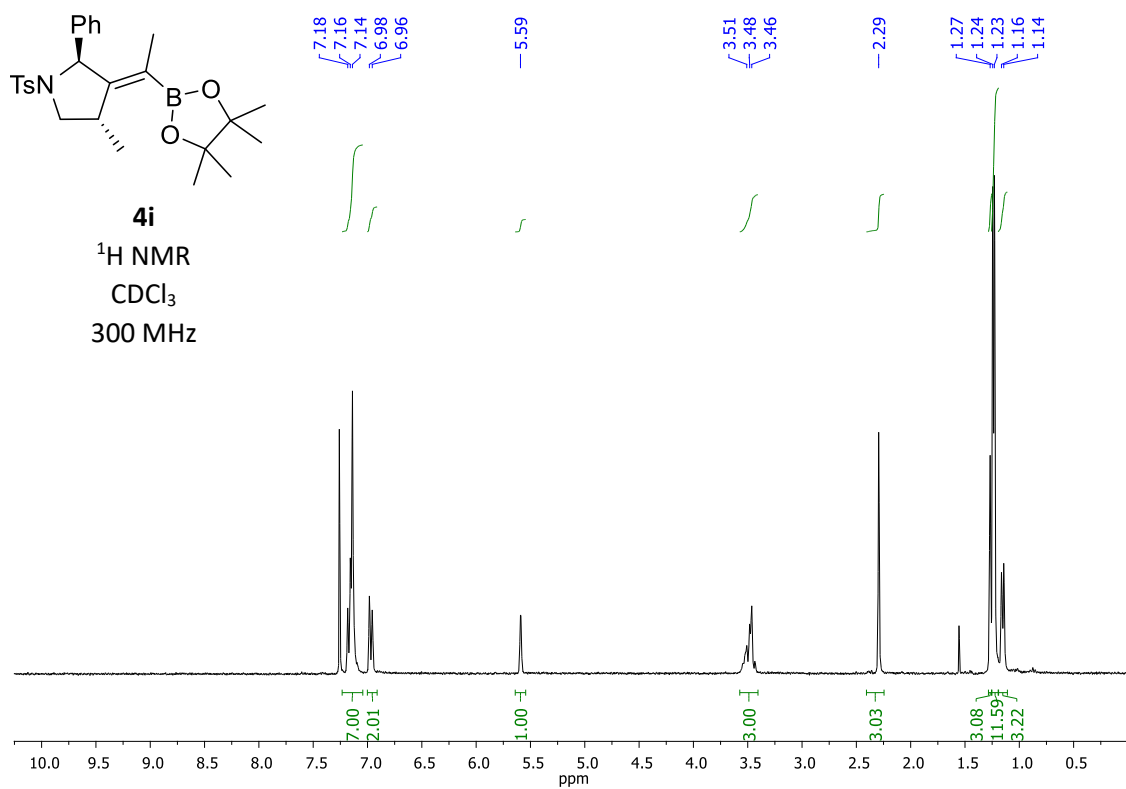
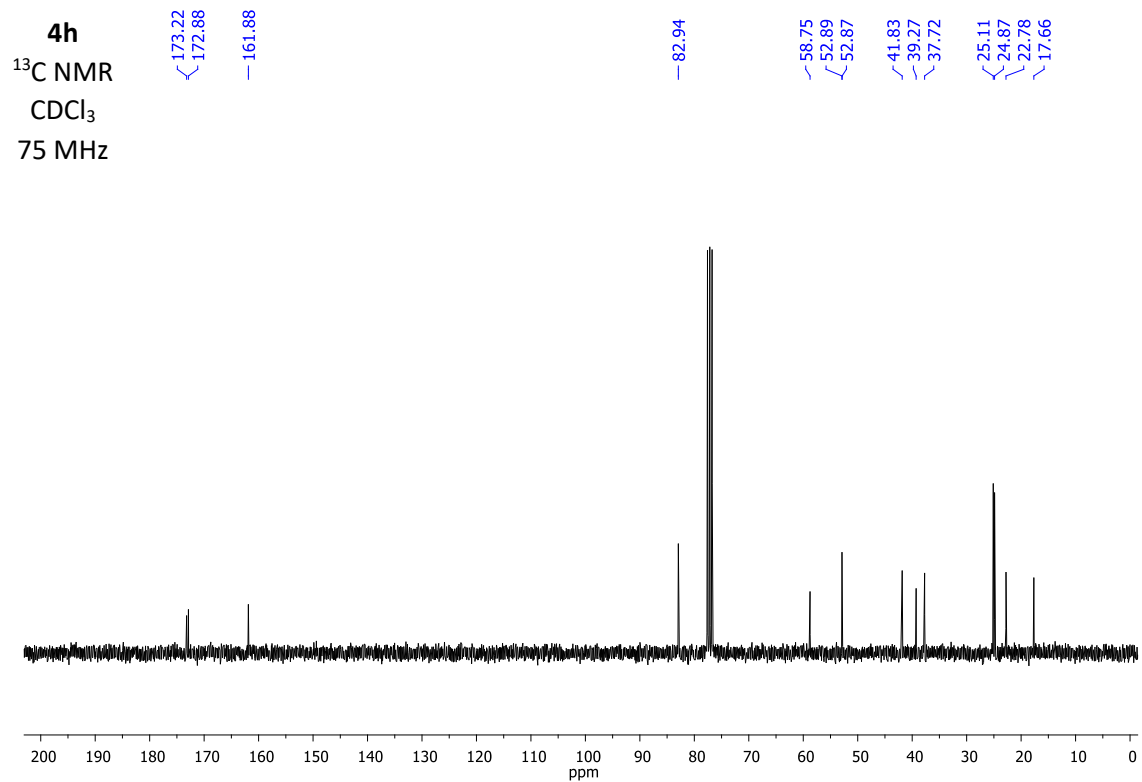
4f
¹³C NMR
 CDCl₃
 75 MHz

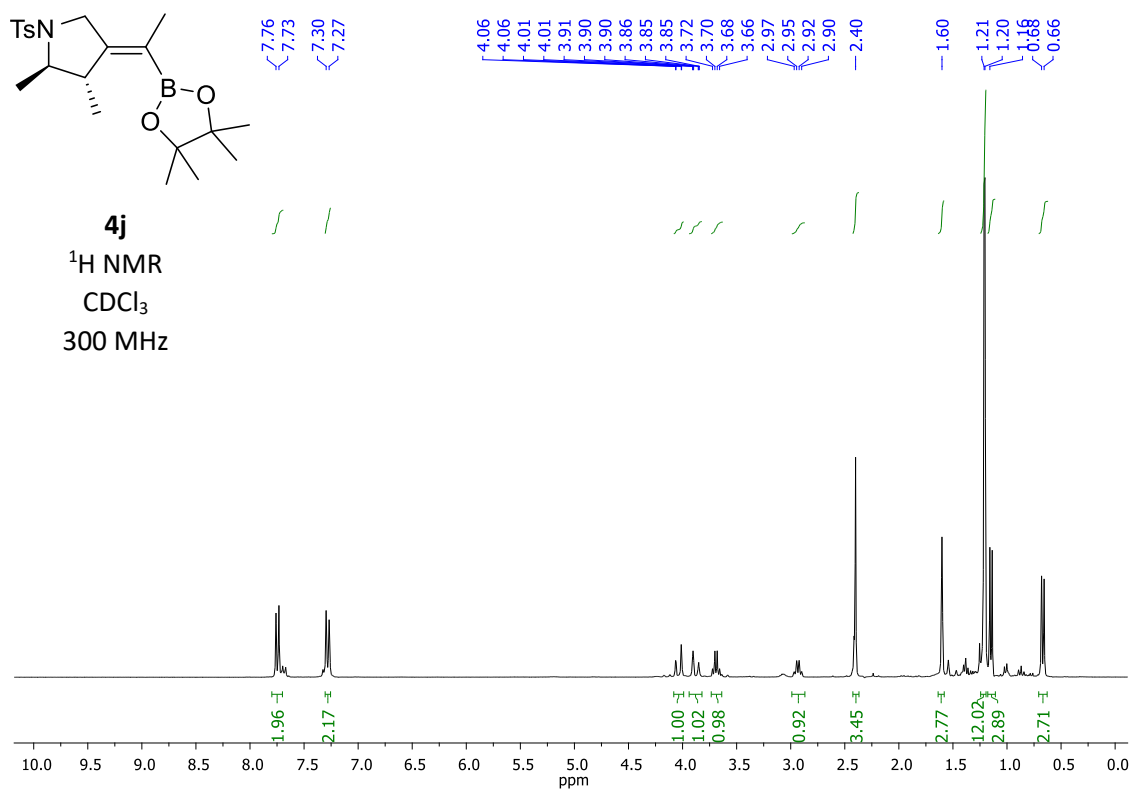
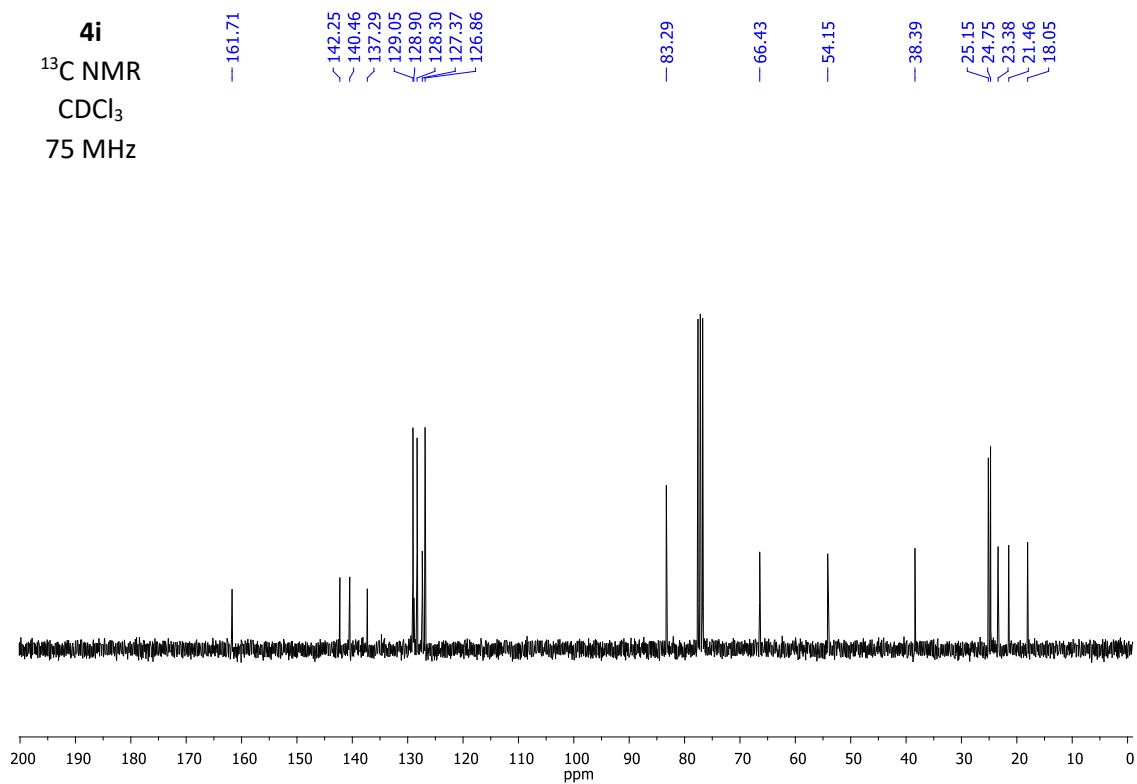


4g
¹H NMR
 CDCl₃
 300 MHz

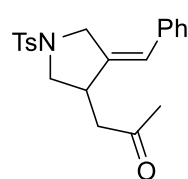
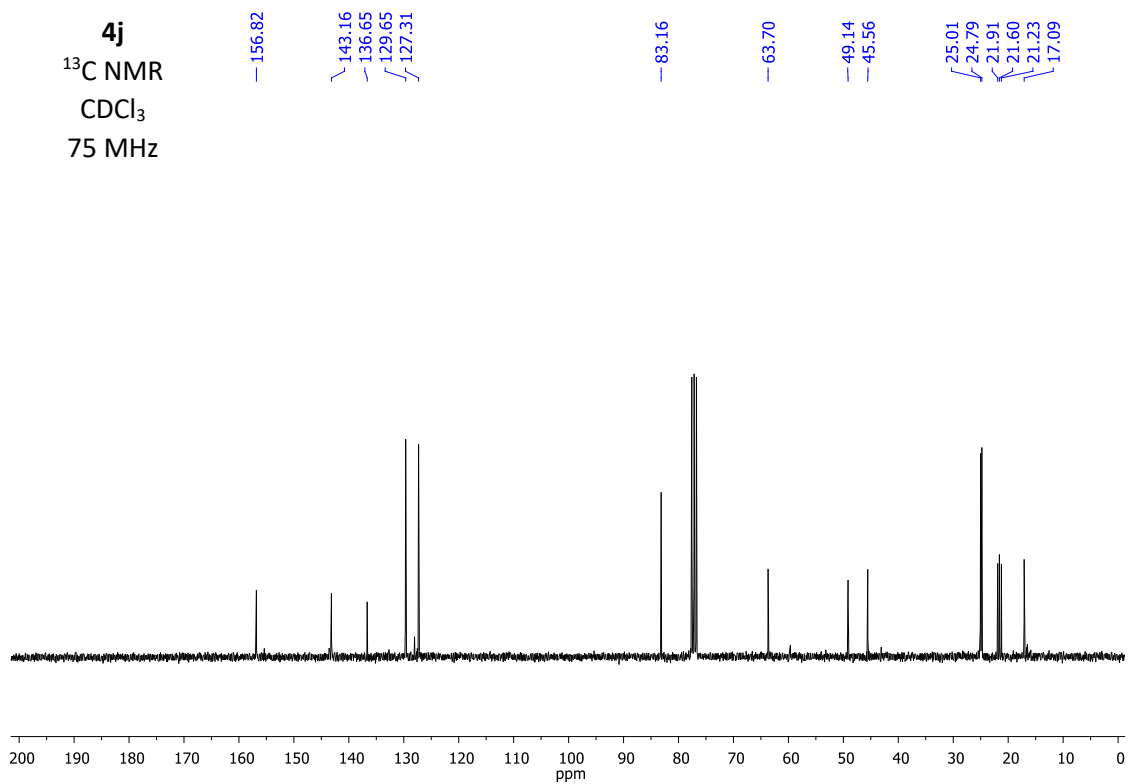




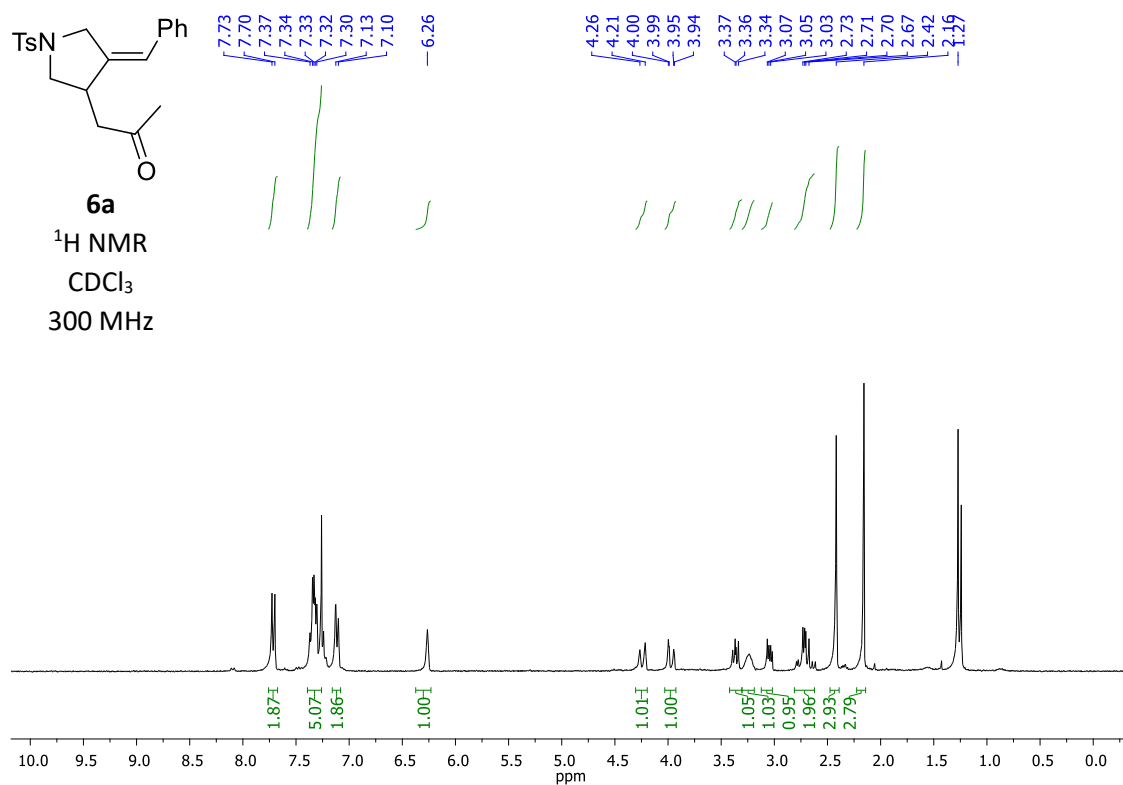


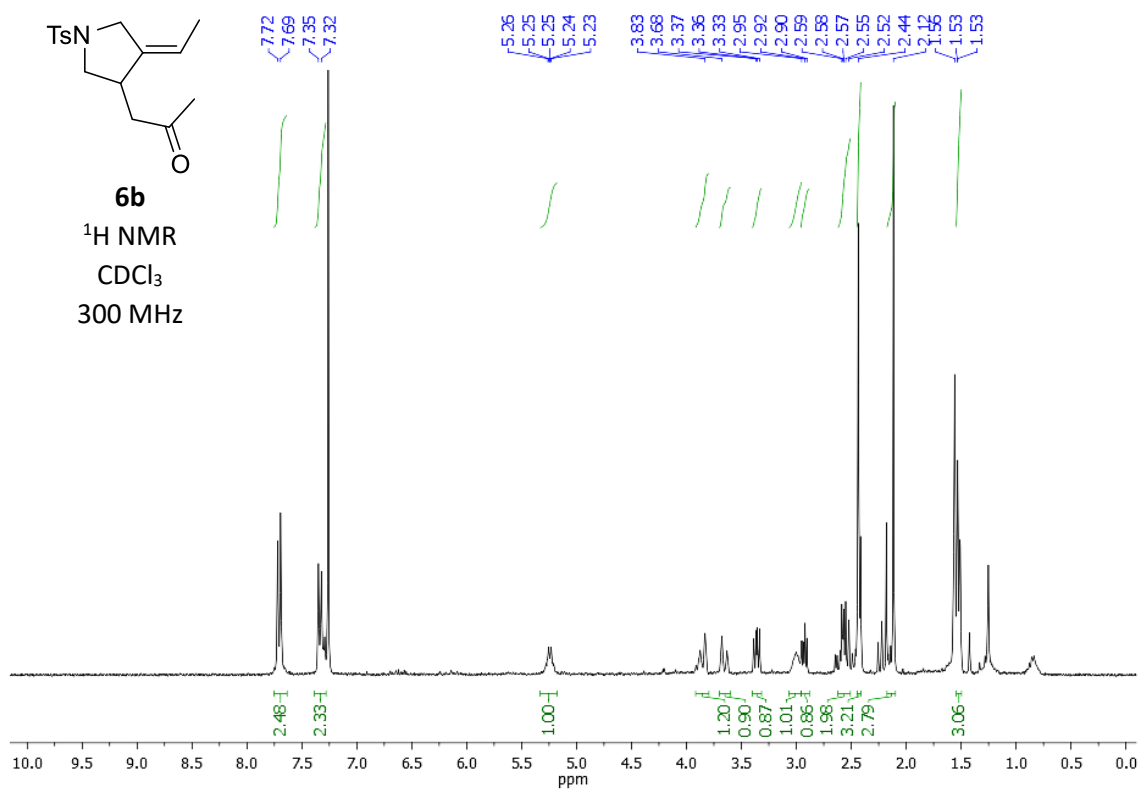
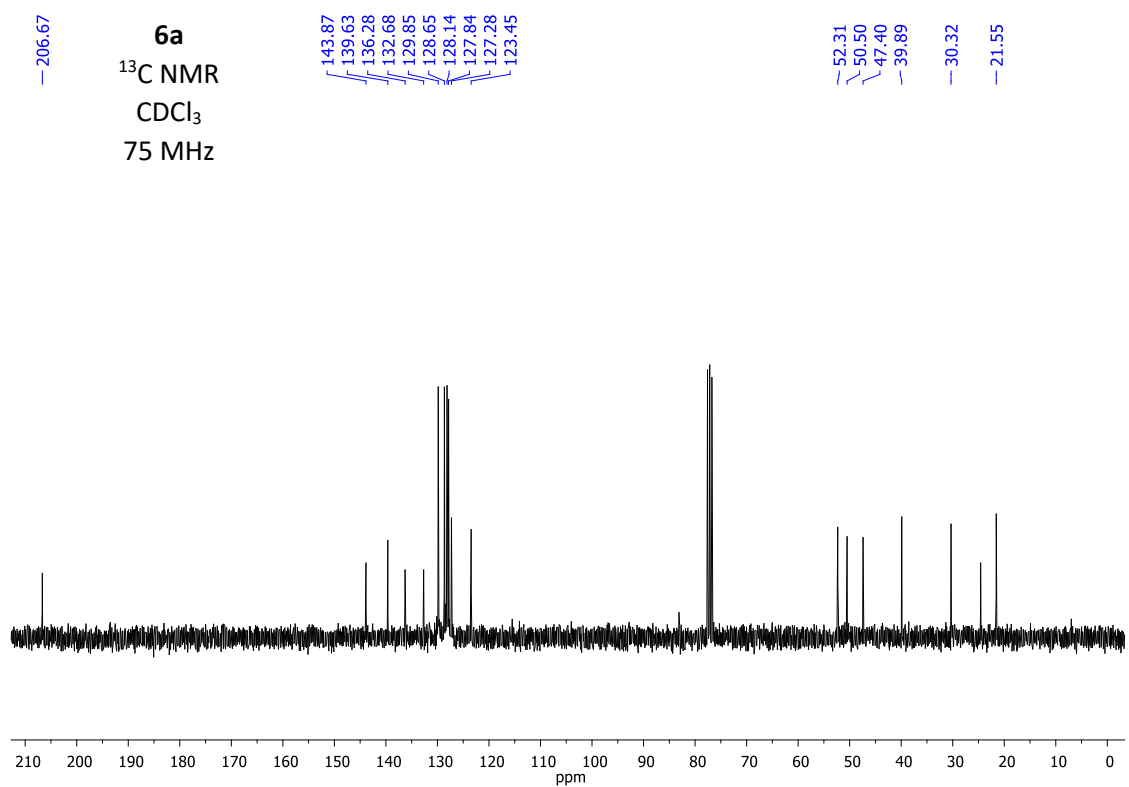


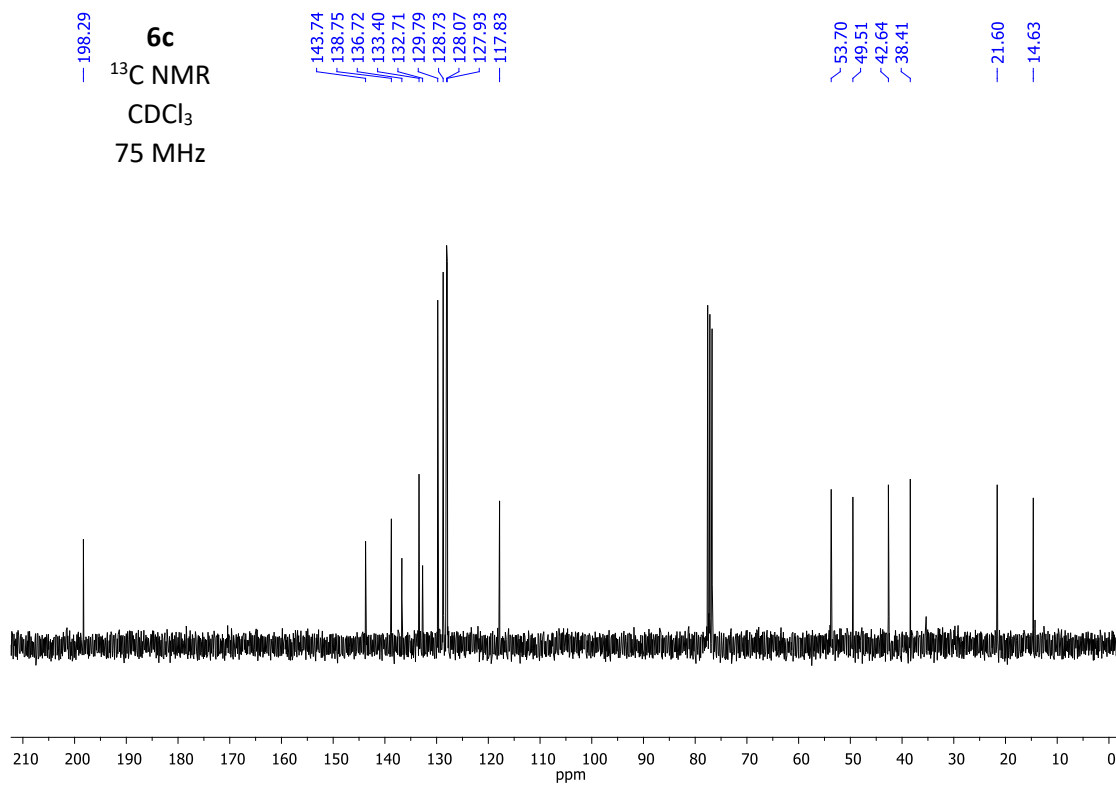
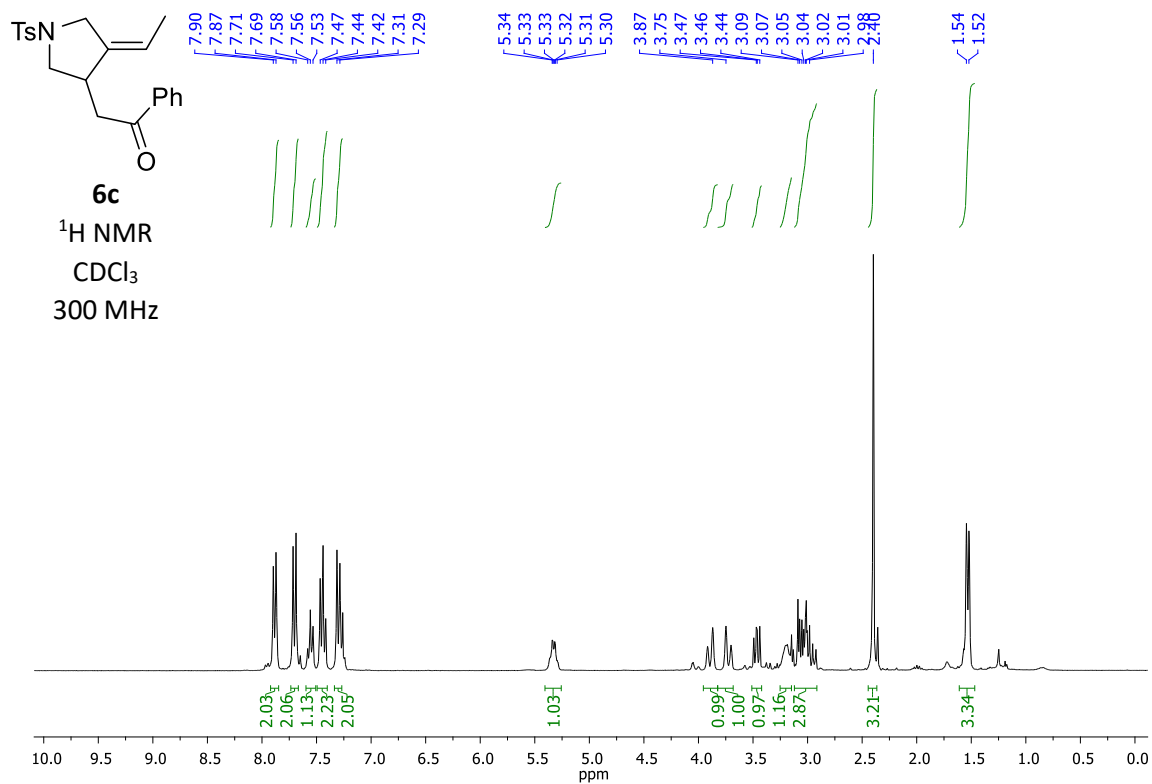
4j
¹³C NMR
 CDCl₃
 75 MHz

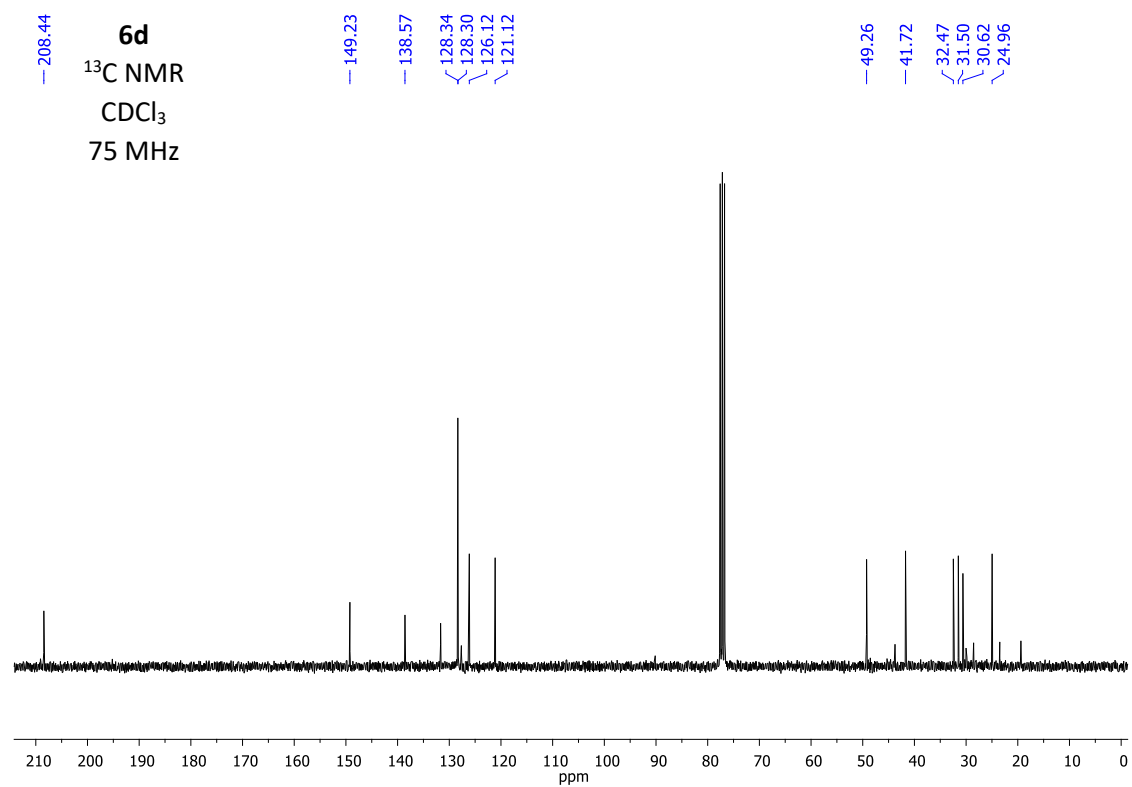
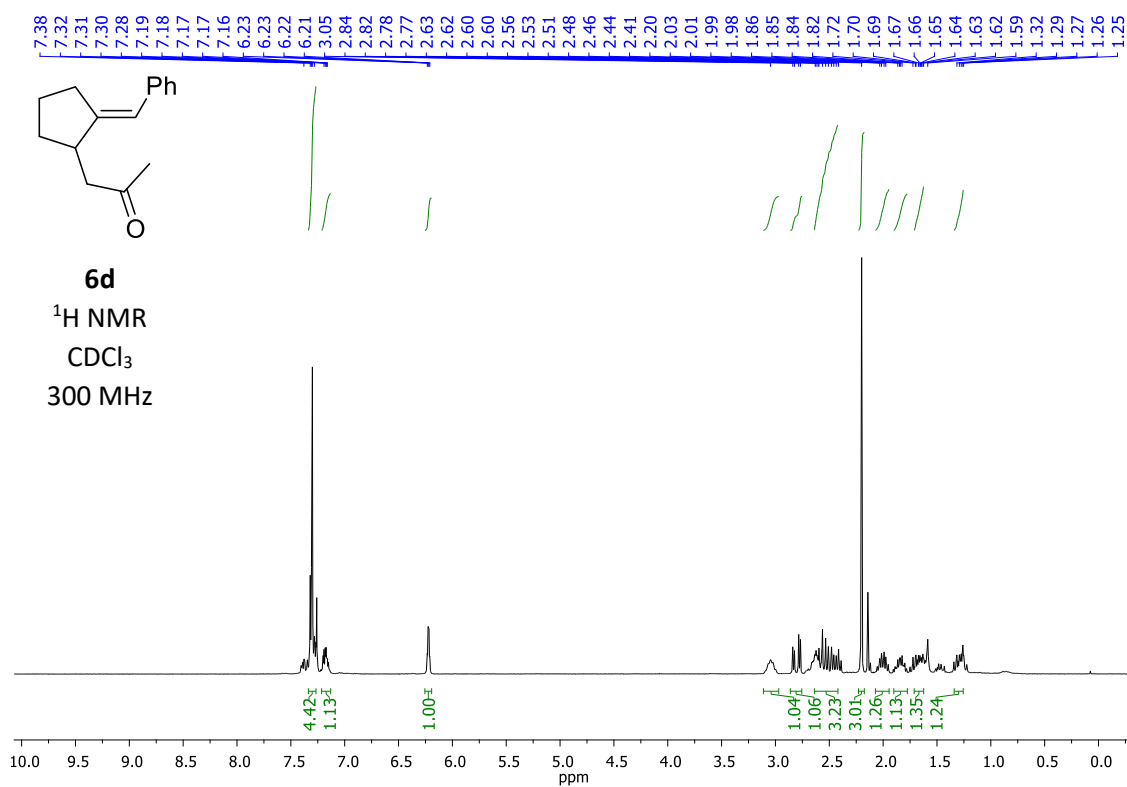


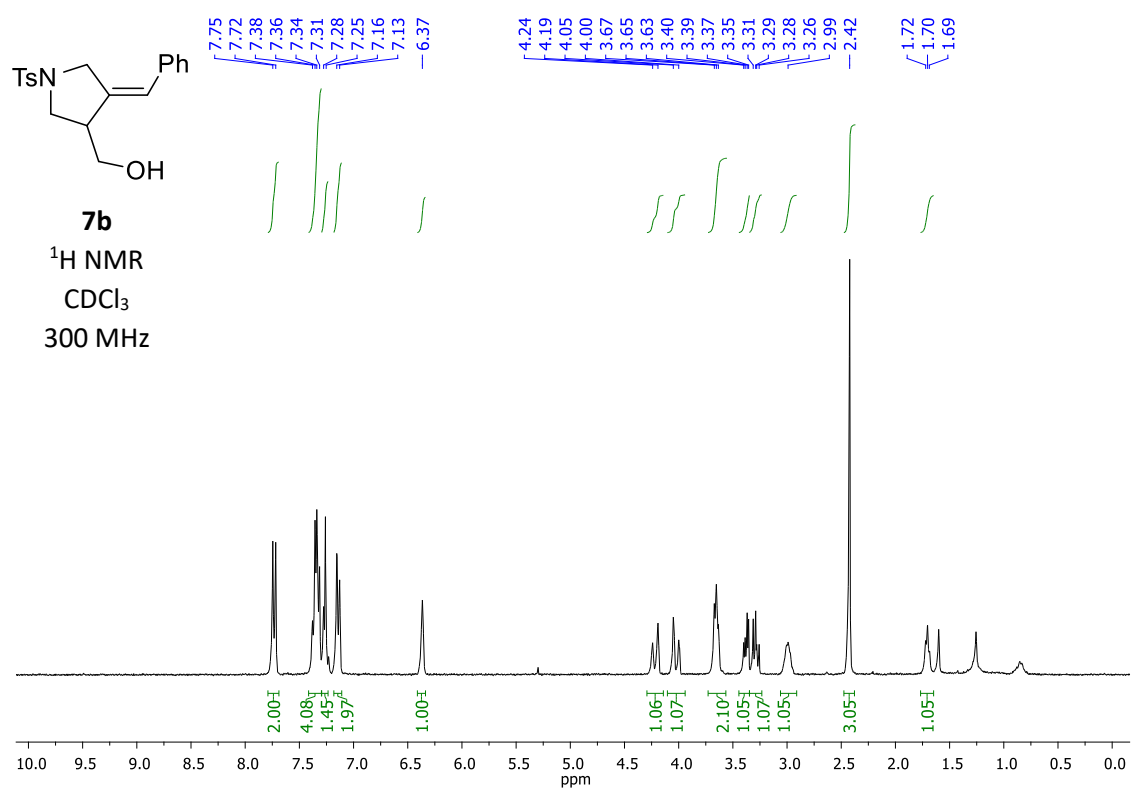
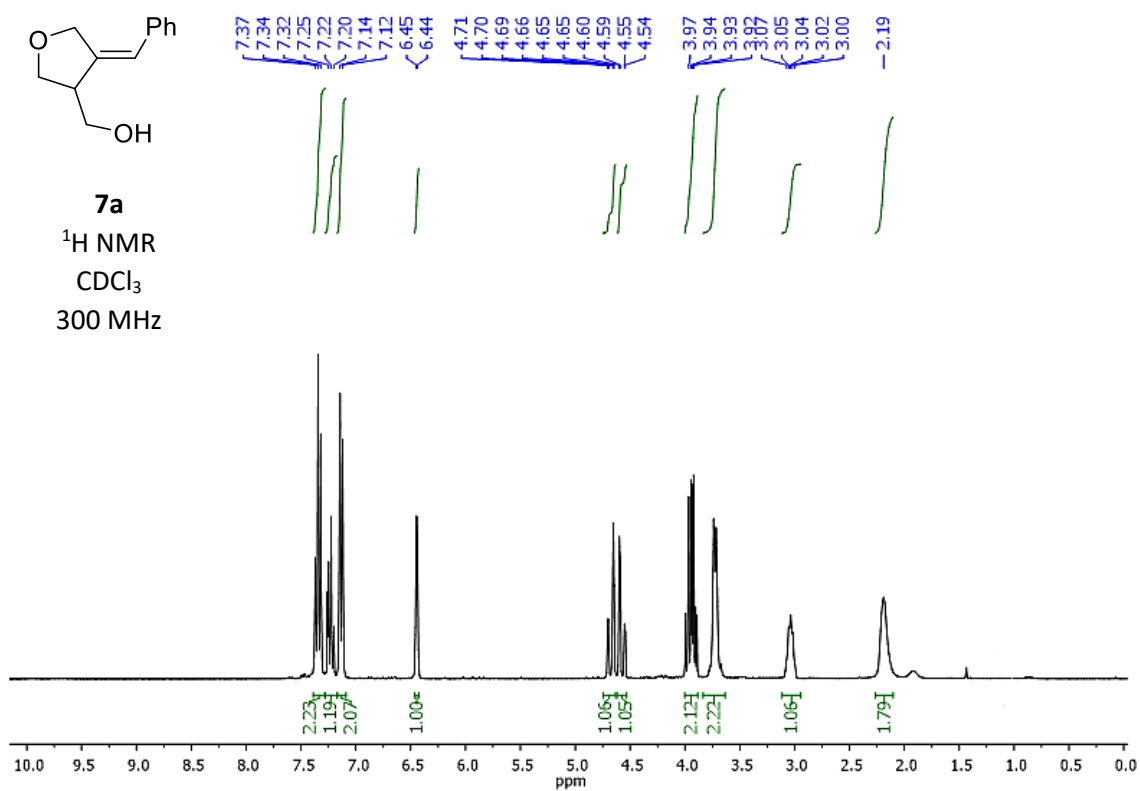
6a
¹H NMR
 CDCl₃
 300 MHz

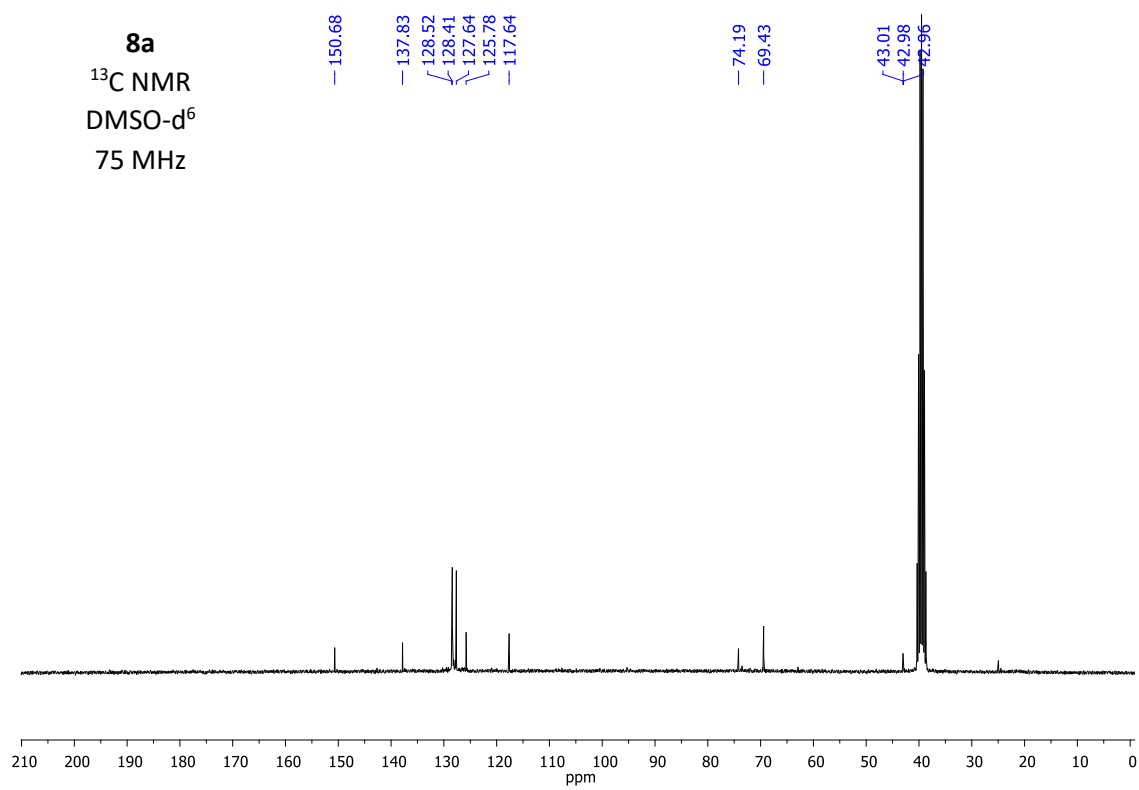
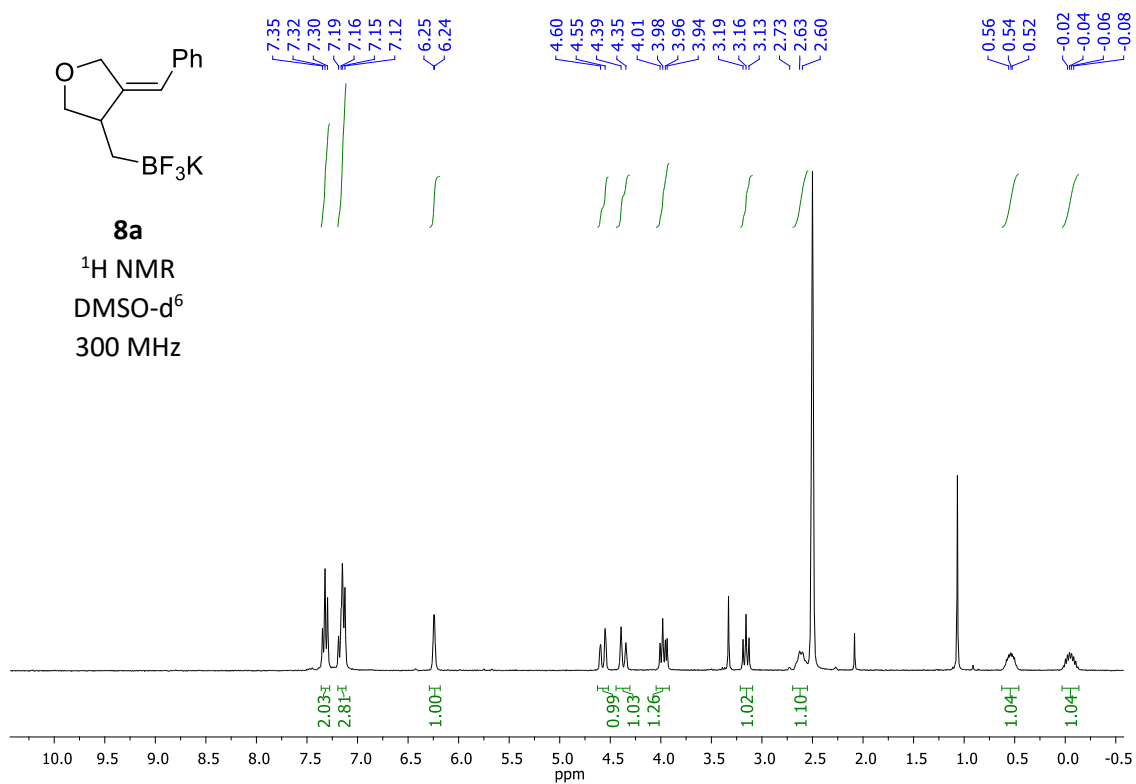


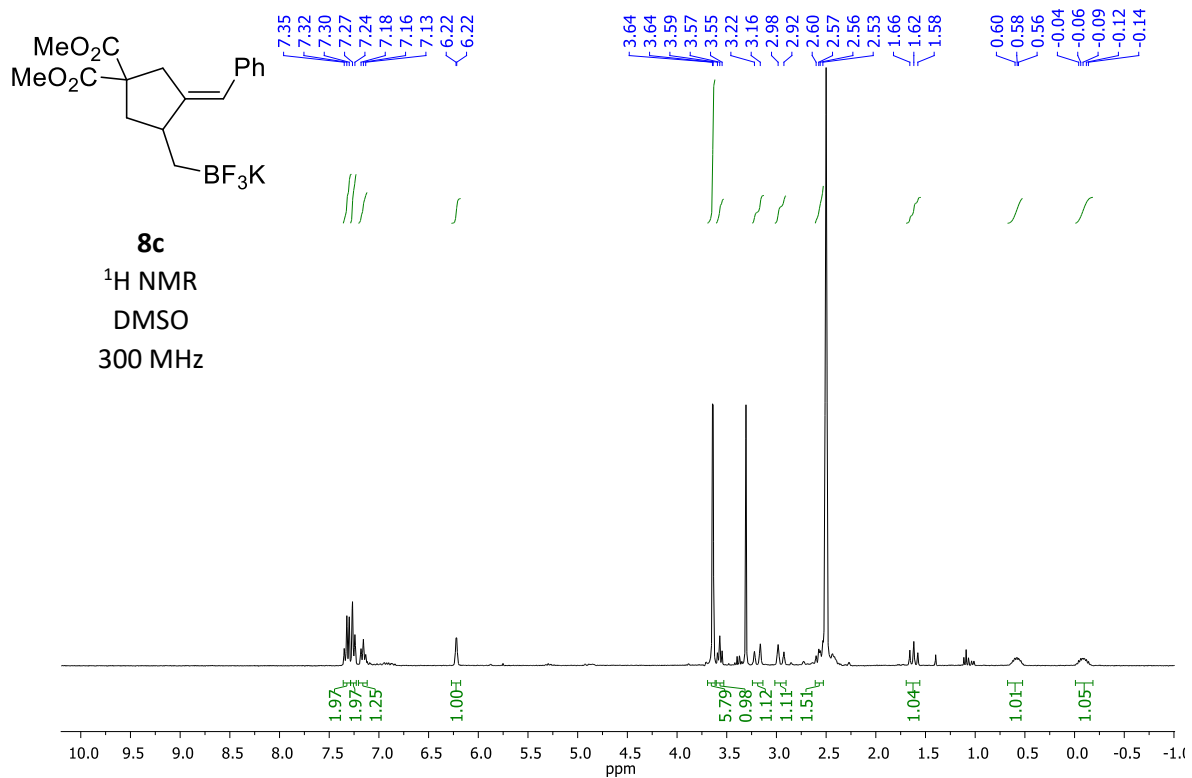
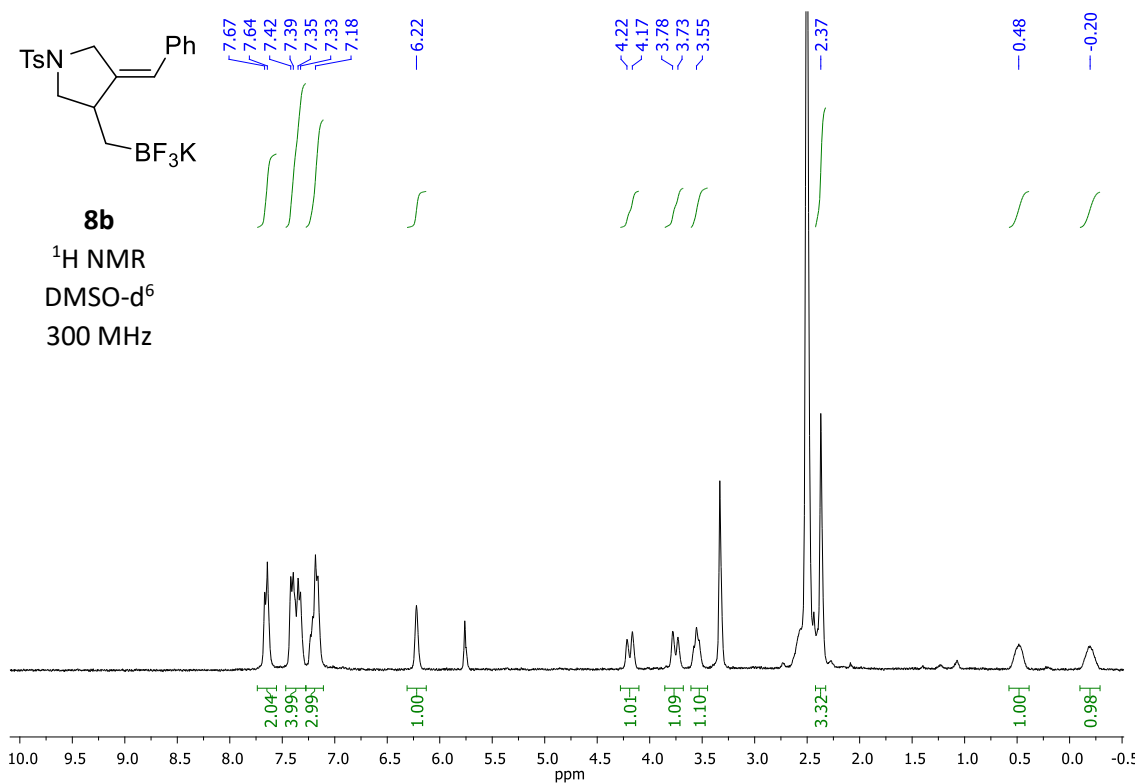


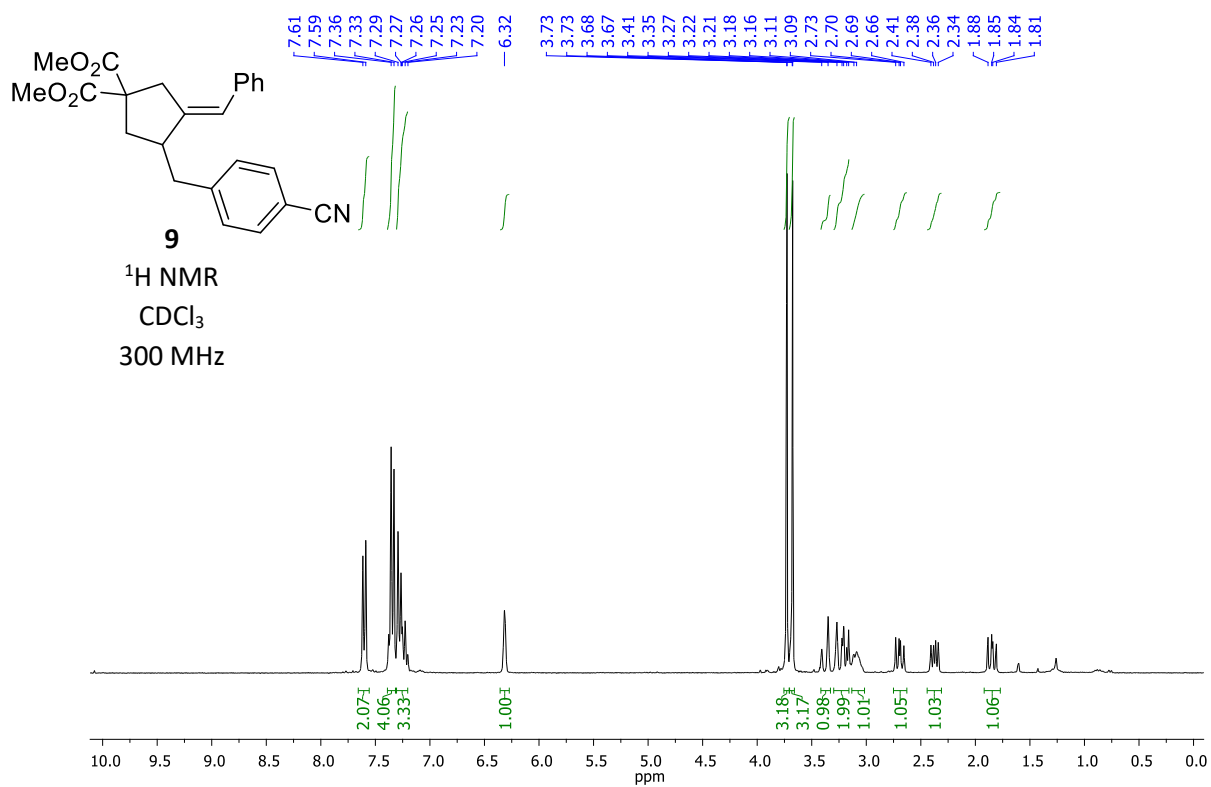
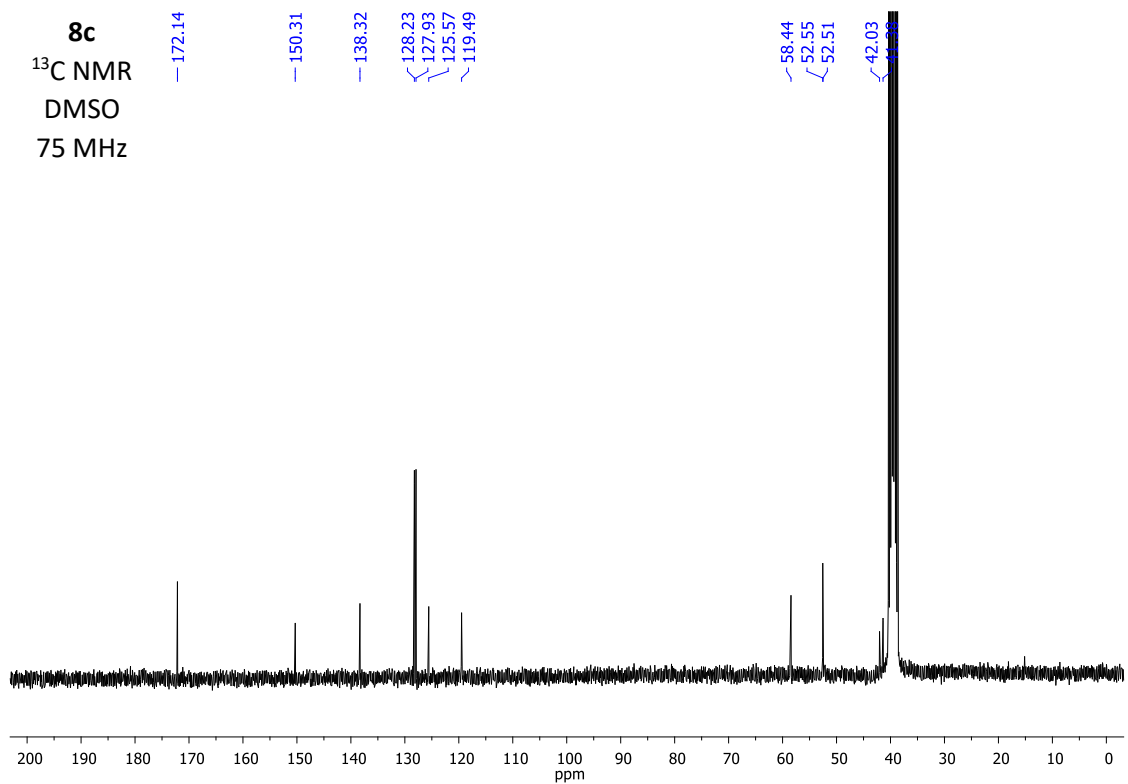


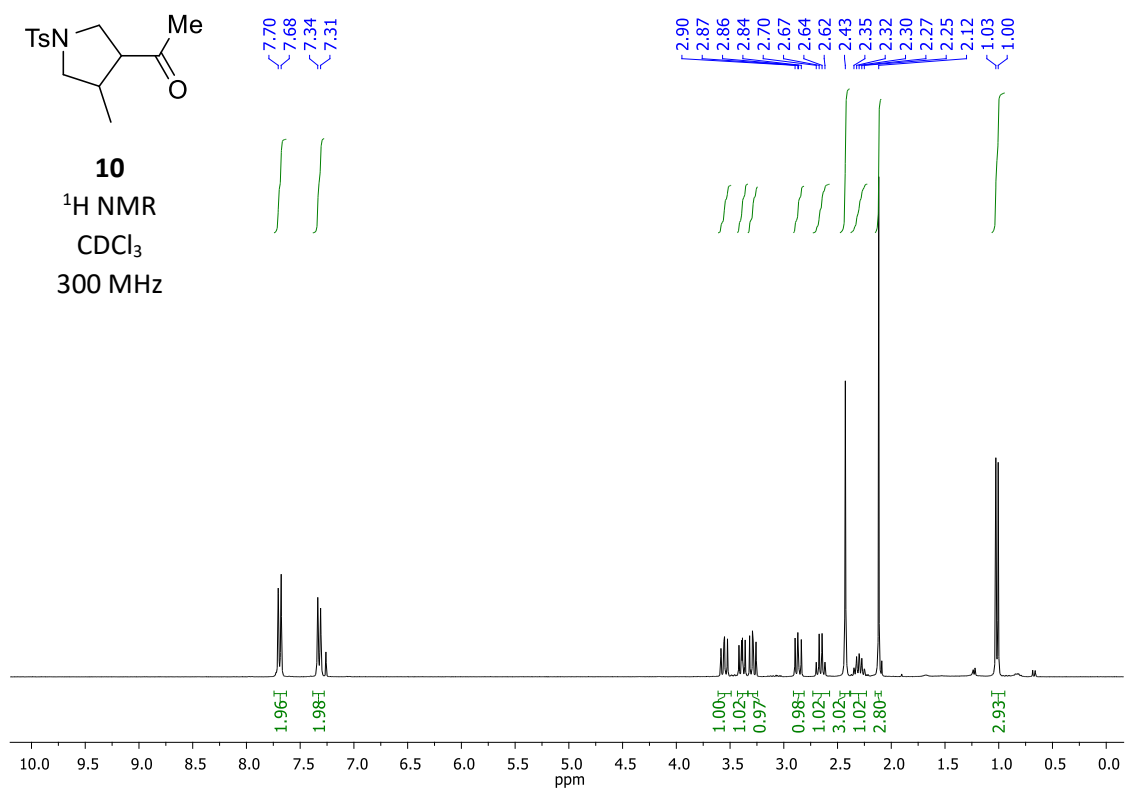
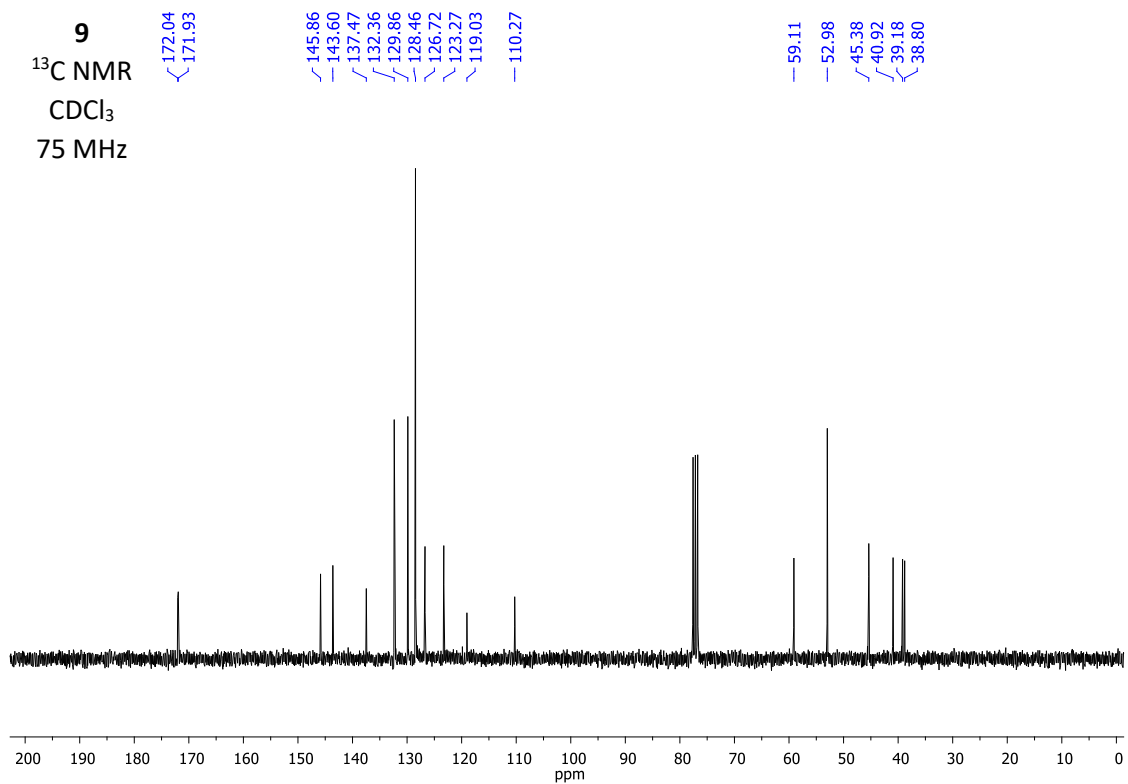


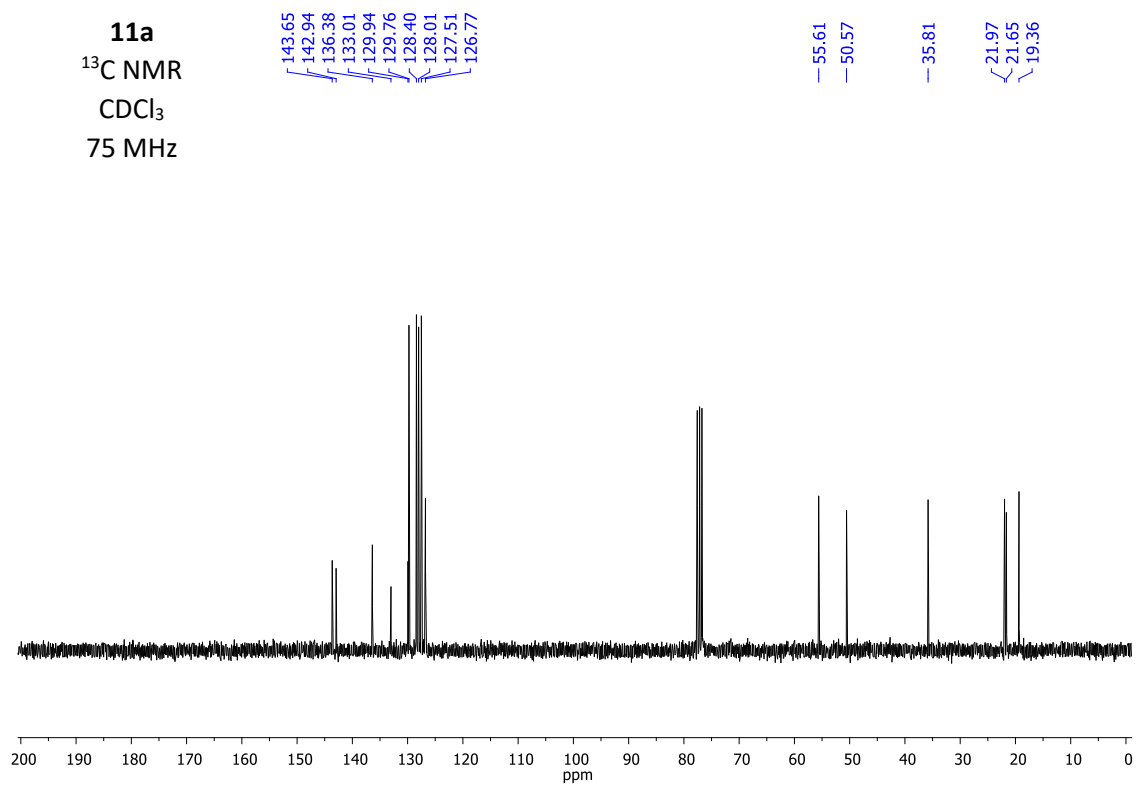
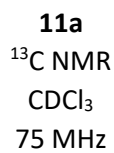
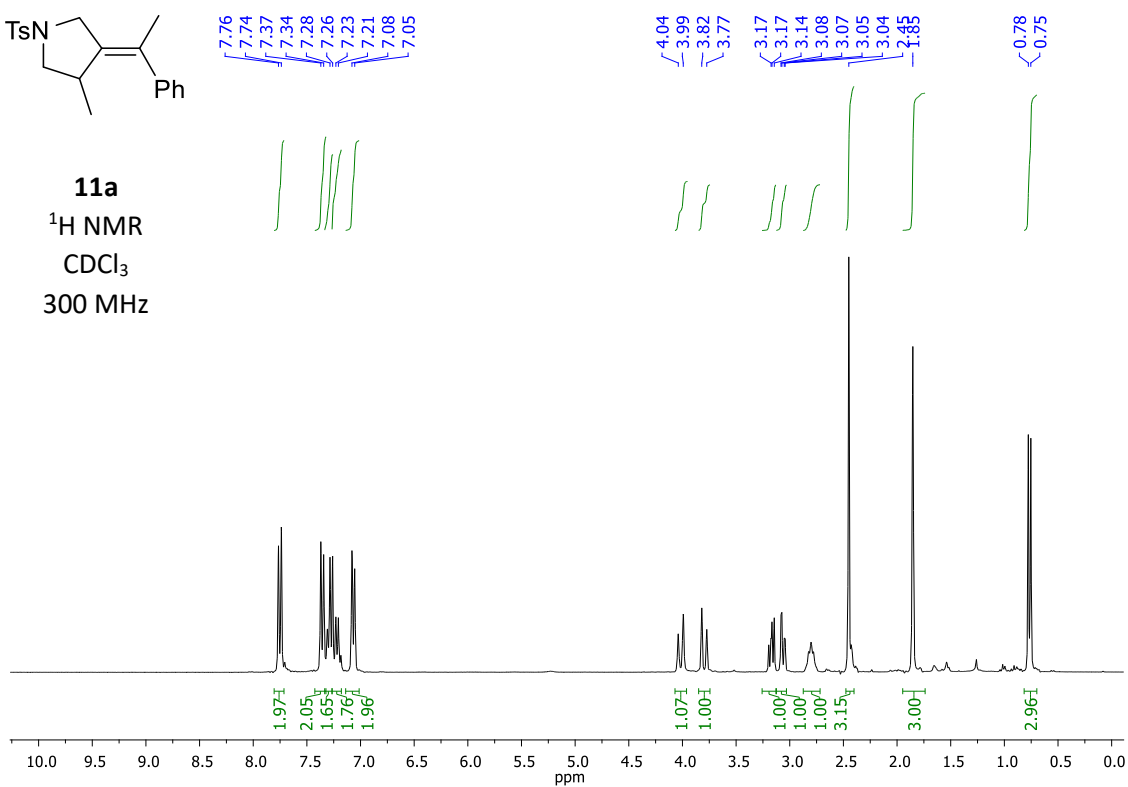
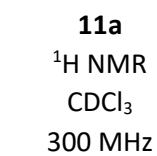


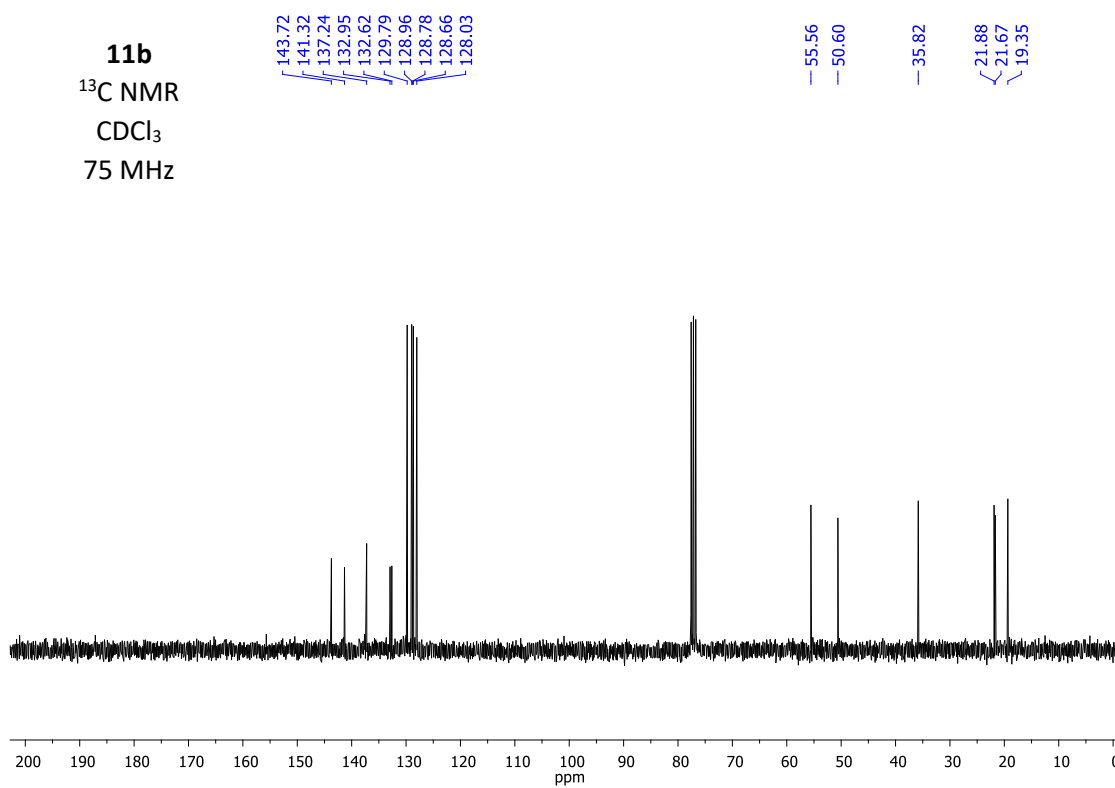
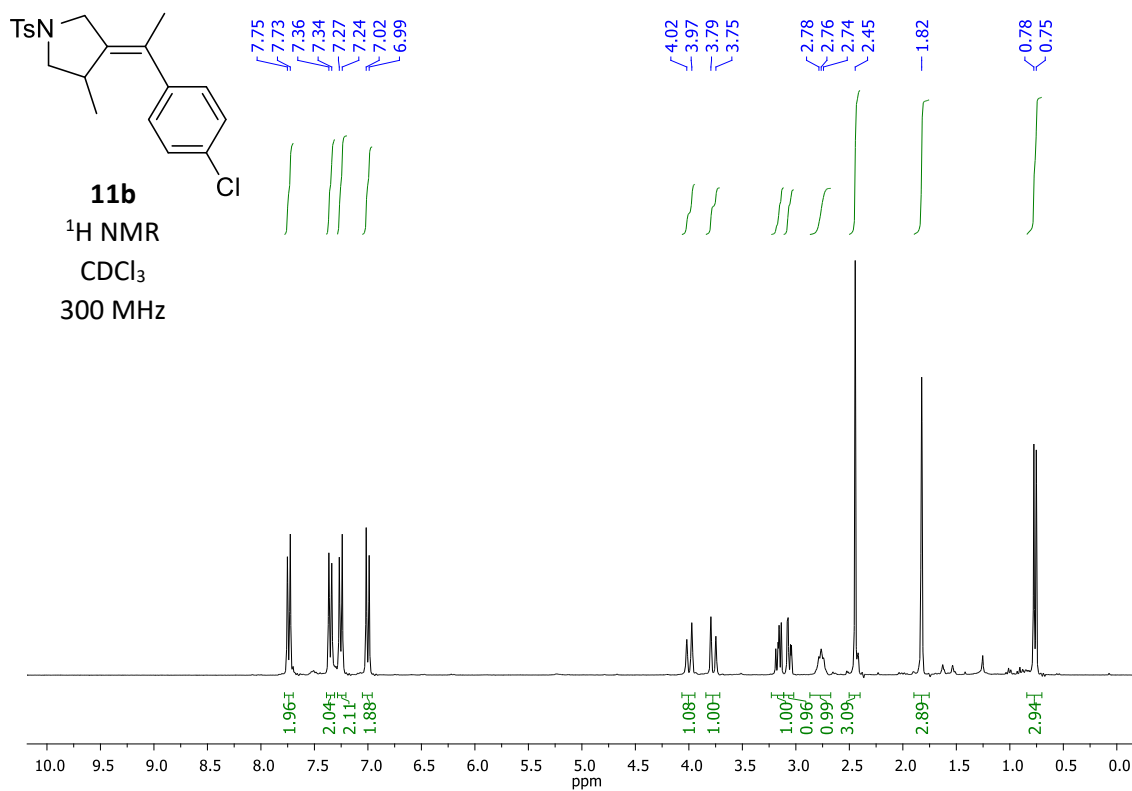


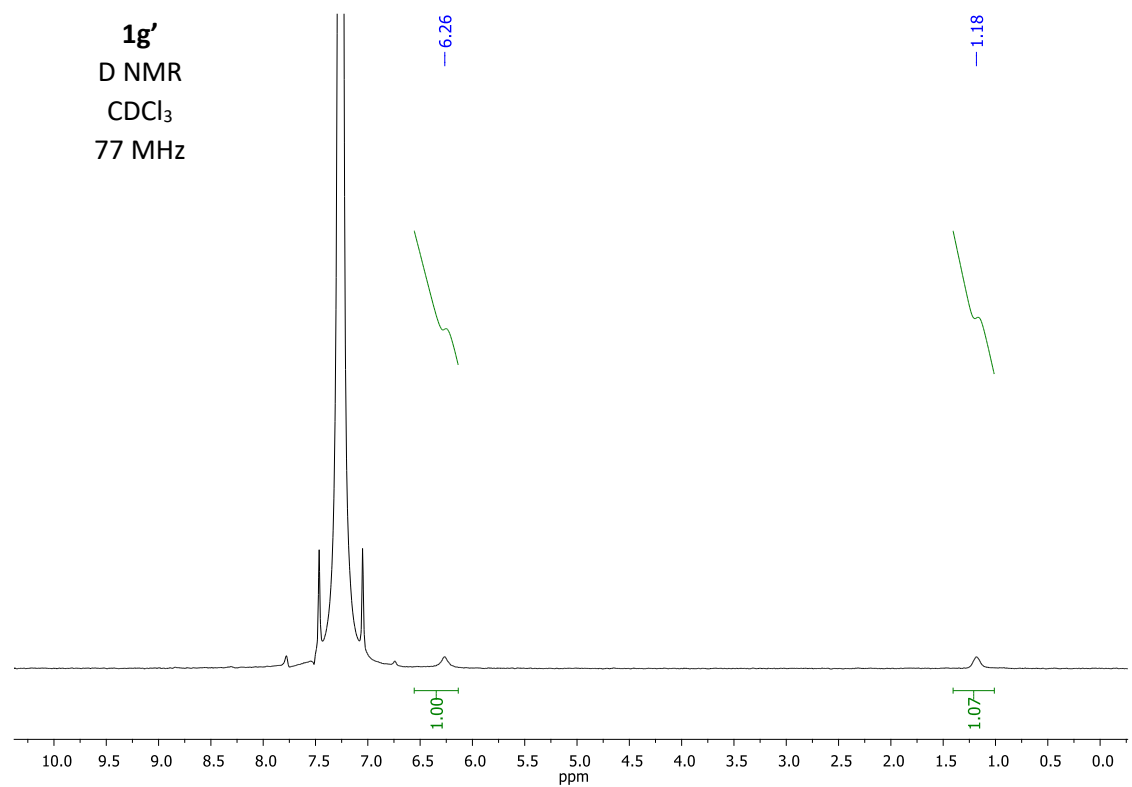
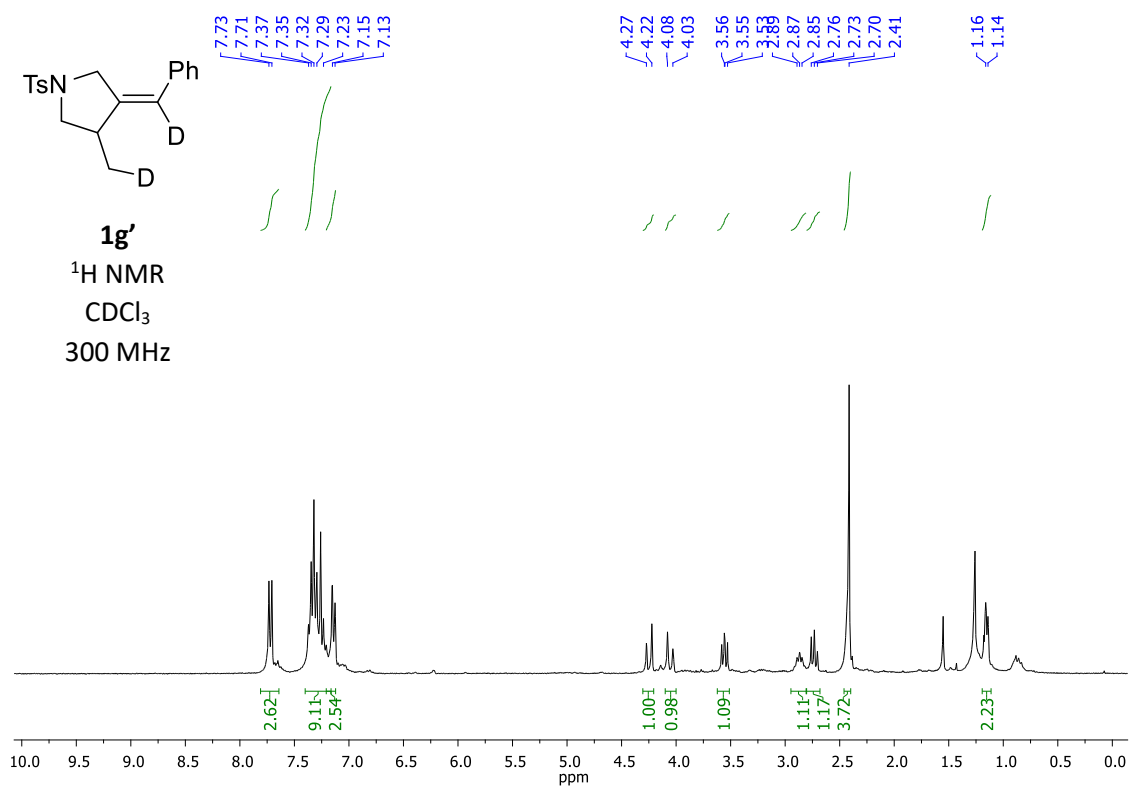




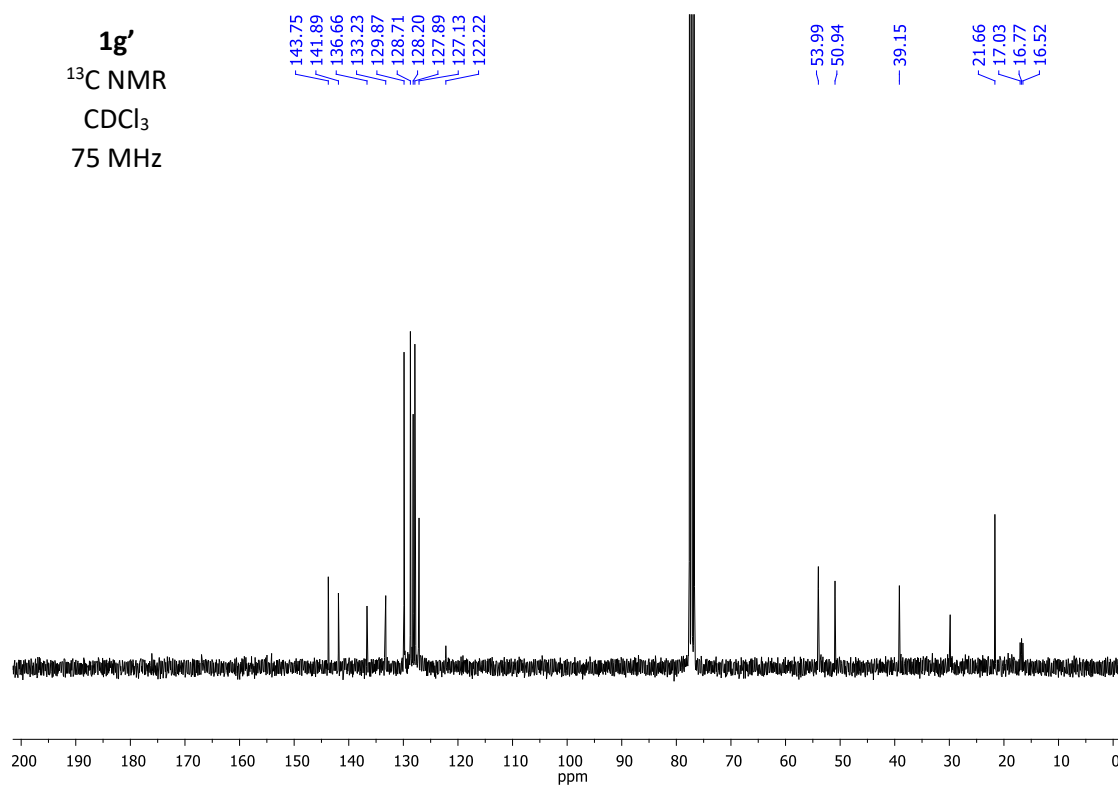








1g'
¹³C NMR
CDCl₃
75 MHz



XIV. X-Ray analysis

Crystal data of alkenylboronate 4i

A clear colourless prismatic-like specimen of $C_{26}H_{34}BNO_4S$, approximate dimensions 0.088 mm x 0.096 mm x 0.139 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 13.57 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 35191 reflections to a maximum θ angle of 25.35° ($0.83 \text{ \AA}$ resolution), of which 4535 were independent (average redundancy 7.760, completeness = 100.0%, $R_{\text{int}} = 13.21\%$, $R_{\text{sig}} = 8.47\%$) and 2886 (63.64%) were greater than $2\sigma(F^2)$. The final cell constants of $a = 6.4192(4) \text{ \AA}$, $b = 32.5924(18) \text{ \AA}$, $c = 11.9890(6) \text{ \AA}$, $\beta = 99.366(4)^\circ$, volume = $2474.9(2) \text{ \AA}^3$, are based upon the refinement of the XYZ-centroids of 1815 reflections above $20 \sigma(I)$ with $4.999^\circ < 2\theta < 40.43^\circ$. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.851. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9780 and 0.9860.

The final anisotropic full-matrix least-squares refinement on F^2 with 305 variables converged at $R1 = 5.14\%$, for the observed data and $wR2 = 12.57\%$ for all data. The goodness-of-fit was 1.005. The largest peak in the final difference electron density synthesis was $0.212 \text{ e}^-/\text{\AA}^3$ and the largest hole was $-0.285 \text{ e}^-/\text{\AA}^3$ with an RMS deviation of $0.056 \text{ e}^-/\text{\AA}^3$. On the basis of the final model, the calculated density was 1.254 g/cm^3 and $F(000)$, 1000 e^- .

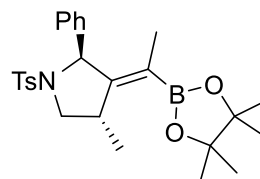
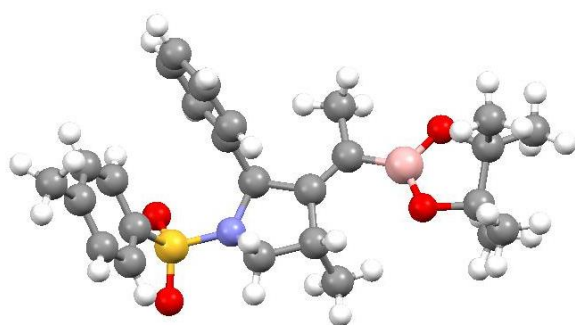


Table 1. Sample and crystal data

Identification code	CCDC 1819416	
Chemical formula	$C_{26}H_{34}BNO_4S$	
Formula weight	467.41 g/mol	
Temperature	200(2) K	
Wavelength	0.71073 $\text{\AA}$	
Crystal size	0.088 x 0.096 x 0.139 mm	
Crystal habit	clear colourless prismatic	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	$a = 6.4192(4) \text{ \AA}$	$\alpha = 90^\circ$
	$b = 32.5924(18) \text{ \AA}$	$\beta = 99.366(4)^\circ$
	$c = 11.9890(6) \text{ \AA}$	$\gamma = 90^\circ$
Volume	$2474.9(2) \text{ \AA}^3$	
Z	4	
Density (calculated)	1.254 g/cm^3	
Absorption coefficient	0.163 mm^{-1}	
$F(000)$	1000	

Table 2. Data collection and structure refinement

Theta range for data collection	1.25 to 25.35°
Index ranges	-7<=h<=7, -39<=k<=39, -12<=l<=14
Reflections collected	35191
Independent reflections	4535 [R(int) = 0.1321]
Coverage of independent reflections	100.0%
Absorption correction	multi-scan
Max. and min. transmission	0.9860 and 0.9780
Refinement method	Full-matrix least-squares on F ²
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\sum w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4535 / 0 / 305
Goodness-of-fit on F ²	1.005
Final R indices	2886 data; I>2σ(I) R1 = 0.0514, wR2 = 0.1000 all data R1 = 0.1042, wR2 = 0.1257
Weighting scheme	w=1/[σ ² (F _o ²)+(0.0360P) ² +1.6820P] where P=(F _o ² +2F _c ²)/3
Largest diff. peak and hole	0.212 and -0.285 eÅ ⁻³
R.M.S. deviation from mean	0.056 eÅ ⁻³

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å²)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x/a	y/b	z/c	U(eq)
B1	0.7624(5)	0.50622(10)	0.2084(3)	0.0257(8)
C1	0.7640(5)	0.29849(8)	0.4246(2)	0.0259(7)
C2	0.8329(5)	0.27589(9)	0.3391(2)	0.0331(8)
C3	0.7040(6)	0.24602(9)	0.2834(3)	0.0400(8)
C4	0.5058(5)	0.23804(10)	0.3108(3)	0.0399(8)
C5	0.4423(5)	0.26053(10)	0.3969(3)	0.0412(8)
C6	0.5691(5)	0.29072(9)	0.4534(3)	0.0343(8)
C7	0.3629(6)	0.20637(12)	0.2467(3)	0.0641(12)
C8	0.6415(4)	0.39762(8)	0.4241(3)	0.0287(7)
C9	0.6707(4)	0.44157(9)	0.3853(2)	0.0260(7)
C10	0.8370(4)	0.43742(8)	0.3085(2)	0.0241(6)
C11	0.9543(4)	0.39650(8)	0.3346(2)	0.0239(7)
C12	0.7469(5)	0.46941(9)	0.4861(2)	0.0351(8)
C13	0.9390(5)	0.36725(8)	0.2349(2)	0.0251(7)
C14	0.7498(5)	0.35963(9)	0.1642(2)	0.0321(7)
C15	0.7394(6)	0.33170(10)	0.0766(3)	0.0457(9)
C16	0.9186(6)	0.31122(10)	0.0577(3)	0.0474(9)
C17	0.1082(6)	0.31855(10)	0.1267(3)	0.0409(9)
C18	0.1176(5)	0.34625(9)	0.2147(3)	0.0329(7)
C19	0.8827(4)	0.46488(9)	0.2336(2)	0.0261(7)

C20	0.0645(5)	0.45855(9)	0.1687(3)	0.0359(8)
C21	0.5767(5)	0.56426(8)	0.2313(2)	0.0275(7)
C22	0.6648(5)	0.56662(9)	0.1186(2)	0.0303(7)
C23	0.3480(5)	0.57679(10)	0.2229(3)	0.0364(8)
C24	0.7142(5)	0.58675(10)	0.3279(3)	0.0398(8)
C25	0.4996(5)	0.55653(10)	0.0166(3)	0.0421(9)
C26	0.7787(5)	0.60631(9)	0.0988(3)	0.0438(9)
N1	0.8544(4)	0.38070(7)	0.42946(19)	0.0251(6)
O1	0.8602(3)	0.34151(6)	0.60467(16)	0.0365(5)
O2	0.1366(3)	0.33083(6)	0.48436(17)	0.0334(5)
O3	0.5982(3)	0.52035(6)	0.25819(16)	0.0290(5)
O4	0.8198(3)	0.53320(6)	0.13159(16)	0.0316(5)
S1	0.92033(12)	0.33797(2)	0.49514(6)	0.0276(2)

Table 4. Bond lengths (Å)

B1-O4	1.367(4)	B1-O3	1.372(4)
B1-C19	1.558(4)	C1-C6	1.374(4)
C1-C2	1.392(4)	C1-S1	1.761(3)
C2-C3	1.378(4)	C2-H2	0.95
C3-C4	1.389(4)	C3-H3	0.95
C4-C5	1.381(4)	C4-C7	1.506(5)
C5-C6	1.382(4)	C5-H5	0.95
C6-H6	0.95	C7-H7A	0.98
C7-H7B	0.98	C7-H7C	0.98
C8-N1	1.465(3)	C8-C9	1.527(4)
C8-H8A	0.99	C8-H8B	0.99
C9-C12	1.526(4)	C9-C10	1.525(4)
C9-H9	1.0	C10-C19	1.334(4)
C10-C11	1.538(4)	C11-N1	1.485(3)
C11-C13	1.520(4)	C11-H11	1.0
C12-H12A	0.98	C12-H12B	0.98
C12-H12C	0.98	C13-C14	1.385(4)
C13-C18	1.390(4)	C14-C15	1.384(4)
C14-H14	0.95	C15-C16	1.380(5)
C15-H15	0.95	C16-C17	1.376(5)
C16-H16	0.95	C17-C18	1.382(4)
C17-H17	0.95	C18-H18	0.95
C19-C20	1.518(4)	C20-H20A	0.98
C20-H20B	0.98	C20-H20C	0.98
C21-O3	1.468(3)	C21-C23	1.511(4)
C21-C24	1.525(4)	C21-C22	1.549(4)
C22-O4	1.467(3)	C22-C25	1.518(4)
C22-C26	1.523(4)	C23-H23A	0.98

C23-H23B	0.98	C23-H23C	0.98
C24-H24A	0.98	C24-H24B	0.98
C24-H24C	0.98	C25-H25A	0.98
C25-H25B	0.98	C25-H25C	0.98
C26-H26A	0.98	C26-H26B	0.98
C26-H26C	0.98	N1-S1	1.622(2)
O1-S1	1.432(2)	O2-S1	1.434(2)

Table 5. Bond angles (°)

O4-B1-O3	112.8(3)	O4-B1-C19	120.5(3)
O3-B1-C19	126.7(3)	C6-C1-C2	119.9(3)
C6-C1-S1	119.0(2)	C2-C1-S1	121.0(2)
C3-C2-C1	119.5(3)	C3-C2-H2	120.2
C1-C2-H2	120.2	C2-C3-C4	121.2(3)
C2-C3-H3	119.4	C4-C3-H3	119.4
C5-C4-C3	118.1(3)	C5-C4-C7	121.1(3)
C3-C4-C7	120.8(3)	C4-C5-C6	121.5(3)
C4-C5-H5	119.2	C6-C5-H5	119.2
C1-C6-C5	119.7(3)	C1-C6-H6	120.1
C5-C6-H6	120.1	C4-C7-H7A	109.5
C4-C7-H7B	109.5	H7A-C7-H7B	109.5
C4-C7-H7C	109.5	H7A-C7-H7C	109.5
H7B-C7-H7C	109.5	N1-C8-C9	101.9(2)
N1-C8-H8A	111.4	C9-C8-H8A	111.4
N1-C8-H8B	111.4	C9-C8-H8B	111.4
H8A-C8-H8B	109.3	C12-C9-C10	111.4(2)
C12-C9-C8	110.8(2)	C10-C9-C8	103.5(2)
C12-C9-H9	110.3	C10-C9-H9	110.3
C8-C9-H9	110.3	C19-C10-C9	126.8(3)
C19-C10-C11	124.4(2)	C9-C10-C11	108.7(2)
N1-C11-C13	113.8(2)	N1-C11-C10	101.4(2)
C13-C11-C10	114.6(2)	N1-C11-H11	108.9
C13-C11-H11	108.9	C10-C11-H11	108.9
C9-C12-H12A	109.5	C9-C12-H12B	109.5
H12A-C12-H12B	109.5	C9-C12-H12C	109.5
H12A-C12-H12C	109.5	H12B-C12-H12C	109.5
C14-C13-C18	118.1(3)	C14-C13-C11	122.1(3)
C18-C13-C11	119.7(3)	C15-C14-C13	120.7(3)
C15-C14-H14	119.6	C13-C14-H14	119.6
C16-C15-C14	120.3(3)	C16-C15-H15	119.8
C14-C15-H15	119.8	C17-C16-C15	119.7(3)
C17-C16-H16	120.1	C15-C16-H16	120.1
C16-C17-C18	119.8(3)	C16-C17-H17	120.1

C18-C17-H17	120.1	C17-C18-C13	121.3(3)
C17-C18-H18	119.3	C13-C18-H18	119.3
C10-C19-C20	121.7(3)	C10-C19-B1	123.7(3)
C20-C19-B1	114.6(2)	C19-C20-H20A	109.5
C19-C20-H20B	109.5	H20A-C20-H20B	109.5
C19-C20-H20C	109.5	H20A-C20-H20C	109.5
H20B-C20-H20C	109.5	O3-C21-C23	109.5(2)
O3-C21-C24	106.2(2)	C23-C21-C24	110.9(2)
O3-C21-C22	101.9(2)	C23-C21-C22	114.6(2)
C24-C21-C22	113.0(3)	O4-C22-C25	107.3(2)
O4-C22-C26	108.2(2)	C25-C22-C26	110.4(3)
O4-C22-C21	102.0(2)	C25-C22-C21	112.7(3)
C26-C22-C21	115.5(3)	C21-C23-H23A	109.5
C21-C23-H23B	109.5	H23A-C23-H23B	109.5
C21-C23-H23C	109.5	H23A-C23-H23C	109.5
H23B-C23-H23C	109.5	C21-C24-H24A	109.5
C21-C24-H24B	109.5	H24A-C24-H24B	109.5
C21-C24-H24C	109.5	H24A-C24-H24C	109.5
H24B-C24-H24C	109.5	C22-C25-H25A	109.5
C22-C25-H25B	109.5	H25A-C25-H25B	109.5
C22-C25-H25C	109.5	H25A-C25-H25C	109.5
H25B-C25-H25C	109.5	C22-C26-H26A	109.5
C22-C26-H26B	109.5	H26A-C26-H26B	109.5
C22-C26-H26C	109.5	H26A-C26-H26C	109.5
H26B-C26-H26C	109.5	C8-N1-C11	110.6(2)
C8-N1-S1	120.82(18)	C11-N1-S1	123.92(18)
B1-O3-C21	106.4(2)	B1-O4-C22	107.3(2)
O1-S1-O2	120.34(13)	O1-S1-N1	106.74(12)
O2-S1-N1	106.01(12)	O1-S1-C1	106.33(13)
O2-S1-C1	108.81(13)	N1-S1-C1	108.12(13)

Table 6. Torsion angles (°)

C6-C1-C2-C3	0.5(4)	S1-C1-C2-C3	-178.1(2)
C1-C2-C3-C4	0.1(5)	C2-C3-C4-C5	-0.9(5)
C2-C3-C4-C7	177.8(3)	C3-C4-C5-C6	1.2(5)
C7-C4-C5-C6	-177.6(3)	C2-C1-C6-C5	-0.2(4)
S1-C1-C6-C5	178.4(2)	C4-C5-C6-C1	-0.6(5)
N1-C8-C9-C12	-86.2(3)	N1-C8-C9-C10	33.3(3)
C12-C9-C10-C19	-77.4(4)	C8-C9-C10-C19	163.4(3)
C12-C9-C10-C11	100.0(3)	C8-C9-C10-C11	-19.1(3)
C19-C10-C11-N1	174.8(3)	C9-C10-C11-N1	-2.8(3)
C19-C10-C11-C13	-62.1(4)	C9-C10-C11-C13	120.4(2)
N1-C11-C13-C14	70.9(3)	C10-C11-C13-C14	-45.3(4)

N1-C11-C13-C18	-107.1(3)	C10-C11-C13-C18	136.8(3)
C18-C13-C14-C15	0.4(4)	C11-C13-C14-C15	-177.6(3)
C13-C14-C15-C16	-0.6(5)	C14-C15-C16-C17	0.3(5)
C15-C16-C17-C18	0.2(5)	C16-C17-C18-C13	-0.4(5)
C14-C13-C18-C17	0.1(4)	C11-C13-C18-C17	178.1(3)
C9-C10-C19-C20	175.0(3)	C11-C10-C19-C20	-2.1(4)
C9-C10-C19-B1	-2.8(5)	C11-C10-C19-B1	-179.9(3)
O4-B1-C19-C10	179.1(3)	O3-B1-C19-C10	0.6(5)
O4-B1-C19-C20	1.2(4)	O3-B1-C19-C20	-177.3(3)
O3-C21-C22-O4	-30.1(3)	C23-C21-C22-O4	-148.3(2)
C24-C21-C22-O4	83.4(3)	O3-C21-C22-C25	84.6(3)
C23-C21-C22-C25	-33.5(3)	C24-C21-C22-C25	-161.9(2)
O3-C21-C22-C26	-147.2(2)	C23-C21-C22-C26	94.6(3)
C24-C21-C22-C26	-33.7(4)	C9-C8-N1-C11	-38.1(3)
C9-C8-N1-S1	165.19(18)	C13-C11-N1-C8	-98.0(3)
C10-C11-N1-C8	25.6(3)	C13-C11-N1-S1	57.9(3)
C10-C11-N1-S1	-178.49(18)	O4-B1-O3-C21	-13.8(3)
C19-B1-O3-C21	164.8(3)	C23-C21-O3-B1	148.8(2)
C24-C21-O3-B1	-91.4(3)	C22-C21-O3-B1	27.1(3)
O3-B1-O4-C22	-7.0(3)	C19-B1-O4-C22	174.3(3)
C25-C22-O4-B1	-95.4(3)	C26-C22-O4-B1	145.5(3)
C21-C22-O4-B1	23.2(3)	C8-N1-S1-O1	-50.2(2)
C11-N1-S1-O1	156.3(2)	C8-N1-S1-O2	-179.6(2)
C11-N1-S1-O2	26.9(2)	C8-N1-S1-C1	63.9(2)
C11-N1-S1-C1	-89.7(2)	C6-C1-S1-O1	27.6(3)
C2-C1-S1-O1	-153.9(2)	C6-C1-S1-O2	158.6(2)
C2-C1-S1-O2	-22.9(3)	C6-C1-S1-N1	-86.7(2)
C2-C1-S1-N1	91.8(2)		

Table 7. Anisotropic atomic displacement parameters (Å²)

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
B1	0.0275(19)	0.0239(18)	0.0243(18)	-0.0005(15)	0.0003(15)	-0.0002(15)
C1	0.0343(18)	0.0150(15)	0.0267(17)	0.0048(13)	-0.0003(14)	0.0008(13)
C2	0.048(2)	0.0211(16)	0.0312(18)	0.0029(14)	0.0102(15)	0.0012(14)
C3	0.068(2)	0.0239(17)	0.0286(18)	-0.0044(14)	0.0098(17)	-0.0040(17)
C4	0.055(2)	0.0272(18)	0.0340(19)	0.0034(15)	-0.0029(16)	-0.0097(16)
C5	0.0358(19)	0.0359(19)	0.050(2)	0.0026(17)	0.0021(16)	-0.0051(16)
C6	0.0370(19)	0.0295(17)	0.0358(19)	-0.0026(15)	0.0046(15)	0.0022(14)
C7	0.080(3)	0.048(2)	0.060(3)	-0.001(2)	0.000(2)	-0.027(2)
C8	0.0283(17)	0.0257(16)	0.0332(18)	-0.0012(14)	0.0083(14)	-0.0003(13)
C9	0.0242(16)	0.0246(16)	0.0292(16)	0.0012(13)	0.0044(13)	0.0019(13)

C10	0.0276(16)	0.0201(15)	0.0233(15)	-0.0028(13)	0.0004(13)	-0.0013(12)
C11	0.0233(16)	0.0216(15)	0.0267(16)	0.0021(13)	0.0037(12)	-0.0002(12)
C12	0.047(2)	0.0266(17)	0.0322(18)	0.0018(14)	0.0064(15)	0.0048(15)
C13	0.0347(18)	0.0170(15)	0.0239(16)	0.0041(12)	0.0054(13)	0.0003(13)
C14	0.0396(19)	0.0226(16)	0.0311(17)	0.0008(14)	-0.0031(14)	0.0024(14)
C15	0.065(2)	0.0308(19)	0.036(2)	-0.0017(16)	-0.0081(17)	-0.0009(18)
C16	0.081(3)	0.0286(19)	0.033(2)	-0.0083(16)	0.012(2)	0.0004(19)
C17	0.058(2)	0.0276(18)	0.041(2)	-0.0026(16)	0.0208(19)	0.0035(16)
C18	0.0396(19)	0.0254(17)	0.0351(18)	0.0020(14)	0.0107(15)	-0.0017(14)
C19	0.0278(16)	0.0229(16)	0.0275(16)	-0.0011(13)	0.0041(13)	0.0027(13)
C20	0.0376(19)	0.0279(17)	0.045(2)	0.0059(15)	0.0152(16)	0.0045(14)
C21	0.0334(17)	0.0183(15)	0.0295(17)	0.0030(13)	0.0008(14)	0.0055(13)
C22	0.0373(18)	0.0201(15)	0.0342(18)	0.0047(14)	0.0083(15)	0.0096(13)
C23	0.0371(19)	0.0348(19)	0.0375(19)	0.0041(15)	0.0068(15)	0.0093(15)
C24	0.047(2)	0.0290(18)	0.040(2)	-0.0046(16)	-0.0041(16)	0.0039(15)
C25	0.056(2)	0.038(2)	0.0296(18)	0.0034(15)	0.0000(16)	0.0097(17)
C26	0.052(2)	0.0274(18)	0.055(2)	0.0139(16)	0.0176(18)	0.0057(16)
N1	0.0300(14)	0.0185(13)	0.0270(13)	0.0030(11)	0.0050(11)	0.0041(10)
O1	0.0563(14)	0.0332(12)	0.0200(11)	0.0002(9)	0.0059(10)	-0.0002(11)
O2	0.0310(12)	0.0311(12)	0.0361(12)	0.0021(10)	-0.0010(9)	0.0059(9)
O3	0.0342(12)	0.0201(11)	0.0336(12)	0.0040(9)	0.0078(10)	0.0052(9)
O4	0.0390(12)	0.0234(11)	0.0346(12)	0.0064(9)	0.0129(10)	0.0079(9)
S1	0.0353(4)	0.0219(4)	0.0240(4)	0.0012(3)	0.0001(3)	0.0017(3)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å²)

Atom	x/a	y/b	z/c	U(eq)
H2	0.9680	0.2810	0.3193	0.04
H3	0.7515	0.2306	0.2251	0.048
H5	0.3084	0.2551	0.4177	0.049
H6	0.5217	0.3060	0.5119	0.041
H7A	0.2552	0.1981	0.2915	0.096
H7B	0.4463	0.1823	0.2322	0.096
H7C	0.2943	0.2180	0.1746	0.096
H8A	0.5959	0.3970	0.4991	0.034
H8B	0.5375	0.3826	0.3690	0.034
H9	0.5356	0.4522	0.3416	0.031
H11	1.1066	0.4023	0.3632	0.029
H12A	0.8741	0.4576	0.5310	0.053
H12B	0.6361	0.4718	0.5331	0.053
H12C	0.7796	0.4966	0.4589	0.053
H14	0.6258	0.3737	0.1761	0.039
H15	0.6084	0.3266	0.0292	0.055
H16	0.9112	0.2921	-0.0027	0.057

H17	1.2321	0.3046	0.1139	0.049
H18	1.2487	0.3510	0.2623	0.039
H20A	1.1345	0.4324	0.1912	0.054
H20B	1.1660	0.4811	0.1856	0.054
H20C	1.0103	0.4581	0.0874	0.054
H23A	0.2594	0.5583	0.1707	0.055
H23B	0.3304	0.6050	0.1947	0.055
H23C	0.3060	0.5751	0.2978	0.055
H24A	0.6730	0.5786	0.4000	0.06
H24B	0.6952	0.6164	0.3176	0.06
H24C	0.8627	0.5797	0.3284	0.06
H25A	0.5687	0.5522	-0.0495	0.063
H25B	0.3992	0.5793	0.0019	0.063
H25C	0.4241	0.5315	0.0317	0.063
H26A	0.8944	0.6109	0.1617	0.066
H26B	0.6792	0.6293	0.0940	0.066
H26C	0.8358	0.6043	0.0281	0.066

Table 9. Hydrogen bond distances (Å) and angles (°)

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
C6-H6...O2	0.95	2.57	3.145(4)	119.2

XV. Computational results

Computational methods

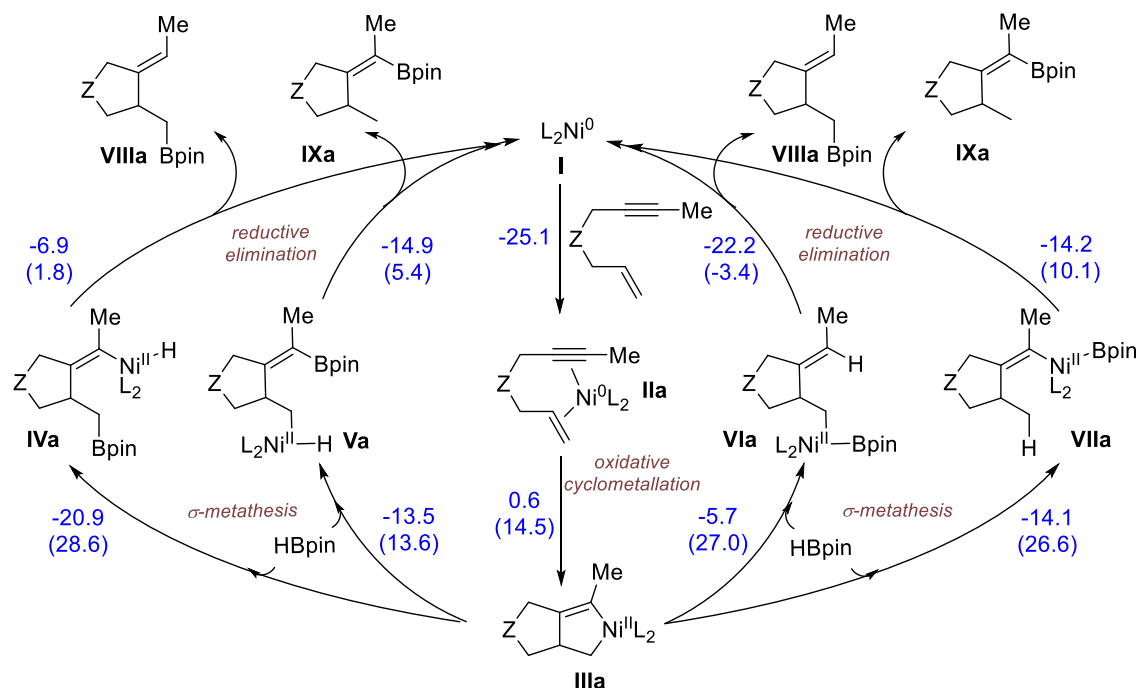
Calculations were performed with Gaussian 09 at DFT level.⁴⁵ The geometries of all complexes here reported were optimized using the M06-2X hybrid functional⁴⁶ that accounts for dispersive interactions. Optimizations were carried out using the standard 6-31G(d) basis set for C, H, N, O, B and P. The LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split-valence (double- ζ) basis set, was used for Ni.⁴⁷ Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE). Gibbs free energy has been used throughout the schemes. The starting approximate geometries for the transition states (TS) were graphically located. Intrinsic reaction coordinate (IRC) studies were performed to confirm the relation of the transition states with the corresponding minima. Solvent effects were considered by performing optimizations in Toluene using the polarized continuum model (PCM).

⁴⁵ Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

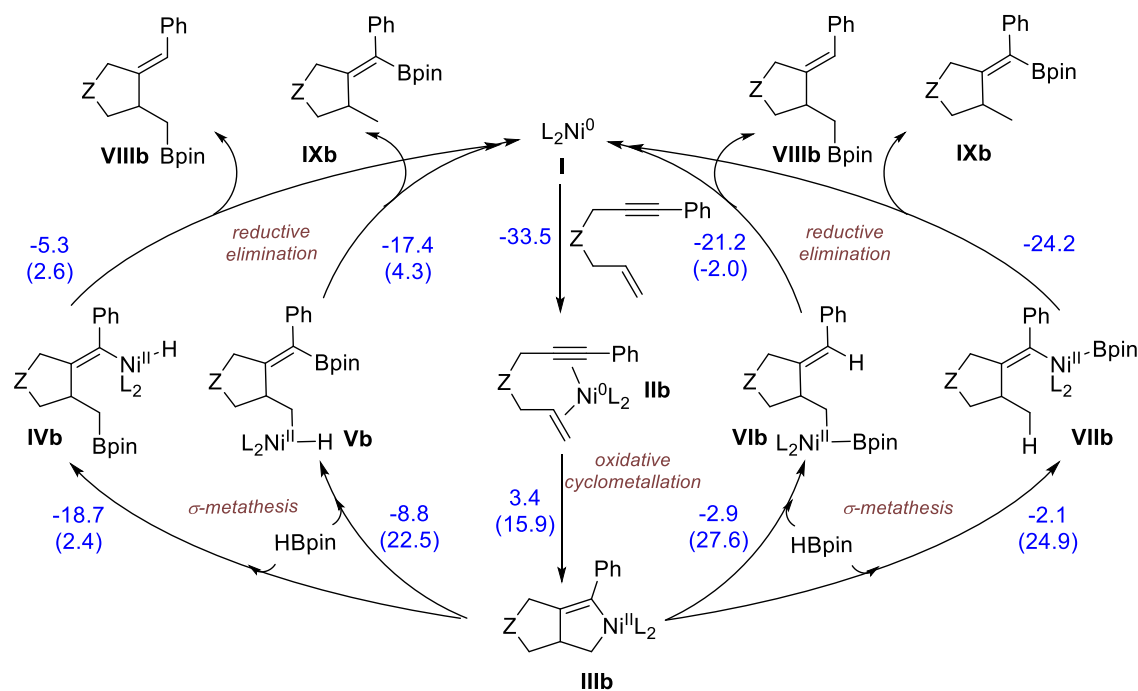
⁴⁶ Y. Zhao, D.G. Truhlar, *Theor Chem Account.* **2006**, 120: 215–241.

⁴⁷ (a) A. D. Becke, *J. Chem. Phys.* **1993**, 98, 5648- 5653. (b) A. D. Becke, *Phys. Rev. A* **1988**, 38, 3098-3100. (c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, 37, 785-789.

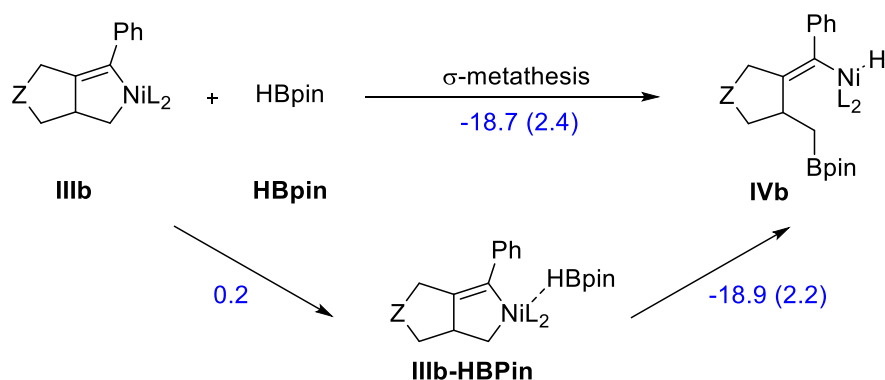
Computed feasible reaction pathways



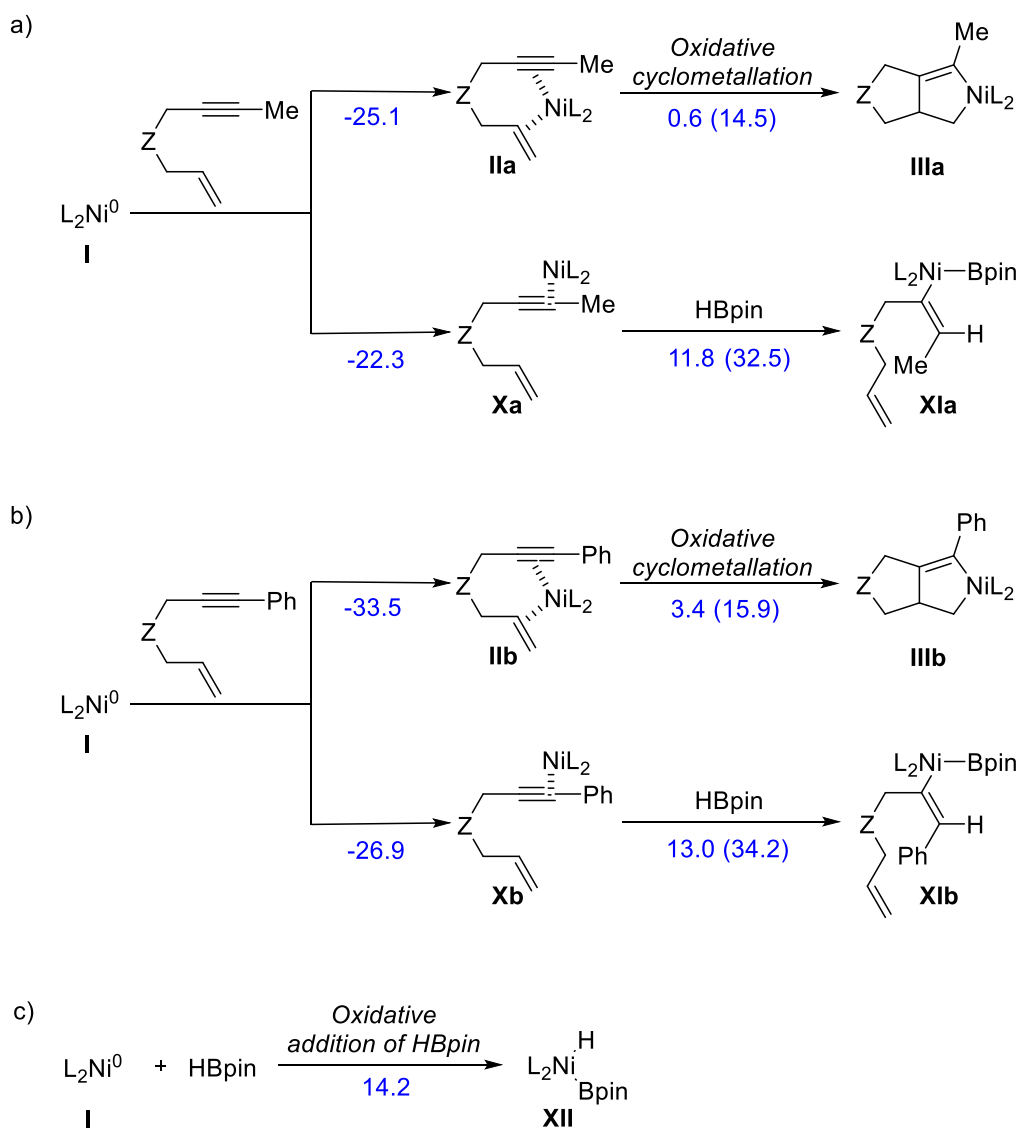
Supplementary Scheme 1. Computed feasible reaction pathways for enyne I. ΔG (kcal mol⁻¹) are calculated in toluene (PCM) at 6-31G(d) (C,H,N,P,O,B), LANL2DZ (Ni) level. Calculated activation energies in toluene are shown in brackets. Z= NMe, L₂=Xantphos.



Supplementary Scheme 2. Computed feasible reaction pathways for enyne I'. ΔG (kcal mol⁻¹) are calculated in toluene (PCM) at 6-31G(d) (C,H,N,P,O,B), LANL2DZ (Ni) level. Calculated activation energies in toluene are shown in brackets. Z= NMe, L₂=Xantphos.

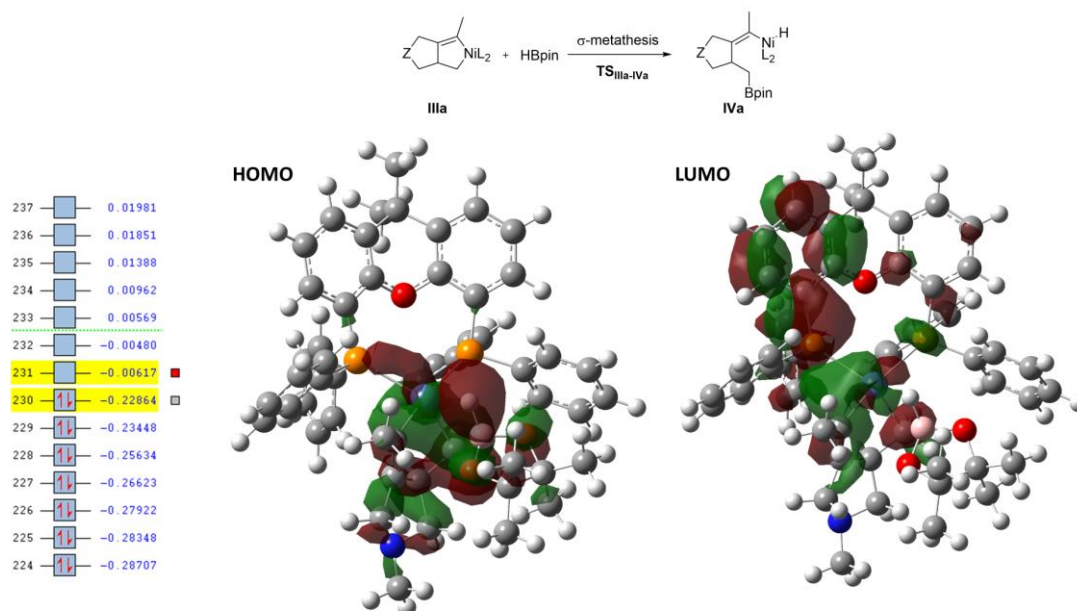


Supplementary Scheme 3. Computed association complex between **IIIb** and HBpin. ΔG (kcal mol⁻¹) are calculated in toluene (PCM) at 6-31G(d) (C,H,N,P,O,B), LANL2DZ (Ni) level. Calculated activation energies in toluene are shown in brackets. Z= NMe, L₂=Xantphos.

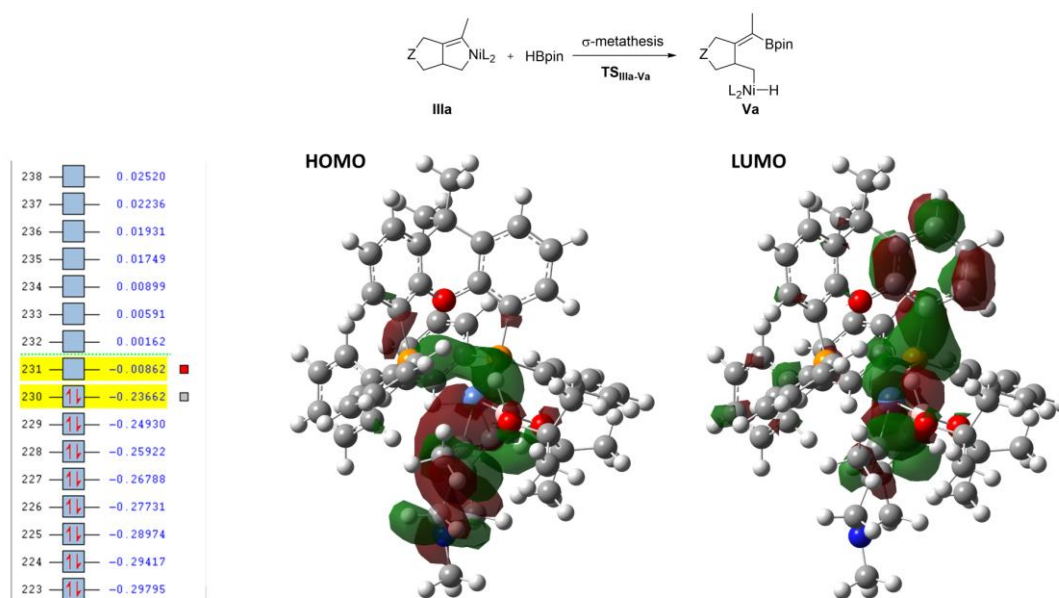


Supplementary Scheme 4. Computed alternative disregarded reaction pathways. ΔG (kcal mol⁻¹) are calculated in toluene (PCM) at 6-31G(d) (C,H,N,P,O,B), LANL2DZ (Ni) level. Calculated activation energies in toluene are shown in brackets. Z= NMe, L₂=Xantphos.

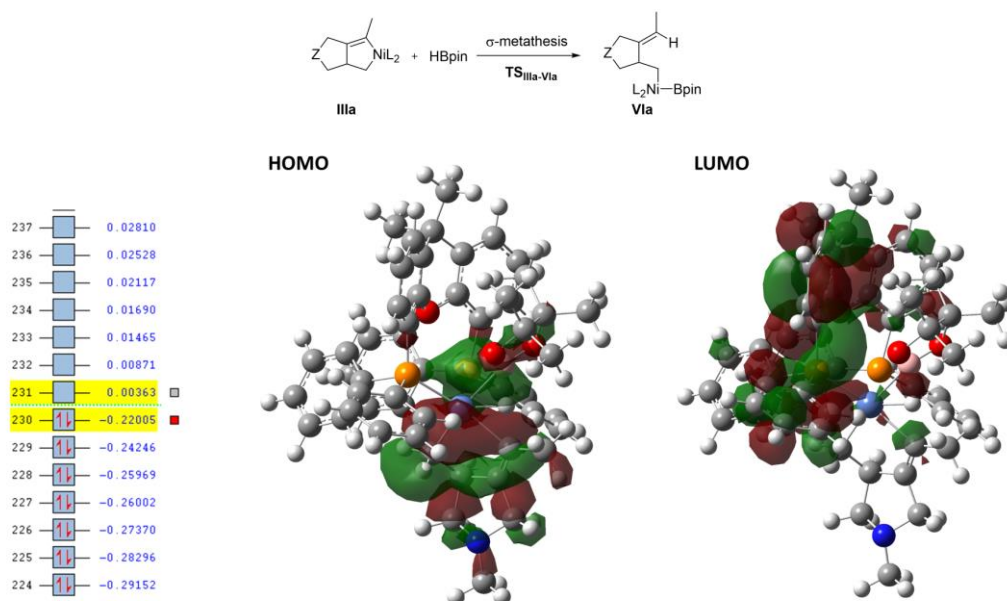
Frontier Orbitals for the σ -metathesis step transition states



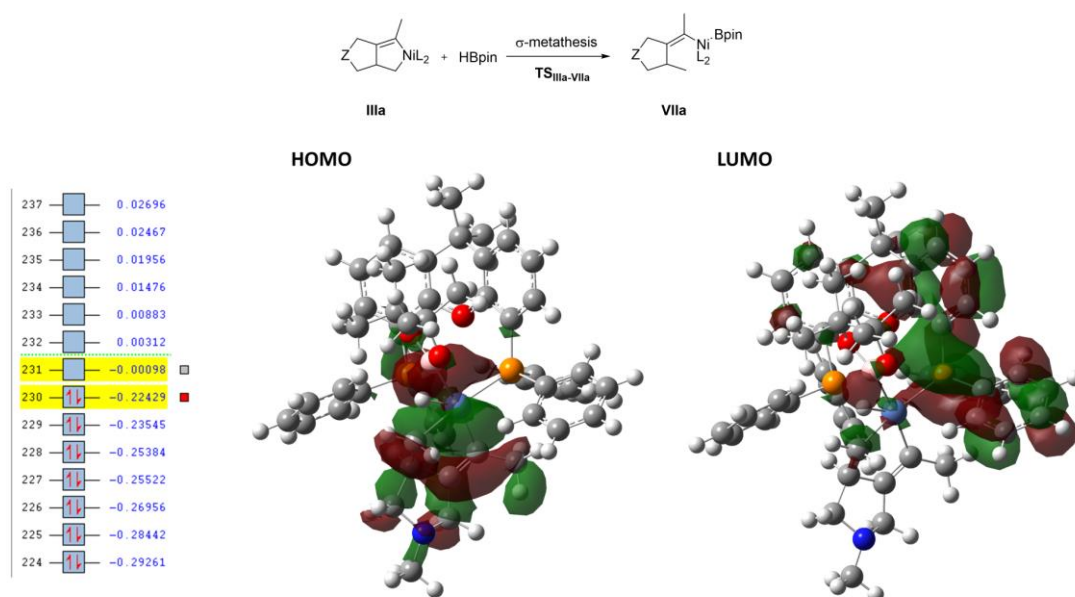
Supplementary Scheme 5. Frontier orbitals for TS_{IIIa-IVa}



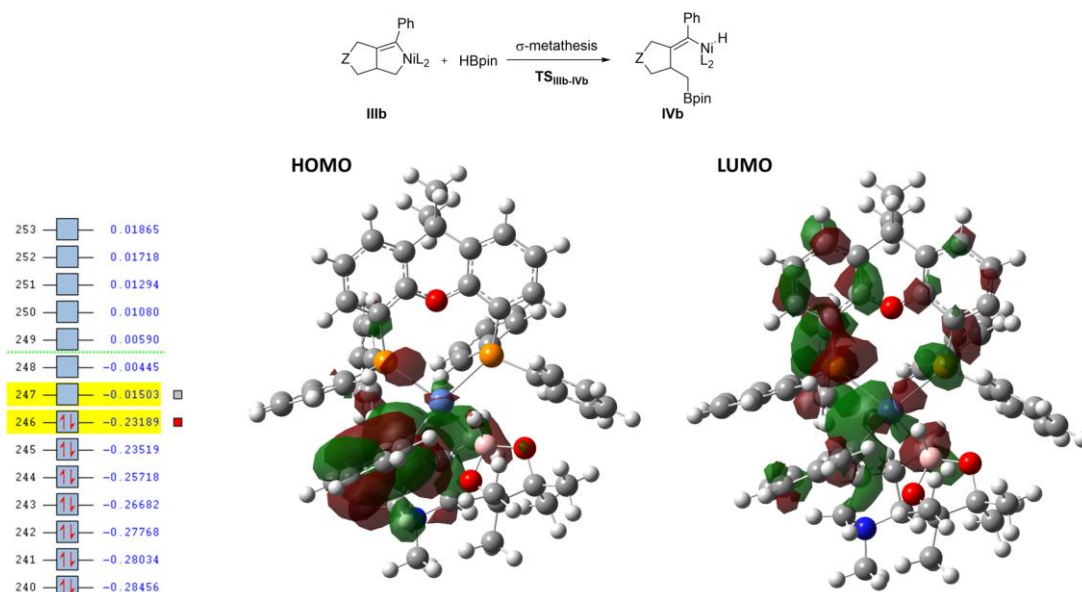
Supplementary Scheme 6. Frontier orbitals for TS_{IIIa-Va}



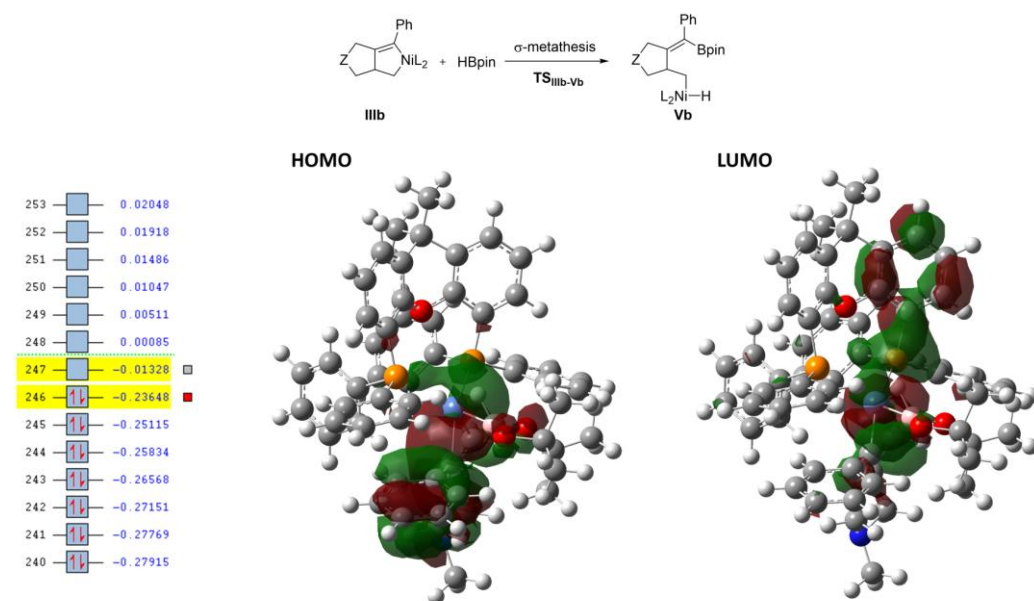
Supplementary Scheme 7. Frontier orbitals for **TS_{IIIa-VIa}**



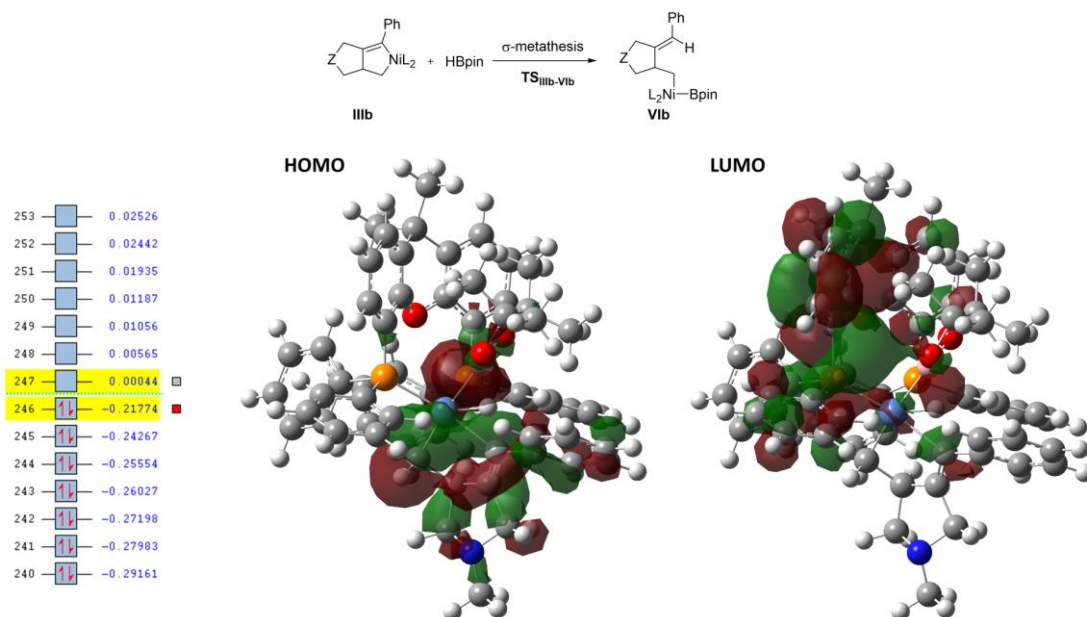
Supplementary Scheme 8. Frontier orbitals for **TS_{IIIa-VIIa}**



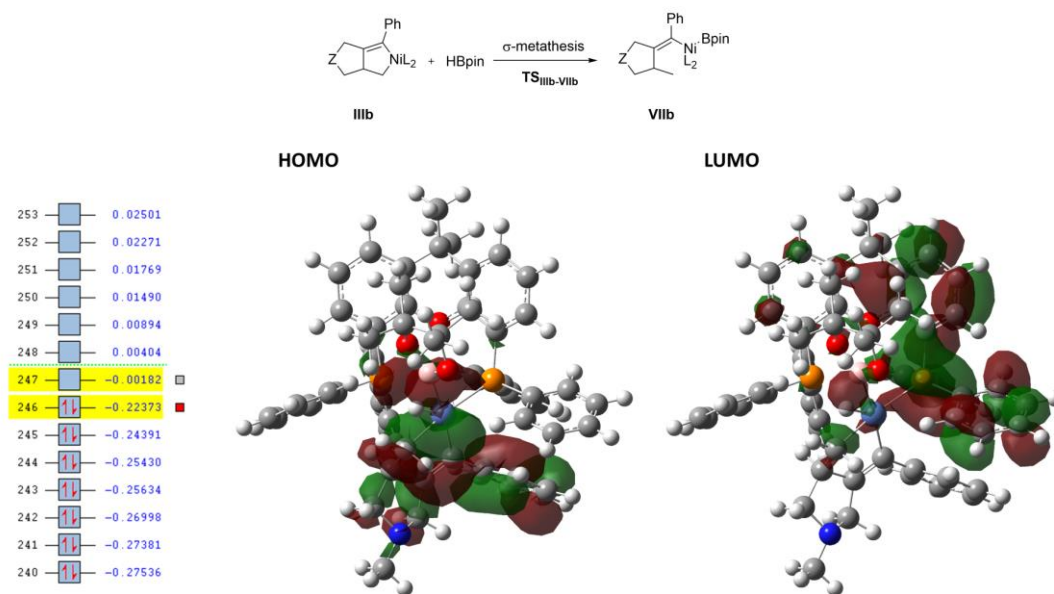
Supplementary Scheme 9. Frontier orbitals for TS_{IIIb-IVb}



Supplementary Scheme 10. Frontier orbitals for TS_{IIIb-Vb}



Supplementary Scheme 11. Frontier orbitals for $TS_{IIIb-VIb}$



Supplementary Scheme 12. Frontier orbitals for $TS_{IIIb-VIIb}$

Atomic coordinates and energies for the stationary points**I - L₂Ni⁰**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	4.255737	3.923287	-0.722320
2	6	0	3.346322	3.376483	-0.495288
3	6	0	1.039047	1.990060	0.065806
4	6	0	2.207467	4.066099	-0.087140
5	6	0	3.325790	1.990222	-0.617144
6	6	0	2.162740	1.262951	-0.343574
7	6	0	1.032385	3.378642	0.211441
8	1	0	2.240778	5.146966	0.000508
9	1	0	4.218457	1.468928	-0.946796
10	6	0	-0.247045	4.019522	0.740593
11	8	0	-0.111492	1.283846	0.342030
12	6	0	-0.306190	3.787036	2.267975
13	1	0	0.546703	4.271271	2.755087
14	1	0	-0.281331	2.718189	2.503518
15	1	0	-1.231703	4.208002	2.674843
16	6	0	-0.298173	5.521064	0.464187
17	1	0	-0.254745	5.735571	-0.608394
18	1	0	0.535137	6.029096	0.957462
19	1	0	-1.217180	5.952500	0.870599
20	6	0	-1.417282	3.274613	0.106739
21	6	0	-3.514993	1.682026	-0.870095
22	6	0	-2.621808	3.854042	-0.292067
23	6	0	-1.293036	1.891987	-0.022717
24	6	0	-2.315965	1.067274	-0.500972
25	6	0	-3.661593	3.064225	-0.776048
26	1	0	-2.757246	4.928226	-0.220771
27	1	0	-4.595152	3.528324	-1.077756
28	1	0	-4.334860	1.076722	-1.244694

29	15	0	1.995942	-0.558454	-0.631711
30	15	0	-1.955576	-0.735740	-0.667505
31	6	0	-3.597188	-1.368186	-1.213096
32	6	0	-6.055040	-2.265504	-2.207502
33	6	0	-3.763644	-1.613704	-2.579672
34	6	0	-4.673742	-1.585402	-0.346584
35	6	0	-5.895307	-2.034093	-0.841890
36	6	0	-4.988260	-2.053465	-3.077333
37	1	0	-2.922641	-1.460598	-3.252787
38	1	0	-4.554284	-1.405861	0.718632
39	1	0	-6.723775	-2.204107	-0.160814
40	1	0	-5.105941	-2.238659	-4.140647
41	1	0	-7.008039	-2.616892	-2.590995
42	6	0	-1.887790	-1.248321	1.102255
43	6	0	-1.694844	-2.144358	3.749330
44	6	0	-2.433553	-0.495604	2.146532
45	6	0	-1.230719	-2.447001	1.402265
46	6	0	-1.144478	-2.898824	2.715320
47	6	0	-2.333489	-0.940263	3.463771
48	1	0	-2.937321	0.444280	1.933729
49	1	0	-0.763266	-3.013690	0.599650
50	1	0	-0.624158	-3.826350	2.932516
51	1	0	-2.758330	-0.344979	4.266737
52	1	0	-1.615715	-2.488761	4.776264
53	6	0	3.678581	-0.976819	-1.254435
54	6	0	6.189339	-1.562609	-2.342786
55	6	0	4.805059	-1.067860	-0.427591
56	6	0	3.824372	-1.188702	-2.627744
57	6	0	5.074745	-1.475867	-3.172357
58	6	0	6.053079	-1.359950	-0.969296
59	1	0	4.700721	-0.909093	0.642993
60	1	0	2.946356	-1.133603	-3.267620
61	1	0	5.175882	-1.639062	-4.240942
62	1	0	6.921302	-1.428217	-0.320795
63	1	0	7.163841	-1.791473	-2.763507

64	6	0	2.073703	-1.260237	1.073798
65	6	0	2.110210	-2.486245	3.596467
66	6	0	1.809109	-0.518202	2.226694
67	6	0	2.346427	-2.629486	1.199873
68	6	0	2.375573	-3.235794	2.450553
69	6	0	1.821254	-1.130690	3.479196
70	1	0	1.596110	0.544254	2.157075
71	1	0	2.553435	-3.220904	0.310042
72	1	0	2.601751	-4.295084	2.531044
73	1	0	1.604429	-0.541516	4.365281
74	1	0	2.124260	-2.959655	4.573789
75	28	0	0.049317	-1.026762	-1.487275

Zero-point correction=
(Hartree/Particle)

0.603934

Thermal correction to Energy=

0.640929

Thermal correction to Enthalpy=

0.641874

Thermal correction to Gibbs Free Energy=

0.533631

Sum of electronic and zero-point Energies=

-2431.311589

Sum of electronic and thermal Energies=

-2431.274594

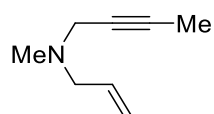
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-2431.273650

Sum of electronic and thermal Free Energies=

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Enyne-Me



Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

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4	6	0	1.029563	-0.864444	0.304829
5	6	0	2.194412	-0.693312	0.040914

6	7	0	-1.334542	-0.631614	-0.335746
7	6	0	-1.594653	0.797192	-0.175310
8	1	0	-2.007859	1.019940	0.828710
9	1	0	-2.371020	1.059296	-0.906747
10	6	0	-0.392694	1.662130	-0.421036
11	1	0	0.155692	1.457649	-1.338623
12	6	0	-0.013906	2.646960	0.387820
13	1	0	0.837976	3.278476	0.156571
14	1	0	-0.543610	2.854862	1.314670
15	6	0	-2.584411	-1.369972	-0.224864
16	1	0	-2.405815	-2.432021	-0.413897
17	1	0	-3.290060	-1.002590	-0.975081
18	6	0	3.600748	-0.458677	-0.288872
19	1	0	4.169454	-1.392977	-0.279592
20	1	0	4.061772	0.226315	0.428649
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22	1	0	-3.056616	-1.266802	0.769630

Zero-point correction=
(Hartree/Particle)

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Thermal correction to Energy=

0.205941

Thermal correction to Enthalpy=

0.206885

Thermal correction to Gibbs Free Energy=

0.158063

Sum of electronic and zero-point Energies=

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Sum of electronic and thermal Energies=

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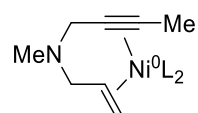
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Sum of electronic and thermal Free Energies=

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IIa



Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

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2	6	0	0.440048	-3.985162	-2.629693
3	1	0	0.080011	-4.198406	-3.643829
4	1	0	1.529892	-4.128236	-2.641914
5	6	0	0.174838	-2.555988	-2.297693
6	6	0	0.074068	-1.324168	-2.478189
7	7	0	-0.124780	-4.982126	-1.736002
8	6	0	0.286413	-4.765974	-0.350636
9	1	0	1.384977	-4.750784	-0.325234
10	1	0	-0.034566	-5.655200	0.211037
11	6	0	-0.235158	-3.529609	0.350556
12	1	0	-1.319441	-3.467490	0.460722
13	6	0	0.558804	-2.814521	1.239250
14	1	0	0.130598	-2.256320	2.067144
15	1	0	1.606662	-3.094967	1.358513
16	6	0	-1.566953	-5.086448	-1.875836
17	1	0	-1.812142	-5.385079	-2.900346
18	1	0	-2.100813	-4.148466	-1.654564
19	1	0	-1.939904	-5.858421	-1.194683
20	1	0	-1.051231	0.359588	-3.147114
21	1	0	0.074166	-0.300030	-4.348519
22	6	0	-0.060947	-0.089253	-3.281826
23	1	0	0.679837	0.661187	-2.984984
24	1	0	4.465126	2.995977	-2.735194
25	6	0	3.528072	2.792373	-2.227119
26	6	0	1.160464	2.279025	-0.946087
27	6	0	2.417149	3.593909	-2.481344
28	6	0	3.444195	1.723333	-1.338508
29	6	0	2.243086	1.437381	-0.682588
30	6	0	1.205246	3.353233	-1.834437
31	1	0	2.500616	4.409537	-3.191778
32	1	0	4.311329	1.091789	-1.173606
33	6	0	-0.065922	4.181344	-2.001102
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35	6	0	-0.188891	5.129454	-0.786941

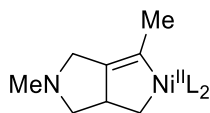
36	1	0	0.663739	5.815799	-0.758354
37	1	0	-0.210401	4.563650	0.150189
38	1	0	-1.112311	5.713677	-0.858969
39	6	0	-0.050476	5.010599	-3.284319
40	1	0	0.038770	4.376658	-4.172409
41	1	0	0.783587	5.717862	-3.273404
42	1	0	-0.966871	5.601820	-3.366514
43	6	0	-1.241564	3.208450	-1.957936
44	6	0	-3.362363	1.397112	-1.566950
45	6	0	-2.409304	3.305437	-2.715560
46	6	0	-1.167480	2.162469	-1.041082
47	6	0	-2.196904	1.249822	-0.811896
48	6	0	-3.458272	2.407585	-2.521976
49	1	0	-2.511498	4.088860	-3.459098
50	1	0	-4.362499	2.502367	-3.114656
51	1	0	-4.187783	0.706845	-1.421750
52	15	0	1.908381	-0.102941	0.280066
53	15	0	-1.829373	-0.119375	0.361171
54	6	0	-3.425442	-1.028594	0.316376
55	6	0	-5.779542	-2.521477	0.068616
56	6	0	-3.560191	-1.979102	-0.703703
57	6	0	-4.480945	-0.833459	1.211101
58	6	0	-5.650643	-1.581106	1.088590
59	6	0	-4.733418	-2.717408	-0.832136
60	1	0	-2.732230	-2.130176	-1.396216
61	1	0	-4.387789	-0.097897	2.005354
62	1	0	-6.464036	-1.426234	1.791082
63	1	0	-4.827308	-3.451462	-1.627244
64	1	0	-6.692368	-3.102333	-0.022186
65	6	0	-1.920040	0.744084	1.986064
66	6	0	-2.002767	1.898281	4.540797
67	6	0	-2.195943	2.105132	2.141358
68	6	0	-1.676724	-0.029164	3.128631
69	6	0	-1.723929	0.540350	4.396284
70	6	0	-2.233782	2.678075	3.411609

71	1	0	-2.395685	2.723492	1.270642
72	1	0	-1.461207	-1.090294	3.024280
73	1	0	-1.528983	-0.073760	5.270349
74	1	0	-2.452354	3.736883	3.516633
75	1	0	-2.033385	2.346405	5.529593
76	6	0	3.553505	-0.927036	0.218682
77	6	0	6.009002	-2.250207	-0.012794
78	6	0	4.660439	-0.500222	0.962131
79	6	0	3.690535	-2.023645	-0.638188
80	6	0	4.913775	-2.681375	-0.756281
81	6	0	5.881028	-1.159619	0.847270
82	1	0	4.562554	0.347829	1.635441
83	1	0	2.825105	-2.358889	-1.207786
84	1	0	5.007748	-3.532201	-1.424417
85	1	0	6.733865	-0.823855	1.429414
86	1	0	6.961765	-2.763759	-0.099154
87	6	0	1.848290	0.478969	2.028091
88	6	0	1.599206	1.188304	4.733558
89	6	0	1.450303	1.768864	2.392594
90	6	0	2.121837	-0.449954	3.041960
91	6	0	2.002173	-0.097811	4.382595
92	6	0	1.324996	2.117971	3.735131
93	1	0	1.234898	2.511822	1.632302
94	1	0	2.448719	-1.452568	2.780542
95	1	0	2.224891	-0.830718	5.152463
96	1	0	1.004312	3.121429	3.998423
97	1	0	1.496481	1.463079	5.779244

Zero-point correction=				0.799787	
(Hartree/Particle)					
Thermal correction to Energy=				0.848150	
Thermal correction to Enthalpy=				0.849095	
Thermal correction to Gibbs Free Energy=				0.717796	
Sum of electronic and zero-point Energies=				-2798.321877	
Sum of electronic and thermal Energies=				-2798.273514	

Sum of electronic and thermal Enthalpies= -2798.272570
 Sum of electronic and thermal Free Energies= -2798.403869

IIIa



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	4.040173	-4.526720	0.737540
2	6	0	3.595017	-3.635252	0.308030
3	6	0	2.476931	-1.365580	-0.750111
4	6	0	4.371187	-2.785981	-0.482744
5	6	0	2.256892	-3.347101	0.550108
6	6	0	1.665303	-2.195893	0.014554
7	6	0	3.819977	-1.632278	-1.031318
8	1	0	5.413269	-3.028897	-0.663308
9	1	0	1.670043	-4.005852	1.183542
10	6	0	4.543394	-0.636557	-1.935648
11	8	0	1.919630	-0.198952	-1.226740
12	6	0	6.060522	-0.802873	-1.880219
13	1	0	6.345120	-1.801957	-2.222228
14	1	0	6.448433	-0.655828	-0.867054
15	1	0	6.545999	-0.086132	-2.548823
16	6	0	4.066882	-0.853810	-3.389255
17	1	0	2.982220	-0.744000	-3.471569
18	1	0	4.340098	-1.859803	-3.723479
19	1	0	4.541462	-0.121717	-4.050678
20	6	0	4.098832	0.746727	-1.470220
21	6	0	3.070320	3.166526	-0.481022
22	6	0	4.920258	1.861843	-1.332585
23	6	0	2.753102	0.890981	-1.123542
24	6	0	2.215551	2.062875	-0.598287

25	6	0	4.404779	3.068681	-0.858563
26	1	0	5.973707	1.794697	-1.584255
27	1	0	5.056872	3.930216	-0.758926
28	1	0	2.693794	4.097397	-0.069847
29	15	0	-0.128738	-1.769449	0.187736
30	15	0	0.507442	1.994308	0.088164
31	6	0	0.123401	3.792472	0.183667
32	6	0	-0.622928	6.494491	0.159981
33	6	0	0.261922	4.561938	-0.979310
34	6	0	-0.385764	4.395552	1.334669
35	6	0	-0.760628	5.739268	1.319571
36	6	0	-0.103679	5.902275	-0.990863
37	1	0	0.657096	4.108393	-1.885450
38	1	0	-0.493458	3.825228	2.251710
39	1	0	-1.158086	6.192719	2.222285
40	1	0	0.009291	6.482751	-1.901236
41	1	0	-0.916250	7.539548	0.150795
42	6	0	0.828971	1.545985	1.848489
43	6	0	1.139424	0.871995	4.550276
44	6	0	2.106562	1.408653	2.399286
45	6	0	-0.292379	1.309188	2.658954
46	6	0	-0.137895	0.989933	4.004651
47	6	0	2.257571	1.068098	3.743771
48	1	0	2.987534	1.571811	1.785001
49	1	0	-1.292069	1.376280	2.231619
50	1	0	-1.014875	0.812078	4.619120
51	1	0	3.254339	0.964096	4.161340
52	1	0	1.262366	0.616531	5.598498
53	6	0	-0.818243	-2.910412	-1.084760
54	6	0	-1.809015	-4.550387	-3.125829
55	6	0	-0.603093	-4.293427	-1.051689
56	6	0	-1.526629	-2.358436	-2.155952
57	6	0	-2.017486	-3.175775	-3.173458
58	6	0	-1.101013	-5.109158	-2.061966
59	1	0	-0.049616	-4.739056	-0.229453

60	1	0	-1.710075	-1.286187	-2.187577
61	1	0	-2.568071	-2.732658	-3.997512
62	1	0	-0.934052	-6.181104	-2.021124
63	1	0	-2.195794	-5.188399	-3.914537
64	6	0	-0.468990	-2.570518	1.802877
65	6	0	-0.940279	-3.597584	4.364509
66	6	0	0.278804	-2.120167	2.897772
67	6	0	-1.458033	-3.536646	2.005295
68	6	0	-1.690471	-4.047018	3.281750
69	6	0	0.045772	-2.631245	4.169744
70	1	0	1.051761	-1.366931	2.753565
71	1	0	-2.048465	-3.895984	1.167566
72	1	0	-2.460463	-4.798427	3.425920
73	1	0	0.633597	-2.270152	5.008671
74	1	0	-1.122221	-3.998369	5.356956
75	28	0	-1.333397	0.327366	-0.241518
76	1	0	-3.180457	-0.204060	1.276923
77	6	0	-2.929515	-0.712593	0.332459
78	1	0	-2.792377	-1.775731	0.561455
79	6	0	-4.035039	-0.491865	-0.685809
80	6	0	-5.509941	-0.456256	-0.269035
81	7	0	-6.123727	0.295809	-1.365983
82	6	0	-5.216797	1.413894	-1.663518
83	6	0	-3.857939	0.894284	-1.226819
84	1	0	-3.947139	-1.231938	-1.497264
85	1	0	-5.610280	0.077172	0.699298
86	1	0	-5.985334	-1.438871	-0.170006
87	1	0	-5.486445	2.315680	-1.078451
88	1	0	-5.287316	1.686573	-2.725207
89	6	0	-7.479687	0.714205	-1.102915
90	1	0	-7.886402	1.236761	-1.975590
91	1	0	-7.552512	1.395118	-0.232251
92	1	0	-8.108677	-0.160347	-0.905335
93	6	0	-2.675834	1.505838	-1.066608
94	1	0	-1.621947	3.051198	-2.171468

95	6	0	-2.512365	2.929387	-1.541663
96	1	0	-2.391457	3.631463	-0.706560
97	1	0	-3.376137	3.265569	-2.133037

Zero-point correction=				0.803540	
(Hartree/Particle)					
Thermal correction to Energy=				0.850132	
Thermal correction to Enthalpy=				0.851076	
Thermal correction to Gibbs Free Energy=				0.724279	
Sum of electronic and zero-point Energies=				-2798.323704	
Sum of electronic and thermal Energies=				-2798.277112	
Sum of electronic and thermal Enthalpies=				-2798.276168	
Sum of electronic and thermal Free Energies=				-2798.402965	

TS_{IIa-IIIa}

Imaginary frequencies = -157.0250 cm⁻¹

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	28	0	0.387341	1.318522	0.043390
2	1	0	1.796001	2.447671	1.962392
3	6	0	0.849287	2.608012	1.439850
4	1	0	0.046950	2.925160	2.106309
5	6	0	0.964462	3.415191	0.190814
6	6	0	2.210911	4.261372	0.015845
7	7	0	2.191436	4.769555	-1.344404
8	6	0	1.995067	3.608089	-2.195073
9	6	0	1.066927	2.644565	-1.500124
10	1	0	0.080790	4.037648	0.027807
11	1	0	3.113206	3.647950	0.220624
12	1	0	2.207287	5.098522	0.722645
13	1	0	2.963900	3.092686	-2.374470
14	1	0	1.603626	3.906590	-3.175446
15	1	0	3.311463	5.873927	-2.719820

16	6	0	0.530154	1.508088	-1.868631
17	6	0	3.384225	5.510169	-1.690119
18	1	0	3.490195	6.373978	-1.026913
19	1	0	4.300009	4.892527	-1.606963
20	1	0	-0.543820	0.396531	-3.354232
21	6	0	0.461793	0.800152	-3.178759
22	1	0	0.730497	1.436909	-4.032704
23	1	0	1.139840	-0.064243	-3.171305
24	1	0	-4.855774	-0.595311	-3.440295
25	6	0	-3.980246	-0.850273	-2.852297
26	6	0	-1.758406	-1.493319	-1.368900
27	6	0	-3.194575	-1.940966	-3.218221
28	6	0	-3.646939	-0.081255	-1.740933
29	6	0	-2.514885	-0.385714	-0.979710
30	6	0	-2.069620	-2.290283	-2.471631
31	1	0	-3.468449	-2.523021	-4.091970
32	1	0	-4.257240	0.776016	-1.476238
33	6	0	-1.186403	-3.507604	-2.731165
34	8	0	-0.651174	-1.788798	-0.607721
35	6	0	-1.606323	-4.623335	-1.747582
36	1	0	-2.649109	-4.906927	-1.924632
37	1	0	-1.508256	-4.287004	-0.710478
38	1	0	-0.971199	-5.504684	-1.886451
39	6	0	-1.323644	-4.025135	-4.162144
40	1	0	-1.036218	-3.263749	-4.894460
41	1	0	-2.354175	-4.331957	-4.361268
42	1	0	-0.696035	-4.908358	-4.310224
43	6	0	0.246570	-3.102113	-2.400932
44	6	0	2.814548	-2.350188	-1.528011
45	6	0	1.386094	-3.537400	-3.078777
46	6	0	0.438492	-2.271966	-1.298553
47	6	0	1.696280	-1.875750	-0.839255
48	6	0	2.657727	-3.169081	-2.644285
49	1	0	1.287736	-4.173831	-3.951988
50	1	0	3.532590	-3.522848	-3.180284

51	1	0	3.808585	-2.059932	-1.200709
52	15	0	-1.852938	0.695703	0.355424
53	15	0	1.721669	-0.630243	0.507821
54	6	0	3.518082	-0.318154	0.706461
55	6	0	6.235054	0.320484	0.891344
56	6	0	4.039029	0.776263	0.006247
57	6	0	4.369545	-1.087702	1.504374
58	6	0	5.722570	-0.767633	1.595709
59	6	0	5.392014	1.092441	0.093991
60	1	0	3.371214	1.380871	-0.605321
61	1	0	3.972304	-1.933887	2.059279
62	1	0	6.376913	-1.367949	2.220511
63	1	0	5.783690	1.946353	-0.451520
64	1	0	7.289177	0.569013	0.968347
65	6	0	1.289440	-1.616698	1.990456
66	6	0	0.622225	-2.970575	4.343134
67	6	0	1.375890	-3.010699	2.049523
68	6	0	0.850888	-0.907168	3.114236
69	6	0	0.530588	-1.581137	4.288741
70	6	0	1.039211	-3.684410	3.221946
71	1	0	1.706559	-3.570675	1.178147
72	1	0	0.750103	0.175012	3.053581
73	1	0	0.189203	-1.022296	5.154548
74	1	0	1.106133	-4.767683	3.259957
75	1	0	0.360895	-3.497783	5.255895
76	6	0	-3.037049	2.096605	0.301363
77	6	0	-4.769882	4.275921	0.045339
78	6	0	-4.263240	2.105143	0.973698
79	6	0	-2.688556	3.186065	-0.505444
80	6	0	-3.554425	4.269825	-0.635284
81	6	0	-5.123488	3.193025	0.848866
82	1	0	-4.544553	1.259728	1.595391
83	1	0	-1.740226	3.170354	-1.040843
84	1	0	-3.276116	5.110920	-1.262660
85	1	0	-6.072096	3.193716	1.377096

86	1	0	-5.442144	5.123257	-0.049164
87	6	0	-2.302471	-0.164363	1.913371
88	6	0	-2.841674	-1.382134	4.377579
89	6	0	-2.563094	-1.534358	1.982214
90	6	0	-2.294783	0.587065	3.096673
91	6	0	-2.576723	-0.014347	4.317810
92	6	0	-2.825481	-2.139421	3.210431
93	1	0	-2.565664	-2.136286	1.078471
94	1	0	-2.080825	1.652906	3.056175
95	1	0	-2.582539	0.583612	5.224328
96	1	0	-3.020729	-3.206744	3.250691
97	1	0	-3.051870	-1.855452	5.332070

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Zero-point correction=                0.800237
(Hartree/Particle)

Thermal correction to Energy=          0.847368

Thermal correction to Enthalpy=        0.848312

Thermal correction to Gibbs Free Energy= 0.718853

Sum of electronic and zero-point Energies= -2798.299450
Sum of electronic and thermal Energies= -2798.252320
Sum of electronic and thermal Enthalpies= -2798.251375
Sum of electronic and thermal Free Energies= -2798.380834

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HBP_{in}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.779744	-0.186336	-0.054694
2	8	0	1.062069	1.185607	-0.422129
3	5	0	-0.000417	1.933337	-0.000328
4	1	0	-0.000821	3.120764	-0.000797
5	8	0	-1.062698	1.185284	0.421553
6	6	0	-0.779573	-0.186760	0.054827
7	6	0	-1.345309	-1.109958	1.121393

8	1	0	-2.436214	-1.034405	1.128103
9	1	0	-0.977221	-0.845424	2.114703
10	1	0	-1.075335	-2.149949	0.909143
11	6	0	-1.468714	-0.433904	-1.285203
12	1	0	-1.061674	0.222551	-2.060739
13	1	0	-2.535125	-0.218213	-1.178165
14	1	0	-1.352868	-1.472608	-1.608194
15	6	0	1.469512	-0.432707	1.285152
16	1	0	1.062994	0.224055	2.060651
17	1	0	2.535893	-0.217189	1.177516
18	1	0	1.353676	-1.471265	1.608641
19	6	0	1.345268	-1.110360	-1.120695
20	1	0	0.976932	-0.846796	-2.114153
21	1	0	1.075129	-2.150109	-0.907339
22	1	0	2.436182	-1.035076	-1.127806

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Zero-point correction=                      0.193501
(Hartree/Particle)

Thermal correction to Energy=                0.202788

Thermal correction to Enthalpy=              0.203732

Thermal correction to Gibbs Free Energy=      0.160716

Sum of electronic and zero-point Energies=   -411.491541

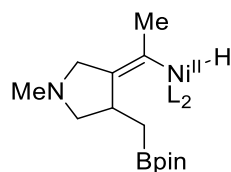
Sum of electronic and thermal Energies=      -411.482254

Sum of electronic and thermal Enthalpies=    -411.481310

Sum of electronic and thermal Free Energies= -411.524326

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IVa



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Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type        X           Y           Z
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1	1	0	4.158600	-3.946121	1.035250
2	6	0	3.179848	-3.481080	1.096534
3	6	0	0.706173	-2.308957	1.247694
4	6	0	2.534182	-3.385827	2.328524
5	6	0	2.588021	-2.971156	-0.055861
6	6	0	1.331324	-2.357961	0.002431
7	6	0	1.275622	-2.795853	2.425327
8	1	0	3.022252	-3.771815	3.217574
9	1	0	3.115296	-3.030477	-1.002679
10	6	0	0.456165	-2.665151	3.705286
11	8	0	-0.539436	-1.728100	1.289288
12	6	0	-0.611934	-3.782745	3.713835
13	1	0	-0.126892	-4.764608	3.717080
14	1	0	-1.257387	-3.717123	2.831945
15	1	0	-1.237905	-3.695410	4.608072
16	6	0	1.322199	-2.790961	4.957256
17	1	0	2.102496	-2.023292	4.986033
18	1	0	1.797157	-3.775329	4.996692
19	1	0	0.707633	-2.700084	5.857225
20	6	0	-0.267230	-1.323302	3.635075
21	6	0	-1.808026	1.009500	3.296771
22	6	0	-0.523522	-0.476715	4.713566
23	6	0	-0.778876	-0.944110	2.396134
24	6	0	-1.549911	0.197869	2.189868
25	6	0	-1.285295	0.678062	4.544704
26	1	0	-0.134877	-0.718899	5.697316
27	1	0	-1.480946	1.321876	5.395882
28	1	0	-2.407950	1.906502	3.179600
29	15	0	0.517738	-1.500544	-1.416833
30	15	0	-2.099128	0.524701	0.467446
31	6	0	-3.194114	1.979319	0.708744
32	6	0	-4.771636	4.270798	1.014513
33	6	0	-2.596108	3.241911	0.820933
34	6	0	-4.586899	1.876429	0.755650
35	6	0	-5.371256	3.019114	0.904524

36	6	0	-3.382326	4.379467	0.979828
37	1	0	-1.516579	3.341621	0.764814
38	1	0	-5.064082	0.904829	0.666817
39	1	0	-6.452753	2.927986	0.932977
40	1	0	-2.903994	5.350693	1.066871
41	1	0	-5.384609	5.160142	1.126105
42	6	0	-3.279181	-0.845286	0.157567
43	6	0	-5.109587	-2.862792	-0.468667
44	6	0	-3.843933	-1.622981	1.171935
45	6	0	-3.629686	-1.094287	-1.174284
46	6	0	-4.549440	-2.091763	-1.484526
47	6	0	-4.751789	-2.631711	0.857746
48	1	0	-3.578398	-1.438681	2.209828
49	1	0	-3.171497	-0.511194	-1.971663
50	1	0	-4.810208	-2.279440	-2.521145
51	1	0	-5.184760	-3.233168	1.651452
52	1	0	-5.818901	-3.648698	-0.710771
53	6	0	1.846359	-1.631739	-2.673128
54	6	0	3.991876	-1.769054	-4.458230
55	6	0	2.055585	-2.785194	-3.435368
56	6	0	2.718321	-0.547151	-2.809423
57	6	0	3.790576	-0.620530	-3.695775
58	6	0	3.122824	-2.850685	-4.328306
59	1	0	1.383335	-3.633015	-3.331387
60	1	0	2.560720	0.352168	-2.218218
61	1	0	4.462726	0.226748	-3.796187
62	1	0	3.275665	-3.747310	-4.921343
63	1	0	4.822356	-1.820945	-5.155800
64	6	0	-0.724440	-2.719347	-2.002932
65	6	0	-2.682934	-4.456916	-2.986363
66	6	0	-1.177847	-3.782721	-1.221504
67	6	0	-1.276847	-2.517004	-3.275664
68	6	0	-2.241712	-3.389469	-3.768037
69	6	0	-2.157614	-4.644840	-1.711668
70	1	0	-0.766046	-3.947184	-0.230115

71	1	0	-0.939893	-1.677493	-3.880039
72	1	0	-2.653526	-3.233159	-4.760621
73	1	0	-2.505241	-5.467753	-1.094489
74	1	0	-3.439459	-5.135564	-3.368861
75	6	0	4.156534	1.226272	1.908315
76	8	0	3.058126	2.161936	1.930850
77	5	0	2.521237	2.183218	0.665929
78	8	0	3.330389	1.552776	-0.253770
79	6	0	4.578348	1.247838	0.404304
80	6	0	5.110853	-0.073727	-0.125415
81	1	0	5.389100	0.034031	-1.178152
82	1	0	4.357087	-0.862025	-0.053003
83	1	0	6.000476	-0.379087	0.436890
84	6	0	5.542762	2.386140	0.077801
85	1	0	5.168901	3.337224	0.470367
86	1	0	5.630932	2.474117	-1.008636
87	1	0	6.536963	2.200569	0.495554
88	6	0	3.591941	-0.126794	2.335455
89	1	0	2.845882	-0.484047	1.616641
90	1	0	3.101726	-0.015751	3.307814
91	1	0	4.376529	-0.885112	2.420331
92	6	0	5.228040	1.692431	2.879866
93	1	0	5.524965	2.723993	2.679280
94	1	0	6.112839	1.050268	2.811902
95	1	0	4.843525	1.638606	3.902402
96	6	0	1.117214	2.767620	0.297645
97	1	0	0.804075	3.539919	1.012140
98	1	0	0.414727	1.928462	0.437012
99	6	0	0.999402	3.291255	-1.145896
100	1	0	1.591941	2.641465	-1.801623
101	6	0	-0.431411	3.377203	-1.673241
102	6	0	-0.775300	4.853248	-1.796369
103	1	0	-1.777663	5.102817	-1.424920
104	1	0	-0.716879	5.197225	-2.851477
105	7	0	0.248431	5.509362	-0.982529

106	6	0	1.466343	4.749050	-1.248178
107	1	0	2.250861	5.013900	-0.527510
108	1	0	1.850880	4.962145	-2.265757
109	6	0	0.382918	6.920779	-1.261076
110	1	0	-0.561544	7.433649	-1.051532
111	1	0	0.653266	7.117088	-2.316696
112	1	0	1.158223	7.355812	-0.621872
113	6	0	-1.207113	2.323729	-1.948319
114	6	0	-2.577972	2.488020	-2.553439
115	1	0	-2.914781	3.533599	-2.584366
116	1	0	-3.341087	1.917430	-2.007158
117	1	0	-2.581292	2.105668	-3.582414
118	28	0	-0.585393	0.589409	-1.421109
119	1	0	-0.014911	0.732447	-2.801423

Zero-point correction=				0.996051	
(Hartree/Particle)					
Thermal correction to Energy=				1.053602	
Thermal correction to Enthalpy=				1.054546	
Thermal correction to Gibbs Free Energy=				0.904755	
Sum of electronic and zero-point Energies=				-3209.869292	
Sum of electronic and thermal Energies=				-3209.811741	
Sum of electronic and thermal Enthalpies=				-3209.810797	
Sum of electronic and thermal Free Energies=				-3209.960588	

TS_{IIIa-IVa}

imaginary frequencies = -267.9386 cm⁻¹

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	28	0	0.655619	0.378319	-0.256222
2	1	0	3.157734	-0.898808	1.004147
3	6	0	2.274335	-0.259417	1.047966
4	1	0	1.606423	-0.829545	1.706129

5	6	0	2.636881	1.104106	1.674561
6	6	0	4.090856	1.309649	2.122893
7	7	0	4.282309	2.756374	2.030437
8	6	0	3.674723	3.133936	0.750271
9	6	0	2.513385	2.179216	0.620286
10	1	0	1.983034	1.309705	2.538521
11	1	0	4.760380	0.779825	1.418609
12	1	0	4.302527	0.955692	3.138512
13	1	0	4.372255	2.958155	-0.097259
14	1	0	3.403040	4.197360	0.744232
15	1	0	5.751322	4.243005	2.059239
16	6	0	1.694528	1.994543	-0.415651
17	6	0	5.667540	3.153883	2.136390
18	1	0	6.070720	2.846709	3.107043
19	1	0	6.295100	2.703667	1.342517
20	1	0	1.216614	2.360463	-2.502726
21	6	0	1.885285	2.725904	-1.717498
22	1	0	1.732013	3.810335	-1.632082
23	1	0	2.915136	2.545063	-2.054282
24	1	0	1.750547	-0.444794	-1.703453
25	5	0	2.761392	-0.579109	-1.003572
26	8	0	3.845530	0.337736	-1.164022
27	6	0	4.909300	-0.382533	-1.778235
28	6	0	4.702697	-1.830658	-1.229078
29	8	0	3.287662	-1.898481	-1.078999
30	6	0	6.234439	0.264090	-1.399193
31	1	0	6.279316	1.277036	-1.812838
32	1	0	7.077761	-0.308507	-1.802646
33	1	0	6.346270	0.336790	-0.314447
34	6	0	4.711808	-0.304408	-3.295803
35	1	0	4.664692	0.749816	-3.585902
36	1	0	3.769733	-0.780732	-3.586336
37	1	0	5.530667	-0.781623	-3.844032
38	6	0	5.376830	-2.058962	0.126331
39	1	0	5.178395	-1.240610	0.823149

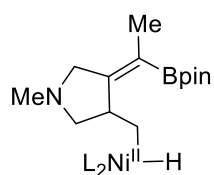
40	1	0	6.462474	-2.162726	0.019842
41	1	0	4.975482	-2.982376	0.556494
42	6	0	5.143660	-2.932672	-2.187251
43	1	0	4.550755	-2.915313	-3.104703
44	1	0	5.004641	-3.908983	-1.712476
45	1	0	6.203526	-2.823069	-2.445846
46	1	0	-5.668166	3.203533	-2.471761
47	6	0	-5.084325	2.407318	-2.021920
48	6	0	-3.617230	0.402483	-0.856432
49	6	0	-5.613265	1.121302	-1.939702
50	6	0	-3.812419	2.680041	-1.531210
51	6	0	-3.033899	1.663303	-0.965726
52	6	0	-4.892040	0.094190	-1.335576
53	1	0	-6.604690	0.928718	-2.335778
54	1	0	-3.418252	3.686779	-1.603761
55	6	0	-5.425088	-1.310276	-1.077863
56	8	0	-2.879009	-0.556898	-0.209593
57	6	0	-5.949435	-1.359156	0.375911
58	1	0	-6.775950	-0.651505	0.499721
59	1	0	-5.158591	-1.098663	1.086728
60	1	0	-6.306933	-2.366859	0.611556
61	6	0	-6.559592	-1.682098	-2.032117
62	1	0	-6.231998	-1.659347	-3.076213
63	1	0	-7.401456	-0.994771	-1.913245
64	1	0	-6.937523	-2.682512	-1.804672
65	6	0	-4.246515	-2.271337	-1.181669
66	6	0	-2.006627	-3.965974	-1.053795
67	6	0	-4.319241	-3.581487	-1.651399
68	6	0	-3.016513	-1.840440	-0.685986
69	6	0	-1.882322	-2.645600	-0.611691
70	6	0	-3.210555	-4.421677	-1.584089
71	1	0	-5.250035	-3.961360	-2.059074
72	1	0	-3.287719	-5.444374	-1.938254
73	1	0	-1.159397	-4.639734	-0.992115
74	15	0	-1.313331	1.905958	-0.329301

75	15	0	-0.389374	-1.887366	0.173299
76	6	0	0.835963	-3.234103	-0.022611
77	6	0	2.784327	-5.202976	-0.406624
78	6	0	1.104165	-3.727850	-1.304300
79	6	0	1.571445	-3.718264	1.060735
80	6	0	2.547611	-4.693108	0.866546
81	6	0	2.057455	-4.720467	-1.492412
82	1	0	0.565573	-3.331774	-2.162518
83	1	0	1.386059	-3.336495	2.060620
84	1	0	3.116446	-5.059120	1.716226
85	1	0	2.249974	-5.101126	-2.491016
86	1	0	3.537268	-5.971865	-0.553817
87	6	0	-0.901663	-2.038069	1.938234
88	6	0	-1.705910	-2.240431	4.608941
89	6	0	-1.406854	-3.245974	2.436712
90	6	0	-0.807522	-0.935907	2.788716
91	6	0	-1.208120	-1.036864	4.121228
92	6	0	-1.804559	-3.347214	3.764379
93	1	0	-1.483945	-4.110526	1.781538
94	1	0	-0.416477	0.006590	2.415760
95	1	0	-1.129566	-0.169159	4.768518
96	1	0	-2.191947	-4.288395	4.142157
97	1	0	-2.018004	-2.320313	5.645856
98	6	0	-0.979312	3.571007	-1.035066
99	6	0	-0.367910	6.014032	-2.260124
100	6	0	-0.998572	3.694132	-2.430629
101	6	0	-0.664171	4.687525	-0.261195
102	6	0	-0.352087	5.901474	-0.873606
103	6	0	-0.703149	4.907085	-3.039799
104	1	0	-1.245931	2.831297	-3.045831
105	1	0	-0.658020	4.622221	0.821399
106	1	0	-0.100135	6.760824	-0.260096
107	1	0	-0.721988	4.985953	-4.122203
108	1	0	-0.125356	6.960244	-2.733731
109	6	0	-1.625999	2.213849	1.459794

110	6	0	-1.954305	2.542368	4.224070
111	6	0	-2.873491	2.003976	2.053935
112	6	0	-0.541107	2.585144	2.267264
113	6	0	-0.706832	2.755675	3.638467
114	6	0	-3.032559	2.163830	3.429625
115	1	0	-3.729404	1.715452	1.451882
116	1	0	0.434334	2.734697	1.812116
117	1	0	0.143602	3.047876	4.247039
118	1	0	-4.006126	1.992863	3.878502
119	1	0	-2.083821	2.667756	5.294998

Zero-point correction=				0.998184	
(Hartree/Particle)					
Thermal correction to Energy=				1.054481	
Thermal correction to Enthalpy=				1.055425	
Thermal correction to Gibbs Free Energy=				0.910540	
Sum of electronic and zero-point Energies=				-3209.794136	
Sum of electronic and thermal Energies=				-3209.737839	
Sum of electronic and thermal Enthalpies=				-3209.736895	
Sum of electronic and thermal Free Energies=				-3209.881780	

Va



Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	-6.729174	2.701214	-0.862700
2	6	0	-5.970391	1.945740	-0.687215
3	6	0	-4.052606	0.037327	-0.249019
4	6	0	-6.285150	0.598632	-0.854885
5	6	0	-4.689680	2.332975	-0.303834

6	6	0	-3.694777	1.374513	-0.082493
7	6	0	-5.325912	-0.387020	-0.629839
8	1	0	-7.287842	0.320513	-1.162249
9	1	0	-4.457034	3.386998	-0.196267
10	6	0	-5.563478	-1.891654	-0.718243
11	8	0	-3.066458	-0.897907	-0.026329
12	6	0	-5.738328	-2.438196	0.717245
13	1	0	-6.616343	-1.982636	1.186817
14	1	0	-4.859765	-2.215962	1.331539
15	1	0	-5.875538	-3.524219	0.689779
16	6	0	-6.805812	-2.233276	-1.539093
17	1	0	-6.724042	-1.863670	-2.566142
18	1	0	-7.698239	-1.798806	-1.080105
19	1	0	-6.959008	-3.315666	-1.566694
20	6	0	-4.296640	-2.505803	-1.305853
21	6	0	-1.827730	-3.571449	-2.136498
22	6	0	-4.248745	-3.590071	-2.181311
23	6	0	-3.079408	-1.972532	-0.886237
24	6	0	-1.837757	-2.465266	-1.282985
25	6	0	-3.025943	-4.120670	-2.587417
26	1	0	-5.169323	-4.033226	-2.546711
27	1	0	-3.006358	-4.973011	-3.258522
28	1	0	-0.882984	-3.996593	-2.459336
29	15	0	-1.922930	1.757951	0.264176
30	15	0	-0.352490	-1.581121	-0.648704
31	6	0	0.987327	-2.627226	-1.335683
32	6	0	3.013708	-4.154657	-2.515266
33	6	0	1.291244	-2.477767	-2.695312
34	6	0	1.710172	-3.546712	-0.573766
35	6	0	2.723532	-4.302767	-1.162781
36	6	0	2.291354	-3.242513	-3.284337
37	1	0	0.739564	-1.755774	-3.294573
38	1	0	1.489174	-3.672456	0.482660
39	1	0	3.285931	-5.008975	-0.559314
40	1	0	2.515983	-3.117992	-4.338962

41	1	0	3.804133	-4.743188	-2.970520
42	6	0	-0.379736	-2.031970	1.131294
43	6	0	-0.314318	-2.632010	3.862383
44	6	0	-1.096816	-3.122983	1.631464
45	6	0	0.365928	-1.240570	2.011981
46	6	0	0.403275	-1.544620	3.370708
47	6	0	-1.065955	-3.418425	2.992097
48	1	0	-1.681100	-3.745208	0.958647
49	1	0	0.908737	-0.376287	1.630114
50	1	0	0.975592	-0.916734	4.046767
51	1	0	-1.628623	-4.266238	3.371327
52	1	0	-0.294539	-2.862048	4.923442
53	6	0	-1.939612	3.586310	0.138436
54	6	0	-2.000010	6.359006	-0.201845
55	6	0	-2.454909	4.407807	1.145391
56	6	0	-1.448809	4.164060	-1.035650
57	6	0	-1.485411	5.545050	-1.208900
58	6	0	-2.481633	5.790314	0.975883
59	1	0	-2.832829	3.965356	2.063945
60	1	0	-1.015053	3.524817	-1.801120
61	1	0	-1.099107	5.984940	-2.123126
62	1	0	-2.876422	6.423758	1.764267
63	1	0	-2.019075	7.436770	-0.331277
64	6	0	-1.751935	1.470388	2.070924
65	6	0	-1.300262	0.998675	4.790866
66	6	0	-2.629802	0.666939	2.801072
67	6	0	-0.633201	2.023619	2.710117
68	6	0	-0.415740	1.795628	4.064802
69	6	0	-2.400564	0.430707	4.155840
70	1	0	-3.497878	0.225676	2.319987
71	1	0	0.063152	2.633783	2.139814
72	1	0	0.447841	2.238643	4.552199
73	1	0	-3.087404	-0.197599	4.714828
74	1	0	-1.127496	0.816379	5.847436
75	6	0	4.159611	1.377113	-2.042024

76	6	0	2.820202	1.765059	-1.414633
77	6	0	2.195164	2.673374	-2.488009
78	7	0	3.307526	3.119900	-3.317986
79	6	0	4.172255	1.952700	-3.441089
80	1	0	2.995603	2.333644	-0.496358
81	1	0	1.469943	2.080590	-3.086969
82	1	0	1.652706	3.525741	-2.065121
83	1	0	5.166018	2.241669	-3.798882
84	1	0	3.755175	1.215670	-4.163304
85	6	0	2.893345	3.661102	-4.590584
86	1	0	2.331307	2.922856	-5.196808
87	1	0	3.767516	3.981502	-5.166725
88	1	0	2.249659	4.532267	-4.431437
89	6	0	5.128375	0.644951	-1.470285
90	6	0	1.929990	0.555991	-1.110279
91	1	0	2.391839	-0.052207	-0.316645
92	1	0	1.911329	-0.078848	-2.009929
93	28	0	0.050596	0.813350	-0.630123
94	1	0	0.522366	2.194608	-0.297307
95	6	0	6.365906	0.195698	-2.217836
96	1	0	6.472816	-0.892816	-2.148244
97	1	0	7.277813	0.623964	-1.783223
98	1	0	6.341109	0.462524	-3.277709
99	5	0	5.032531	0.189526	0.012377
100	8	0	5.664723	-0.946056	0.477119
101	8	0	4.402061	0.877804	1.026401
102	6	0	5.209117	-1.161270	1.827914
103	6	0	4.811972	0.281379	2.270379
104	6	0	4.007715	-2.102988	1.750694
105	1	0	3.621067	-2.350728	2.744995
106	1	0	4.314707	-3.026326	1.250529
107	1	0	3.197035	-1.657116	1.163129
108	6	0	6.328862	-1.793792	2.638153
109	1	0	6.032988	-1.892700	3.688370
110	1	0	7.243532	-1.199882	2.584697

111	1	0	6.544290	-2.792502	2.247564
112	6	0	3.655687	0.353513	3.253523
113	1	0	3.898483	-0.180896	4.178962
114	1	0	3.447216	1.398929	3.499972
115	6	0	6.001830	1.089629	2.785923
116	1	0	6.332725	0.735962	3.767304
117	1	0	5.703513	2.137821	2.873228
118	1	0	6.843782	1.029702	2.088966
119	1	0	2.754171	-0.081849	2.819506

Zero-point correction=			0.996023		
(Hartree/Particle)					
Thermal correction to Energy=			1.053943		
Thermal correction to Enthalpy=			1.054887		
Thermal correction to Gibbs Free Energy=			0.901459		
Sum of electronic and zero-point Energies=			-3209.854235		
Sum of electronic and thermal Energies=			-3209.796315		
Sum of electronic and thermal Enthalpies=			-3209.795371		
Sum of electronic and thermal Free Energies=			-3209.948799		

TS_{IIIa-Va}

imaginary frequencies = -134.8575 cm⁻¹

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	28	0	0.860966	-0.236654	0.136907
2	1	0	2.481484	-1.911313	0.862403
3	6	0	1.848021	-1.286624	1.500326
4	1	0	1.291625	-1.931319	2.190866
5	6	0	2.651435	-0.240463	2.234468
6	6	0	3.941171	-0.567210	2.992298
7	7	0	4.504923	0.769075	3.196666
8	6	0	4.290008	1.516043	1.950516
9	6	0	3.134044	0.802762	1.274617

10	1	0	2.000771	0.271012	2.967532
11	1	0	4.595148	-1.204720	2.364348
12	1	0	3.788480	-1.067519	3.954881
13	1	0	5.176478	1.471728	1.285225
14	1	0	4.107704	2.580198	2.160645
15	1	0	6.220632	1.792260	3.810488
16	6	0	2.649514	1.011562	0.032449
17	6	0	5.881610	0.765940	3.634291
18	1	0	5.970300	0.211265	4.574029
19	1	0	6.560937	0.302835	2.893095
20	1	0	2.694724	2.546227	-1.544737
21	6	0	3.183496	2.291762	-0.607520
22	1	0	3.074270	3.143475	0.076754
23	1	0	4.255466	2.186231	-0.833246
24	1	0	1.049028	-0.054499	-1.739533
25	5	0	2.294760	-0.142815	-1.602550
26	8	0	3.041003	0.516477	-2.610754
27	6	0	3.920341	-0.432488	-3.214742
28	6	0	4.082580	-1.504927	-2.095300
29	8	0	2.799501	-1.468121	-1.470324
30	6	0	5.211891	0.267558	-3.614610
31	1	0	5.007566	0.993512	-4.407482
32	1	0	5.944638	-0.454585	-3.992239
33	1	0	5.647590	0.802681	-2.767723
34	6	0	3.219090	-0.989894	-4.455197
35	1	0	2.942871	-0.154816	-5.105535
36	1	0	2.304933	-1.521641	-4.172788
37	1	0	3.865013	-1.671115	-5.018956
38	6	0	5.146779	-1.118173	-1.064868
39	1	0	5.011107	-0.086232	-0.727623
40	1	0	6.157255	-1.231162	-1.471818
41	1	0	5.044341	-1.773090	-0.193367
42	6	0	4.335029	-2.921738	-2.592017
43	1	0	3.505410	-3.275930	-3.208908
44	1	0	4.436624	-3.594004	-1.733505

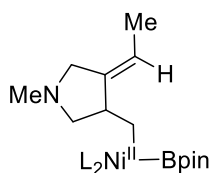
45	1	0	5.259421	-2.973967	-3.178109
46	1	0	-4.429966	4.331216	-2.498760
47	6	0	-4.089125	3.406074	-2.045517
48	6	0	-3.247200	1.072627	-0.872200
49	6	0	-4.862296	2.251134	-2.164973
50	6	0	-2.870789	3.372426	-1.376182
51	6	0	-2.413141	2.184920	-0.792540
52	6	0	-4.453441	1.057582	-1.575607
53	1	0	-5.791116	2.288520	-2.724799
54	1	0	-2.252673	4.264025	-1.332416
55	6	0	-5.229265	-0.255581	-1.610921
56	8	0	-2.816895	-0.069297	-0.240229
57	6	0	-5.990479	-0.407635	-0.273855
58	1	0	-6.709384	0.410019	-0.156873
59	1	0	-5.300026	-0.388288	0.575481
60	1	0	-6.532434	-1.359180	-0.258277
61	6	0	-6.228076	-0.303546	-2.765838
62	1	0	-5.730055	-0.193290	-3.734230
63	1	0	-6.971929	0.491196	-2.661519
64	1	0	-6.774892	-1.250576	-2.757890
65	6	0	-4.201140	-1.381141	-1.689707
66	6	0	-2.286347	-3.435047	-1.459646
67	6	0	-4.351987	-2.577892	-2.389843
68	6	0	-3.047954	-1.238977	-0.921038
69	6	0	-2.092767	-2.240583	-0.762018
70	6	0	-3.398981	-3.589806	-2.283710
71	1	0	-5.223790	-2.732990	-3.017170
72	1	0	-3.534871	-4.515729	-2.832706
73	1	0	-1.567983	-4.242449	-1.359081
74	15	0	-0.725877	1.965400	-0.075310
75	15	0	-0.716723	-1.909757	0.416047
76	6	0	-0.003393	-3.592001	0.550054
77	6	0	1.060608	-6.174327	0.554830
78	6	0	1.034644	-3.924796	-0.328039
79	6	0	-0.496008	-4.553054	1.436105

80	6	0	0.038661	-5.839444	1.439595
81	6	0	1.557227	-5.215942	-0.326840
82	1	0	1.454011	-3.167892	-0.989208
83	1	0	-1.291372	-4.300848	2.131025
84	1	0	-0.345028	-6.578915	2.135659
85	1	0	2.362653	-5.468798	-1.010030
86	1	0	1.474276	-7.178199	0.557519
87	6	0	-1.655125	-1.616222	1.967874
88	6	0	-3.092959	-1.007514	4.288112
89	6	0	-2.879992	-2.243657	2.225128
90	6	0	-1.164218	-0.676335	2.877984
91	6	0	-1.880963	-0.372506	4.033516
92	6	0	-3.591257	-1.944914	3.383480
93	1	0	-3.286204	-2.955963	1.510660
94	1	0	-0.226775	-0.166016	2.675043
95	1	0	-1.492076	0.372471	4.720839
96	1	0	-4.539819	-2.437165	3.575012
97	1	0	-3.655272	-0.768174	5.185425
98	6	0	0.110923	3.359677	-0.926261
99	6	0	1.385022	5.367467	-2.399576
100	6	0	0.353087	3.190879	-2.295888
101	6	0	0.506850	4.543765	-0.303824
102	6	0	1.149249	5.540241	-1.038964
103	6	0	0.977947	4.191790	-3.030488
104	1	0	0.064036	2.262722	-2.785097
105	1	0	0.320065	4.692455	0.755801
106	1	0	1.461335	6.455147	-0.544236
107	1	0	1.164216	4.046683	-4.089943
108	1	0	1.885719	6.145421	-2.967592
109	6	0	-0.922230	2.557135	1.652090
110	6	0	-1.094259	3.295502	4.347909
111	6	0	-2.152900	2.908247	2.209643
112	6	0	0.224765	2.574417	2.459552
113	6	0	0.139853	2.946614	3.797369
114	6	0	-2.237196	3.272385	3.553231

115	1	0	-3.050538	2.895258	1.598463
116	1	0	1.184778	2.289524	2.030437
117	1	0	1.037064	2.956419	4.409186
118	1	0	-3.200445	3.539999	3.977133
119	1	0	-1.162637	3.581199	5.393282

Zero-point correction=				0.997986	
(Hartree/Particle)					
Thermal correction to Energy=				1.054557	
Thermal correction to Enthalpy=				1.055501	
Thermal correction to Gibbs Free Energy=				0.907461	
Sum of electronic and zero-point Energies=				-3209.815106	
Sum of electronic and thermal Energies=				-3209.758535	
Sum of electronic and thermal Enthalpies=				-3209.757591	
Sum of electronic and thermal Free Energies=				-3209.905630	

Vla



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.868258	-4.109518	1.863232
2	6	0	2.778030	-4.054823	0.773090
3	6	0	1.495828	-3.343536	0.312441
4	6	0	1.908033	-2.934868	-1.099515
5	6	0	3.423323	-2.904958	-1.152356
6	7	0	3.833154	-3.208861	0.217390
7	1	0	2.836812	-5.083422	0.360233
8	1	0	3.836064	-1.940247	-1.478476
9	1	0	3.785393	-3.675816	-1.862814

10	6	0	5.158445	-3.773543	0.311966
11	1	0	5.893597	-3.069727	-0.092880
12	1	0	5.405743	-3.961830	1.361612
13	6	0	1.082619	-2.733225	-2.130303
14	6	0	1.497745	-2.375559	-3.529491
15	1	0	1.250435	-3.183380	-4.229507
16	1	0	2.575379	-2.191795	-3.595864
17	1	0	0.969893	-1.475239	-3.865865
18	28	0	0.312795	-0.789303	-0.082912
19	5	0	-0.452753	0.479727	-1.530698
20	8	0	-1.170067	1.638869	-1.281510
21	6	0	-1.748320	2.138803	-2.493751
22	6	0	-0.820804	1.504383	-3.574491
23	8	0	-0.358373	0.304654	-2.916733
24	1	0	0.650819	-4.041571	0.260132
25	6	0	1.132060	-2.131330	1.185878
26	1	0	0.013790	-2.874664	-1.961119
27	1	0	2.052135	-1.745621	1.632381
28	1	0	0.490706	-2.452795	2.014686
29	6	0	-1.737046	3.659671	-2.431477
30	1	0	-2.391298	3.983665	-1.614842
31	1	0	-2.105320	4.097072	-3.366330
32	1	0	-0.733783	4.041320	-2.226752
33	6	0	-3.187416	1.628205	-2.547733
34	1	0	-3.710206	1.964489	-1.646235
35	1	0	-3.215113	0.533214	-2.560579
36	1	0	-3.719210	2.006734	-3.427053
37	6	0	0.412374	2.357804	-3.862474
38	1	0	0.152865	3.268324	-4.412095
39	1	0	1.116697	1.774332	-4.463982
40	1	0	0.915440	2.636616	-2.929434
41	6	0	-1.516615	1.116288	-4.869527
42	1	0	-2.309893	0.386411	-4.688568
43	1	0	-0.791435	0.672252	-5.558477
44	1	0	-1.953628	1.996771	-5.353742

45	1	0	5.253349	-4.726956	-0.242849
46	1	0	1.517728	5.781755	0.127608
47	6	0	1.041643	4.852215	0.422412
48	6	0	-0.188160	2.481149	1.137070
49	6	0	-0.205485	4.872820	1.040011
50	6	0	1.685893	3.639298	0.199733
51	6	0	1.082724	2.430121	0.552753
52	6	0	-0.831340	3.687555	1.421410
53	1	0	-0.690839	5.824880	1.226975
54	1	0	2.664010	3.630315	-0.271342
55	6	0	-2.148645	3.608004	2.179678
56	8	0	-0.822028	1.293250	1.441483
57	6	0	-1.835565	3.300580	3.662332
58	1	0	-1.246997	4.115385	4.097318
59	1	0	-1.266154	2.371201	3.759182
60	1	0	-2.767543	3.196929	4.228109
61	6	0	-2.939100	4.913513	2.105586
62	1	0	-3.189155	5.176107	1.072231
63	1	0	-2.363286	5.732427	2.545696
64	1	0	-3.865556	4.834594	2.680947
65	6	0	-2.919793	2.429063	1.600535
66	6	0	-4.201627	0.119397	0.690781
67	6	0	-4.301257	2.408716	1.425048
68	6	0	-2.191483	1.276555	1.284241
69	6	0	-2.809508	0.106395	0.823252
70	6	0	-4.944076	1.258018	0.978142
71	1	0	-4.886752	3.293758	1.650086
72	1	0	-6.021802	1.249469	0.852627
73	1	0	-4.711665	-0.766791	0.328256
74	15	0	1.891821	0.797684	0.297277
75	15	0	-1.822301	-1.386520	0.363007
76	6	0	-2.888500	-2.230440	-0.884379
77	6	0	-4.472039	-3.460486	-2.848271
78	6	0	-2.583752	-2.080390	-2.242534
79	6	0	-3.991442	-3.017675	-0.524254

80	6	0	-4.777648	-3.625667	-1.498486
81	6	0	-3.374833	-2.687916	-3.217066
82	1	0	-1.727776	-1.483029	-2.545494
83	1	0	-4.233739	-3.162104	0.524905
84	1	0	-5.629019	-4.230575	-1.202199
85	1	0	-3.123817	-2.560379	-4.265932
86	1	0	-5.084388	-3.937362	-3.607485
87	6	0	-2.065641	-2.456653	1.840451
88	6	0	-2.141045	-4.102509	4.107598
89	6	0	-2.286144	-1.909049	3.105659
90	6	0	-1.875524	-3.839147	1.723789
91	6	0	-1.918695	-4.657112	2.847866
92	6	0	-2.323269	-2.728632	4.232872
93	1	0	-2.426347	-0.837192	3.217679
94	1	0	-1.700546	-4.280592	0.745181
95	1	0	-1.774212	-5.727839	2.740355
96	1	0	-2.494994	-2.288428	5.210412
97	1	0	-2.169285	-4.739078	4.986378
98	6	0	3.159066	1.091678	-0.999393
99	6	0	5.051294	1.408689	-3.038179
100	6	0	2.918534	0.572322	-2.275040
101	6	0	4.365993	1.758234	-0.749603
102	6	0	5.302881	1.921327	-1.765516
103	6	0	3.860961	0.733012	-3.290703
104	1	0	1.990231	0.041236	-2.469544
105	1	0	4.577103	2.137839	0.246884
106	1	0	6.234324	2.440571	-1.561980
107	1	0	3.663469	0.320340	-4.276257
108	1	0	5.787844	1.530284	-3.826575
109	6	0	2.948278	0.707295	1.805715
110	6	0	4.565363	0.447946	4.079426
111	6	0	2.733346	1.516618	2.923471
112	6	0	3.976313	-0.245475	1.841954
113	6	0	4.780271	-0.369095	2.969871
114	6	0	3.537883	1.385205	4.055179

115	1	0	1.940483	2.259062	2.918208
116	1	0	4.126653	-0.921556	1.001388
117	1	0	5.571537	-1.113149	2.984659
118	1	0	3.359677	2.022907	4.915877
119	1	0	5.192951	0.349885	4.960161

Zero-point correction= 1.000377
(Hartree/Particle)

Thermal correction to Energy= 1.057551

Thermal correction to Enthalpy= 1.058496

Thermal correction to Gibbs Free Energy= 0.911266

Sum of electronic and zero-point Energies= -3209.847185

Sum of electronic and thermal Energies= -3209.790011

Sum of electronic and thermal Enthalpies= -3209.789067

Sum of electronic and thermal Free Energies= -3209.936296

TS_{IIIa-VIa}

Imaginary frequency: -1142.1454

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	5.351273	1.069590	1.329151
2	6	0	5.250138	0.607682	0.340671
3	6	0	3.778282	0.333400	-0.047385
4	6	0	3.710832	0.780204	-1.488273
5	6	0	5.127768	1.048618	-1.938976
6	7	0	5.748624	1.510687	-0.698802
7	1	0	5.832594	-0.335853	0.342527
8	1	0	5.227075	1.804293	-2.723847
9	1	0	5.605285	0.111803	-2.302823
10	6	0	7.190740	1.566253	-0.763765
11	1	0	7.504259	2.259260	-1.551337
12	1	0	7.590948	1.927356	0.188876
13	6	0	2.549644	1.058593	-2.089687

14	6	0	2.452938	1.632602	-3.483599
15	1	0	1.921277	0.948467	-4.159951
16	1	0	3.433251	1.842228	-3.923169
17	1	0	1.879487	2.569501	-3.474507
18	28	0	1.106860	0.836643	-0.490334
19	5	0	-0.388218	0.816765	-2.099919
20	8	0	-0.772460	-0.134903	-3.013237
21	6	0	-2.013850	0.289908	-3.623405
22	6	0	-2.029789	1.826693	-3.329077
23	8	0	-1.195782	1.932163	-2.151299
24	1	0	3.598864	-0.752442	-0.000107
25	6	0	2.666752	1.068042	0.709245
26	1	0	1.089570	0.779923	-2.048343
27	1	0	2.911986	2.141667	0.742082
28	1	0	2.569632	0.710407	1.741153
29	6	0	-3.136675	-0.464842	-2.923140
30	1	0	-2.924268	-1.536877	-2.972059
31	1	0	-4.106115	-0.271306	-3.395120
32	1	0	-3.198776	-0.176955	-1.869982
33	6	0	-1.976769	-0.077222	-5.099088
34	1	0	-1.967213	-1.166144	-5.201366
35	1	0	-1.085010	0.320020	-5.588337
36	1	0	-2.863957	0.307899	-5.613488
37	6	0	-3.401225	2.399843	-3.010582
38	1	0	-4.077502	2.274481	-3.863545
39	1	0	-3.307410	3.469531	-2.800289
40	1	0	-3.840512	1.919169	-2.133396
41	6	0	-1.347763	2.653562	-4.417594
42	1	0	-0.355488	2.252431	-4.646708
43	1	0	-1.226060	3.678606	-4.055779
44	1	0	-1.939490	2.675187	-5.337885
45	1	0	7.640792	0.576309	-0.973732
46	1	0	-5.229740	2.996872	0.598054
47	6	0	-4.519190	2.179368	0.665732
48	6	0	-2.721028	0.114006	0.806508

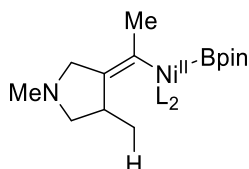
49	6	0	-4.966455	0.864242	0.549259
50	6	0	-3.168206	2.454950	0.859727
51	6	0	-2.236218	1.416322	0.935769
52	6	0	-4.069460	-0.199994	0.629090
53	1	0	-6.023200	0.672296	0.395981
54	1	0	-2.834702	3.484893	0.928106
55	6	0	-4.448776	-1.678146	0.583555
56	8	0	-1.790792	-0.898739	0.853854
57	6	0	-4.463875	-2.213354	2.033668
58	1	0	-5.210597	-1.675681	2.627338
59	1	0	-3.484778	-2.085214	2.507903
60	1	0	-4.710085	-3.280418	2.036253
61	6	0	-5.821908	-1.898381	-0.048907
62	1	0	-5.851929	-1.526519	-1.078676
63	1	0	-6.598243	-1.390970	0.530582
64	1	0	-6.074864	-2.962083	-0.053209
65	6	0	-3.344191	-2.409830	-0.173140
66	6	0	-1.132175	-3.703928	-1.338582
67	6	0	-3.526118	-3.500507	-1.023879
68	6	0	-2.035628	-1.986000	0.042041
69	6	0	-0.912466	-2.612874	-0.496145
70	6	0	-2.430445	-4.134433	-1.607923
71	1	0	-4.526485	-3.862564	-1.237528
72	1	0	-2.589939	-4.979684	-2.269824
73	1	0	-0.285921	-4.215856	-1.786410
74	15	0	-0.409410	1.654599	1.070240
75	15	0	0.718832	-1.890950	-0.042464
76	6	0	1.869504	-3.102127	-0.809029
77	6	0	3.623941	-4.861061	-2.091655
78	6	0	2.578328	-2.690941	-1.942390
79	6	0	2.053352	-4.400378	-0.318126
80	6	0	2.925459	-5.275643	-0.957196
81	6	0	3.451336	-3.569809	-2.582554
82	1	0	2.458544	-1.672431	-2.307704
83	1	0	1.511712	-4.720662	0.568851

84	1	0	3.063757	-6.280366	-0.569394
85	1	0	4.001252	-3.242179	-3.459642
86	1	0	4.307642	-5.544263	-2.586616
87	6	0	0.819970	-2.381882	1.737574
88	6	0	1.147704	-3.027300	4.449762
89	6	0	-0.157785	-3.114131	2.418263
90	6	0	1.965588	-1.980520	2.436333
91	6	0	2.129953	-2.301080	3.779795
92	6	0	0.005611	-3.433071	3.765632
93	1	0	-1.050657	-3.450947	1.898816
94	1	0	2.737733	-1.415461	1.921902
95	1	0	3.022898	-1.976065	4.305234
96	1	0	-0.763656	-4.003613	4.278313
97	1	0	1.271360	-3.271910	5.500666
98	6	0	-0.246987	3.481012	1.047364
99	6	0	0.039146	6.258707	0.920583
100	6	0	0.350211	4.078228	-0.065763
101	6	0	-0.694748	4.287325	2.101631
102	6	0	-0.554068	5.669626	2.037403
103	6	0	0.490908	5.463822	-0.128578
104	1	0	0.709043	3.453780	-0.880603
105	1	0	-1.147570	3.827515	2.976930
106	1	0	-0.901141	6.287365	2.859904
107	1	0	0.961010	5.918948	-0.994701
108	1	0	0.154212	7.337367	0.873757
109	6	0	-0.056702	1.251871	2.832454
110	6	0	0.656640	0.600960	5.465428
111	6	0	-0.764522	0.275598	3.538896
112	6	0	1.016292	1.897212	3.461804
113	6	0	1.368786	1.574623	4.768661
114	6	0	-0.408762	-0.045463	4.846782
115	1	0	-1.592944	-0.248369	3.076044
116	1	0	1.578989	2.657067	2.926699
117	1	0	2.201163	2.086806	5.241498
118	1	0	-0.964297	-0.812801	5.377112

119	1	0	0.932269	0.346897	6.484604

Zero-point correction=				0.994380	
(Hartree/Particle)					
Thermal correction to Energy=				1.051876	
Thermal correction to Enthalpy=				1.052820	
Thermal correction to Gibbs Free Energy=				0.903618	
Sum of electronic and zero-point Energies=				-3209.791984	
Sum of electronic and thermal Energies=				-3209.734487	
Sum of electronic and thermal Enthalpies=				-3209.733543	
Sum of electronic and thermal Free Energies=				-3209.882746	

VIIa



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-5.347434	0.706661	-2.791540
2	6	0	-4.970451	0.420674	-1.802005
3	6	0	-3.453790	0.581904	-1.644748
4	6	0	-3.317362	0.744017	-0.134287
5	6	0	-4.697659	1.051498	0.414206
6	7	0	-5.516604	1.298550	-0.772246
7	1	0	-5.262996	-0.635061	-1.617978
8	1	0	-4.713403	1.920789	1.086895
9	1	0	-5.082029	0.184003	0.997183
10	6	0	-6.929364	1.105161	-0.547349
11	1	0	-7.282134	1.792192	0.228630
12	1	0	-7.487983	1.311099	-1.466493
13	6	0	-2.200020	0.573106	0.581045
14	6	0	-2.295360	0.670047	2.091445

15	1	0	-1.326726	0.516006	2.582276
16	1	0	-2.988502	-0.089637	2.485743
17	1	0	-2.673708	1.649319	2.420980
18	28	0	-0.532674	0.174085	-0.409441
19	5	0	1.174788	-0.239284	-1.485905
20	8	0	1.331684	-0.301807	-2.873085
21	6	0	2.732075	-0.483838	-3.182453
22	6	0	3.288885	-1.088932	-1.857603
23	8	0	2.383553	-0.552748	-0.882304
24	1	0	-2.926044	-0.320874	-1.988116
25	6	0	-2.918367	1.788073	-2.418565
26	1	0	-1.860080	1.949603	-2.181744
27	1	0	-3.476458	2.688922	-2.139979
28	1	0	-3.007657	1.646013	-3.502518
29	6	0	3.315454	0.894054	-3.487206
30	1	0	2.750019	1.350157	-4.305894
31	1	0	4.366197	0.825313	-3.787199
32	1	0	3.240229	1.551412	-2.614343
33	6	0	2.847763	-1.390661	-4.397845
34	1	0	2.428644	-0.886666	-5.273903
35	1	0	2.301874	-2.325205	-4.245259
36	1	0	3.897090	-1.626217	-4.607699
37	6	0	4.699762	-0.658403	-1.481987
38	1	0	5.425453	-0.974568	-2.239706
39	1	0	4.969608	-1.124864	-0.528393
40	1	0	4.761931	0.424997	-1.355027
41	6	0	3.168779	-2.610914	-1.793097
42	1	0	2.149282	-2.934154	-2.033623
43	1	0	3.390070	-2.936000	-0.771395
44	1	0	3.867104	-3.101382	-2.479401
45	1	0	-7.165453	0.071775	-0.223502
46	1	0	2.682714	-5.278235	1.579348
47	6	0	2.363294	-4.241316	1.588788
48	6	0	1.558975	-1.591075	1.596925
49	6	0	3.120827	-3.283468	2.257324

50	6	0	1.195411	-3.866526	0.935930
51	6	0	0.775045	-2.533687	0.917789
52	6	0	2.722037	-1.948501	2.286368
53	1	0	4.026439	-3.587078	2.771548
54	1	0	0.613616	-4.615764	0.408288
55	6	0	3.425073	-0.861594	3.088180
56	8	0	1.159261	-0.271306	1.595344
57	6	0	2.632605	-0.641031	4.397474
58	1	0	2.635439	-1.557366	4.997071
59	1	0	1.593977	-0.368369	4.186520
60	1	0	3.091243	0.164664	4.980396
61	6	0	4.862851	-1.240444	3.442836
62	1	0	5.470024	-1.406731	2.546666
63	1	0	4.880445	-2.148343	4.051569
64	1	0	5.328994	-0.452714	4.040944
65	6	0	3.350112	0.420043	2.269528
66	6	0	2.969638	2.825446	0.891068
67	6	0	4.367336	1.369626	2.203209
68	6	0	2.155441	0.684419	1.595015
69	6	0	1.932385	1.889165	0.913678
70	6	0	4.184329	2.564788	1.514348
71	1	0	5.313922	1.182178	2.698340
72	1	0	4.984733	3.296162	1.471205
73	1	0	2.831713	3.761118	0.358546
74	15	0	-0.749402	-2.013399	0.024479
75	15	0	0.334712	2.185747	0.049355
76	6	0	0.709976	3.427845	-1.250435
77	6	0	1.232651	5.283499	-3.279353
78	6	0	0.784154	3.014305	-2.583730
79	6	0	0.879354	4.785469	-0.945223
80	6	0	1.146165	5.705831	-1.953145
81	6	0	1.048914	3.940164	-3.592519
82	1	0	0.636310	1.966424	-2.832841
83	1	0	0.791130	5.123875	0.083946
84	1	0	1.278233	6.754498	-1.705356

85	1	0	1.101332	3.607925	-4.625017
86	1	0	1.432243	6.004321	-4.066377
87	6	0	-0.597042	3.217529	1.249645
88	6	0	-2.221971	4.644069	3.021678
89	6	0	-0.198652	3.403313	2.572595
90	6	0	-1.814837	3.758328	0.815009
91	6	0	-2.620146	4.470219	1.694336
92	6	0	-1.012083	4.114277	3.456845
93	1	0	0.742787	2.988985	2.922759
94	1	0	-2.140589	3.598279	-0.209683
95	1	0	-3.563830	4.880570	1.347936
96	1	0	-0.696194	4.249977	4.486767
97	1	0	-2.855613	5.193367	3.711421
98	6	0	-0.977959	-3.281909	-1.285761
99	6	0	-1.296211	-5.170817	-3.328380
100	6	0	-0.624100	-2.966496	-2.602450
101	6	0	-1.515827	-4.545616	-1.007577
102	6	0	-1.668759	-5.485529	-2.022352
103	6	0	-0.777772	-3.911690	-3.616517
104	1	0	-0.223298	-1.983797	-2.836756
105	1	0	-1.824659	-4.791354	0.005124
106	1	0	-2.085312	-6.461920	-1.794596
107	1	0	-0.500186	-3.655085	-4.634477
108	1	0	-1.420707	-5.903995	-4.119332
109	6	0	-2.072030	-2.479724	1.211663
110	6	0	-4.188673	-2.950054	2.981127
111	6	0	-1.817188	-2.814149	2.541140
112	6	0	-3.399284	-2.388483	0.771102
113	6	0	-4.449962	-2.625496	1.647746
114	6	0	-2.874340	-3.047570	3.423170
115	1	0	-0.794554	-2.885863	2.900492
116	1	0	-3.608785	-2.114301	-0.260393
117	1	0	-5.473827	-2.546472	1.293768
118	1	0	-2.663935	-3.301934	4.457548
119	1	0	-5.009685	-3.126476	3.669286

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Zero-point correction=                                0.999738
(Hartree/Particle)

Thermal correction to Energy=                          1.057288

Thermal correction to Enthalpy=                       1.058232

Thermal correction to Gibbs Free Energy=              0.908939

Sum of electronic and zero-point Energies=            -3209.859026

Sum of electronic and thermal Energies=               -3209.801476

Sum of electronic and thermal Enthalpies=             -3209.800532

Sum of electronic and thermal Free Energies=          -3209.949825

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TS_{IIIa-VIIa}

Imaginary frequency: -1006.4562

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-4.852651	0.413745	-3.212712
2	6	0	-4.906861	0.479769	-2.119267
3	6	0	-3.526061	0.380754	-1.430314
4	6	0	-3.530249	1.520129	-0.436159
5	6	0	-4.962667	1.989939	-0.340169
6	7	0	-5.439068	1.781994	-1.711160
7	1	0	-5.564657	-0.339064	-1.766074
8	1	0	-5.078927	3.039143	-0.050075
9	1	0	-5.547922	1.373393	0.378844
10	6	0	-6.874082	1.872075	-1.845702
11	1	0	-7.217681	2.865510	-1.539381
12	1	0	-7.160771	1.718121	-2.891377
13	6	0	-2.372296	2.010013	0.029185
14	6	0	-2.386058	3.154691	1.014049
15	1	0	-2.232508	2.793208	2.040265
16	1	0	-3.335911	3.707595	1.004887
17	1	0	-1.582896	3.878173	0.823246
18	28	0	-0.852903	1.029088	-0.835629

19	5	0	0.613239	0.012169	-2.127141
20	8	0	1.264587	0.613156	-3.174614
21	6	0	2.377445	-0.230378	-3.566255
22	6	0	1.985689	-1.614654	-2.948139
23	8	0	1.127948	-1.232914	-1.846809
24	1	0	-3.470861	-0.584716	-0.908796
25	6	0	-2.302178	0.529338	-2.325665
26	1	0	-0.807538	0.173942	-2.157528
27	1	0	-2.314680	1.493116	-2.847848
28	1	0	-2.269048	-0.266769	-3.082664
29	6	0	3.635937	0.350549	-2.938540
30	1	0	3.728297	1.402633	-3.224071
31	1	0	4.529483	-0.185974	-3.274016
32	1	0	3.581684	0.292917	-1.850395
33	6	0	2.482176	-0.213617	-5.083126
34	1	0	2.756773	0.790826	-5.417507
35	1	0	1.534994	-0.484603	-5.553940
36	1	0	3.256836	-0.910996	-5.420078
37	6	0	3.145130	-2.434200	-2.404353
38	1	0	3.831760	-2.709371	-3.212942
39	1	0	2.755862	-3.350651	-1.949216
40	1	0	3.699829	-1.885691	-1.638682
41	6	0	1.138156	-2.470553	-3.889103
42	1	0	0.273584	-1.906348	-4.257706
43	1	0	0.772693	-3.344512	-3.341269
44	1	0	1.720231	-2.817246	-4.748165
45	1	0	-7.403437	1.117821	-1.230640
46	1	0	1.668869	-5.885805	0.496428
47	6	0	1.665353	-4.810004	0.639150
48	6	0	1.665448	-2.075329	0.988706
49	6	0	2.853870	-4.143640	0.923068
50	6	0	0.471918	-4.098819	0.545796
51	6	0	0.450109	-2.713157	0.717678
52	6	0	2.873214	-2.761388	1.113907
53	1	0	3.774634	-4.712145	0.998108

54	1	0	-0.454037	-4.620379	0.320580
55	6	0	4.108389	-1.971201	1.526188
56	8	0	1.630066	-0.705374	1.133685
57	6	0	4.065877	-1.786721	3.060711
58	1	0	4.095488	-2.763050	3.556162
59	1	0	3.150797	-1.270115	3.367005
60	1	0	4.925256	-1.193855	3.391517
61	6	0	5.403960	-2.691359	1.149542
62	1	0	5.479524	-2.847492	0.068123
63	1	0	5.459908	-3.662750	1.647389
64	1	0	6.274400	-2.121132	1.484013
65	6	0	4.013543	-0.586357	0.895227
66	6	0	3.707021	2.063322	0.033881
67	6	0	5.120585	0.170187	0.510086
68	6	0	2.751630	0.010094	0.805174
69	6	0	2.568608	1.345076	0.411875
70	6	0	4.969745	1.482042	0.074643
71	1	0	6.113807	-0.262872	0.557111
72	1	0	5.837241	2.055100	-0.235489
73	1	0	3.608730	3.075258	-0.337190
74	15	0	-1.054411	-1.669638	0.492940
75	15	0	0.849995	2.034395	0.369566
76	6	0	1.065912	3.730375	-0.293605
77	6	0	1.251452	6.295494	-1.412442
78	6	0	0.272991	4.089341	-1.389724
79	6	0	1.952557	4.680445	0.236774
80	6	0	2.044873	5.952205	-0.318438
81	6	0	0.366175	5.364135	-1.945835
82	1	0	-0.435213	3.371198	-1.797672
83	1	0	2.579437	4.425425	1.086749
84	1	0	2.736353	6.674868	0.103163
85	1	0	-0.257169	5.625962	-2.794676
86	1	0	1.324798	7.288401	-1.845217
87	6	0	0.453631	2.247275	2.161402
88	6	0	-0.370220	2.414683	4.839743

89	6	0	-0.029802	1.121629	2.835278
90	6	0	0.500570	3.466410	2.843368
91	6	0	0.095528	3.545650	4.174275
92	6	0	-0.436034	1.199140	4.163657
93	1	0	-0.114525	0.180035	2.311799
94	1	0	0.809177	4.373835	2.338689
95	1	0	0.131079	4.502783	4.685712
96	1	0	-0.825088	0.308760	4.650925
97	1	0	-0.694574	2.485208	5.873532
98	6	0	-2.130990	-2.824542	-0.454777
99	6	0	-3.752732	-4.407780	-2.103201
100	6	0	-1.877989	-2.916393	-1.829939
101	6	0	-3.206997	-3.533472	0.084796
102	6	0	-4.014948	-4.318133	-0.739164
103	6	0	-2.676316	-3.707532	-2.648168
104	1	0	-1.048451	-2.354426	-2.250760
105	1	0	-3.422900	-3.469355	1.147557
106	1	0	-4.852119	-4.860201	-0.309427
107	1	0	-2.465819	-3.768662	-3.712271
108	1	0	-4.385594	-5.017763	-2.740399
109	6	0	-1.835452	-1.725584	2.160794
110	6	0	-3.158809	-1.652195	4.627511
111	6	0	-1.486297	-2.621097	3.175811
112	6	0	-2.842818	-0.779548	2.398987
113	6	0	-3.507434	-0.752047	3.621699
114	6	0	-2.143246	-2.580481	4.405696
115	1	0	-0.701166	-3.353327	3.006953
116	1	0	-3.082725	-0.046335	1.628481
117	1	0	-4.285812	-0.014713	3.793445
118	1	0	-1.863560	-3.278710	5.189139
119	1	0	-3.671043	-1.625023	5.584691

Zero-point correction=
(Hartree/Particle)

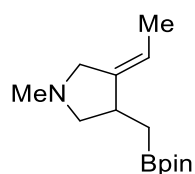
0.996196

Thermal correction to Energy=

1.053159

Thermal correction to Enthalpy=	1.054103
Thermal correction to Gibbs Free Energy=	0.906562
Sum of electronic and zero-point Energies=	-3209.795207
Sum of electronic and thermal Energies=	-3209.738244
Sum of electronic and thermal Enthalpies=	-3209.737300
Sum of electronic and thermal Free Energies=	-3209.884841

VIIIa

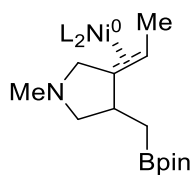


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.153086	-0.527651	-0.545367
2	8	0	-1.902794	-0.716347	-1.242999
3	5	0	-0.894176	-0.501726	-0.335857
4	8	0	-1.356626	0.022007	0.848616
5	6	0	-2.734335	0.401297	0.638189
6	6	0	-3.513833	0.187382	1.925115
7	1	0	-3.155910	0.881960	2.690272
8	1	0	-3.390700	-0.830014	2.301393
9	1	0	-4.580090	0.376917	1.761672
10	6	0	-2.729726	1.880870	0.257837
11	1	0	-2.181975	2.042425	-0.676511
12	1	0	-2.230580	2.445178	1.050620
13	1	0	-3.745811	2.269013	0.139620
14	6	0	-3.615603	-1.906399	-0.077838
15	1	0	-2.896920	-2.341904	0.623622
16	1	0	-3.690578	-2.566174	-0.946434
17	1	0	-4.594023	-1.855982	0.409374
18	6	0	-4.168932	0.075146	-1.502356
19	1	0	-3.785296	0.985072	-1.967999

20	1	0	-5.099276	0.312630	-0.975182
21	1	0	-4.397750	-0.644326	-2.293617
22	6	0	0.620339	-0.813542	-0.609436
23	1	0	0.919611	-0.362629	-1.565011
24	1	0	0.750180	-1.895977	-0.742893
25	6	0	1.560318	-0.308588	0.497445
26	1	0	1.234219	-0.708709	1.463073
27	6	0	3.014668	-0.658994	0.218409
28	6	0	3.708484	0.602333	-0.257750
29	1	0	4.301384	0.464645	-1.169490
30	1	0	4.394657	0.974462	0.531349
31	7	0	2.611910	1.538190	-0.491333
32	6	0	1.619036	1.224161	0.530359
33	1	0	0.659248	1.699717	0.300199
34	1	0	1.944010	1.575775	1.529582
35	6	0	3.029872	2.921471	-0.489919
36	1	0	3.766963	3.088848	-1.281488
37	1	0	3.483837	3.222996	0.473522
38	1	0	2.168957	3.569274	-0.681663
39	6	0	3.570812	-1.856973	0.383630
40	6	0	5.006357	-2.196593	0.104834
41	1	0	5.565286	-1.328397	-0.254964
42	1	0	5.087649	-2.987948	-0.649238
43	1	0	5.505486	-2.566502	1.007971
44	1	0	2.944074	-2.667859	0.756981

Zero-point correction=				0.395059	
(Hartree/Particle)					
Thermal correction to Energy=				0.414789	
Thermal correction to Enthalpy=				0.415733	
Thermal correction to Gibbs Free Energy=				0.347067	
Sum of electronic and zero-point Energies=				-778.541735	
Sum of electronic and thermal Energies=				-778.522005	
Sum of electronic and thermal Enthalpies=				-778.521061	
Sum of electronic and thermal Free Energies=				-778.589727	

VIIIa-Ni



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.542292	3.193679	-4.966432
2	6	0	-2.557611	2.440736	-4.184900
3	6	0	-2.611177	0.543746	-2.204735
4	6	0	-3.147496	1.202176	-4.430405
5	6	0	-1.975731	2.716923	-2.951130
6	6	0	-1.974912	1.756159	-1.934227
7	6	0	-3.190348	0.228608	-3.434463
8	1	0	-3.579056	1.001805	-5.405608
9	1	0	-1.500717	3.678445	-2.785209
10	6	0	-3.855172	-1.139077	-3.560833
11	8	0	-2.648001	-0.381004	-1.186036
12	6	0	-5.237543	-1.068835	-2.873212
13	1	0	-5.870530	-0.333107	-3.380491
14	1	0	-5.138534	-0.777929	-1.823020
15	1	0	-5.727767	-2.046984	-2.916877
16	6	0	-4.044314	-1.556755	-5.017957
17	1	0	-3.088239	-1.617885	-5.547606
18	1	0	-4.689461	-0.844494	-5.539966
19	1	0	-4.538596	-2.530801	-5.072988
20	6	0	-2.986391	-2.126747	-2.786264
21	6	0	-1.467127	-3.812978	-1.128283
22	6	0	-2.732692	-3.446210	-3.157436
23	6	0	-2.444283	-1.685890	-1.578505
24	6	0	-1.687306	-2.491405	-0.728586
25	6	0	-1.980252	-4.282860	-2.334560

26	1	0	-3.123532	-3.831526	-4.093481
27	1	0	-1.792768	-5.308265	-2.636628
28	1	0	-0.876187	-4.470933	-0.497628
29	15	0	-1.058790	1.922831	-0.338298
30	15	0	-1.042218	-1.726273	0.825978
31	6	0	0.167294	-3.017241	1.328143
32	6	0	2.197144	-4.842737	1.964090
33	6	0	1.413031	-2.956795	0.685625
34	6	0	-0.040816	-3.989816	2.307542
35	6	0	0.972809	-4.897154	2.623109
36	6	0	2.418424	-3.866029	0.991950
37	1	0	1.610484	-2.173228	-0.045747
38	1	0	-0.989762	-4.041186	2.833448
39	1	0	0.801366	-5.647220	3.389392
40	1	0	3.375721	-3.786414	0.484855
41	1	0	2.981951	-5.549969	2.214868
42	6	0	-2.498170	-1.955879	1.926316
43	6	0	-4.712168	-2.179914	3.622857
44	6	0	-3.262786	-3.130097	1.943442
45	6	0	-2.871138	-0.888483	2.747717
46	6	0	-3.972834	-1.001681	3.594936
47	6	0	-4.358918	-3.244044	2.792095
48	1	0	-3.000909	-3.955458	1.285066
49	1	0	-2.304424	0.039720	2.715963
50	1	0	-4.252797	-0.160871	4.222240
51	1	0	-4.942888	-4.159314	2.801758
52	1	0	-5.570416	-2.268700	4.282238
53	6	0	-0.296094	3.575656	-0.589009
54	6	0	1.018007	6.002942	-1.064767
55	6	0	-0.859916	4.780046	-0.159725
56	6	0	0.930126	3.601728	-1.262554
57	6	0	1.580644	4.806955	-1.508309
58	6	0	-0.200010	5.986651	-0.389490
59	1	0	-1.813964	4.777868	0.359699
60	1	0	1.381815	2.665585	-1.586806

61	1	0	2.532857	4.811343	-2.030318
62	1	0	-0.641957	6.915853	-0.042759
63	1	0	1.528902	6.944212	-1.242518
64	6	0	-2.387720	2.252169	0.891871
65	6	0	-4.261525	2.538066	2.958193
66	6	0	-3.736505	1.969728	0.667426
67	6	0	-1.987710	2.685449	2.164999
68	6	0	-2.917626	2.833806	3.189083
69	6	0	-4.665832	2.107211	1.698101
70	1	0	-4.070669	1.636656	-0.310472
71	1	0	-0.938344	2.905258	2.351501
72	1	0	-2.591190	3.173542	4.167528
73	1	0	-5.710039	1.875610	1.511419
74	1	0	-4.989184	2.645427	3.757016
75	6	0	6.523879	-0.804352	-1.221565
76	8	0	5.961782	-0.069459	-0.113250
77	5	0	4.772685	-0.673121	0.220174
78	8	0	4.404418	-1.635710	-0.699718
79	6	0	5.259443	-1.469129	-1.849746
80	6	0	5.500517	-2.823656	-2.494997
81	1	0	4.560327	-3.209285	-2.899487
82	1	0	5.884243	-3.545418	-1.770845
83	1	0	6.217573	-2.734729	-3.318243
84	6	0	4.523642	-0.538197	-2.812384
85	1	0	4.363225	0.444071	-2.354107
86	1	0	3.546364	-0.971314	-3.043538
87	1	0	5.077657	-0.403178	-3.746173
88	6	0	7.497056	-1.823712	-0.632657
89	1	0	6.971876	-2.538648	0.008658
90	1	0	8.235049	-1.294914	-0.023507
91	1	0	8.022844	-2.375035	-1.417967
92	6	0	7.258932	0.161722	-2.136705
93	1	0	6.620058	0.997360	-2.429793
94	1	0	7.603238	-0.353605	-3.039929
95	1	0	8.133581	0.564955	-1.618450

96	6	0	3.836410	-0.271194	1.404197
97	1	0	4.370813	0.126446	2.273956
98	1	0	3.289169	-1.163569	1.723660
99	6	0	2.846361	0.809263	0.905302
100	1	0	2.501895	0.530996	-0.103153
101	6	0	1.643719	1.062224	1.844393
102	6	0	1.772549	2.503581	2.317266
103	1	0	1.477480	2.642484	3.365162
104	1	0	1.179670	3.210810	1.701369
105	7	0	3.199174	2.788163	2.149147
106	6	0	3.530358	2.187973	0.860745
107	1	0	4.617363	2.117999	0.733059
108	1	0	3.126492	2.798881	0.031883
109	6	0	3.497625	4.202495	2.199277
110	1	0	3.223383	4.606227	3.179362
111	1	0	2.948617	4.772494	1.423902
112	1	0	4.570415	4.362857	2.050834
113	6	0	1.076794	0.024215	2.599330
114	6	0	0.326021	0.249680	3.894159
115	1	0	-0.312858	1.139044	3.860184
116	1	0	1.017505	0.372535	4.740589
117	1	0	-0.319830	-0.605388	4.124073
118	28	0	-0.002864	0.313874	0.926053
119	1	0	1.525068	-0.966003	2.529959

Zero-point correction=				1.002152	
(Hartree/Particle)					
Thermal correction to Energy=				1.059407	
Thermal correction to Enthalpy=				1.060351	
Thermal correction to Gibbs Free Energy=				0.909839	
Sum of electronic and zero-point Energies=				-3209.896540	
Sum of electronic and thermal Energies=				-3209.839286	
Sum of electronic and thermal Enthalpies=				-3209.838342	
Sum of electronic and thermal Free Energies=				-3209.988854	

TS_{IVa-VIIIa}Imaginary frequencies = -604.92 cm⁻¹

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	28	0	0.249466	0.192056	0.283197
2	1	0	3.879452	0.733691	2.915441
3	6	0	3.372398	0.621793	1.945693
4	1	0	2.517223	-0.041507	2.129067
5	6	0	2.876934	1.992471	1.457145
6	6	0	3.941190	3.093763	1.549773
7	7	0	3.562523	4.041278	0.504394
8	6	0	3.222978	3.201573	-0.645763
9	6	0	2.485466	2.035050	-0.017674
10	1	0	2.012426	2.296039	2.068170
11	1	0	4.942661	2.665440	1.353362
12	1	0	3.967486	3.588892	2.527443
13	1	0	4.139781	2.858655	-1.171011
14	1	0	2.616513	3.770371	-1.363052
15	1	0	4.256227	5.692060	-0.572916
16	6	0	1.560442	1.272237	-0.617059
17	6	0	4.594666	5.012029	0.215775
18	1	0	4.809623	5.604728	1.110903
19	1	0	5.536364	4.536462	-0.118613
20	1	0	1.579305	-0.342252	-0.195657
21	5	0	4.310735	-0.092633	0.905093
22	8	0	5.163396	0.546603	0.034357
23	6	0	5.542750	-0.417940	-0.968585
24	6	0	5.396140	-1.768992	-0.196933
25	8	0	4.357346	-1.461540	0.754593
26	6	0	6.949613	-0.105691	-1.450716
27	1	0	6.952588	0.860720	-1.963313
28	1	0	7.292045	-0.869628	-2.157165
29	1	0	7.654516	-0.053993	-0.618342

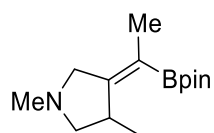
30	6	0	4.540483	-0.282088	-2.114406
31	1	0	4.554861	0.752866	-2.469564
32	1	0	3.523399	-0.504741	-1.774084
33	1	0	4.793650	-0.943317	-2.949191
34	6	0	6.643177	-2.133095	0.605265
35	1	0	6.973242	-1.286148	1.214828
36	1	0	7.466037	-2.438521	-0.048054
37	1	0	6.403171	-2.964919	1.273956
38	6	0	4.945190	-2.943980	-1.050299
39	1	0	3.961671	-2.758313	-1.488170
40	1	0	4.879633	-3.845256	-0.433182
41	1	0	5.664004	-3.132438	-1.855126
42	1	0	-2.696522	3.638592	-4.134471
43	6	0	-2.618547	2.745209	-3.523458
44	6	0	-2.412610	0.486537	-1.984451
45	6	0	-2.792382	1.491729	-4.107560
46	6	0	-2.332897	2.862599	-2.165760
47	6	0	-2.211819	1.721948	-1.366514
48	6	0	-2.702492	0.331501	-3.339789
49	1	0	-3.002708	1.424653	-5.169893
50	1	0	-2.173742	3.843955	-1.730563
51	6	0	-2.952328	-1.086459	-3.849319
52	8	0	-2.301105	-0.627058	-1.184386
53	6	0	-4.389304	-1.491202	-3.447511
54	1	0	-5.114878	-0.818344	-3.916400
55	1	0	-4.520120	-1.440407	-2.361447
56	1	0	-4.594850	-2.516480	-3.772596
57	6	0	-2.808973	-1.187610	-5.366832
58	1	0	-1.804366	-0.903711	-5.695819
59	1	0	-3.537486	-0.540980	-5.863864
60	1	0	-3.012167	-2.208821	-5.701298
61	6	0	-1.984318	-2.010775	-3.116105
62	6	0	-0.366523	-3.672655	-1.513198
63	6	0	-1.373000	-3.144617	-3.653306
64	6	0	-1.740545	-1.738859	-1.772510

65	6	0	-0.943771	-2.534340	-0.949520
66	6	0	-0.576728	-3.968646	-2.859096
67	1	0	-1.520442	-3.395609	-4.698604
68	1	0	-0.116768	-4.849928	-3.294224
69	1	0	0.260758	-4.315304	-0.902428
70	15	0	-1.571356	1.727053	0.364469
71	15	0	-0.644024	-1.902045	0.749908
72	6	0	0.396101	-3.228979	1.476021
73	6	0	2.094916	-5.194381	2.509797
74	6	0	1.781806	-3.052520	1.445262
75	6	0	-0.136054	-4.400433	2.026962
76	6	0	0.712400	-5.378080	2.540245
77	6	0	2.628504	-4.031505	1.960142
78	1	0	2.203759	-2.150622	1.013668
79	1	0	-1.212381	-4.547154	2.058617
80	1	0	0.293475	-6.283949	2.967958
81	1	0	3.701174	-3.862619	1.938237
82	1	0	2.751860	-5.956440	2.918564
83	6	0	-2.261417	-2.200097	1.568465
84	6	0	-4.630816	-2.657149	2.984509
85	6	0	-3.291766	-2.951077	0.997382
86	6	0	-2.437376	-1.663732	2.848677
87	6	0	-3.609618	-1.901071	3.557514
88	6	0	-4.473670	-3.174148	1.701819
89	1	0	-3.170204	-3.373559	0.003470
90	1	0	-1.652388	-1.051795	3.288913
91	1	0	-3.735255	-1.476718	4.548785
92	1	0	-5.268422	-3.759049	1.248238
93	1	0	-5.550860	-2.833959	3.533738
94	6	0	-1.373157	3.529469	0.673521
95	6	0	-0.998015	6.271553	1.086419
96	6	0	-0.088724	4.077586	0.663317
97	6	0	-2.474439	4.369546	0.889249
98	6	0	-2.286143	5.732521	1.091767
99	6	0	0.099126	5.443668	0.872719

100	1	0	0.768765	3.436258	0.487643
101	1	0	-3.478647	3.953451	0.902974
102	1	0	-3.144571	6.376210	1.259186
103	1	0	1.111140	5.837791	0.872110
104	1	0	-0.855958	7.335439	1.252024
105	6	0	-3.050630	1.382479	1.405918
106	6	0	-5.222234	0.933861	3.116797
107	6	0	-4.213307	0.777045	0.926289
108	6	0	-2.977472	1.737956	2.759280
109	6	0	-4.059052	1.525369	3.606632
110	6	0	-5.291369	0.550999	1.781152
111	1	0	-4.290382	0.490290	-0.118181
112	1	0	-2.076169	2.208578	3.146651
113	1	0	-3.993642	1.822113	4.649278
114	1	0	-6.189776	0.078076	1.396037
115	1	0	-6.066869	0.762512	3.777663
116	1	0	0.776513	0.586766	-2.528199
117	1	0	2.165224	1.679353	-2.680656
118	1	0	0.570846	2.310308	-2.228469
119	6	0	1.263448	1.466252	-2.090522

Zero-point correction=				0.995533	
(Hartree/Particle)					
Thermal correction to Energy=				1.052758	
Thermal correction to Enthalpy=				1.053702	
Thermal correction to Gibbs Free Energy=				0.904354	
Sum of electronic and zero-point Energies=				-3209.866612	
Sum of electronic and thermal Energies=				-3209.809387	
Sum of electronic and thermal Enthalpies=				-3209.808443	
Sum of electronic and thermal Free Energies=				-3209.957790	

IXa



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.805795	0.529689	-0.181568
2	6	0	1.946300	-0.957505	-0.454702
3	6	0	3.382829	-1.039902	-1.017151
4	7	0	4.157229	0.067340	-0.441282
5	6	0	3.190916	1.153893	-0.270065
6	1	0	1.214339	-1.278923	-1.201483
7	1	0	3.872846	-1.996426	-0.810004
8	1	0	3.353836	-0.908950	-2.106683
9	1	0	3.220583	1.832844	-1.137225
10	1	0	3.436337	1.761548	0.609461
11	6	0	4.859180	-0.256787	0.792884
12	1	0	4.204225	-0.424094	1.664066
13	1	0	5.540381	0.562588	1.044064
14	1	0	5.462441	-1.156055	0.639850
15	6	0	0.685609	1.233645	0.059392
16	6	0	1.736208	-1.803507	0.808184
17	1	0	0.708820	-1.694999	1.164715
18	1	0	2.412137	-1.502471	1.613307
19	6	0	0.785743	2.723627	0.326175
20	1	0	-0.202839	3.177024	0.424351
21	1	0	1.315797	3.241769	-0.482991
22	1	0	1.339411	2.929851	1.250788
23	5	0	-0.726585	0.592099	0.031615
24	8	0	-1.858935	1.300199	0.366596
25	8	0	-1.016864	-0.702443	-0.342503
26	6	0	-2.996463	0.499625	-0.014443
27	6	0	-2.399393	-0.944184	-0.007106
28	6	0	-4.122446	0.730140	0.980701

29	1	0	-4.966550	0.066278	0.764850
30	1	0	-4.472377	1.763566	0.904762
31	1	0	-3.789910	0.555513	2.005839
32	6	0	-3.417672	0.957064	-1.409597
33	1	0	-4.318566	0.435455	-1.746143
34	1	0	-2.617870	0.781189	-2.135705
35	1	0	-3.625692	2.030040	-1.380839
36	6	0	-2.418623	-1.582456	1.380424
37	1	0	-3.436146	-1.843193	1.686538
38	1	0	-1.817097	-2.495672	1.358904
39	6	0	-3.000260	-1.889715	-1.034659
40	1	0	-4.073431	-2.017526	-0.856711
41	1	0	-2.521388	-2.869755	-0.954500
42	1	0	-2.853326	-1.518137	-2.050725
43	1	0	-1.990516	-0.904973	2.126518
44	1	0	1.916943	-2.862169	0.592333

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Zero-point correction=                0.395277
(Hartree/Particle)

Thermal correction to Energy=         0.415304

Thermal correction to Enthalpy=       0.416248

Thermal correction to Gibbs Free Energy= 0.347156

Sum of electronic and zero-point Energies= -778.542452
Sum of electronic and thermal Energies= -778.522425
Sum of electronic and thermal Enthalpies= -778.521481
Sum of electronic and thermal Free Energies= -778.590573

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TS_{Va-IXa}

Imaginary frequencies = -778.2777 cm⁻¹

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	1	0	-6.589448	2.926392	-0.900658
2	6	0	-5.863199	2.140380	-0.721095

3	6	0	-4.026469	0.152867	-0.271029
4	6	0	-6.226515	0.808560	-0.909203
5	6	0	-4.574599	2.472450	-0.313045
6	6	0	-3.619513	1.475579	-0.085894
7	6	0	-5.309443	-0.215276	-0.679127
8	1	0	-7.233581	0.572673	-1.237059
9	1	0	-4.302926	3.515748	-0.191184
10	6	0	-5.603480	-1.708424	-0.795064
11	8	0	-3.087864	-0.829138	-0.041666
12	6	0	-5.818995	-2.271199	0.628430
13	1	0	-6.687189	-1.791726	1.092546
14	1	0	-4.942719	-2.090375	1.258670
15	1	0	-5.994782	-3.350951	0.581218
16	6	0	-6.847580	-1.989267	-1.635840
17	1	0	-6.740620	-1.604934	-2.655161
18	1	0	-7.728945	-1.530634	-1.178814
19	1	0	-7.039165	-3.064881	-1.684513
20	6	0	-4.353468	-2.359249	-1.379290
21	6	0	-1.916969	-3.489316	-2.217501
22	6	0	-4.335729	-3.418484	-2.286114
23	6	0	-3.123327	-1.883630	-0.927986
24	6	0	-1.896265	-2.413670	-1.326544
25	6	0	-3.128951	-3.981225	-2.697482
26	1	0	-5.267846	-3.815570	-2.674433
27	1	0	-3.133519	-4.811394	-3.396344
28	1	0	-0.981962	-3.933005	-2.546096
29	15	0	-1.836520	1.789787	0.279983
30	15	0	-0.389359	-1.602873	-0.649548
31	6	0	0.943150	-2.582571	-1.448482
32	6	0	3.017971	-3.915673	-2.778009
33	6	0	1.248831	-2.277201	-2.782224
34	6	0	1.694077	-3.557650	-0.788623
35	6	0	2.728948	-4.217803	-1.450829
36	6	0	2.271974	-2.945612	-3.446376
37	1	0	0.680695	-1.506700	-3.300785

38	1	0	1.478177	-3.801229	0.247702
39	1	0	3.308945	-4.970100	-0.924581
40	1	0	2.496189	-2.700317	-4.479861
41	1	0	3.825683	-4.429186	-3.290076
42	6	0	-0.402284	-2.238494	1.073679
43	6	0	-0.317992	-3.125023	3.724740
44	6	0	-0.936539	-3.484963	1.418721
45	6	0	0.163670	-1.438833	2.069319
46	6	0	0.211249	-1.881711	3.390221
47	6	0	-0.893619	-3.925464	2.738192
48	1	0	-1.384663	-4.112234	0.651701
49	1	0	0.554781	-0.457651	1.806882
50	1	0	0.647417	-1.244725	4.154132
51	1	0	-1.310385	-4.893953	2.998001
52	1	0	-0.288675	-3.470140	4.753863
53	6	0	-1.781928	3.625819	0.221686
54	6	0	-1.669453	6.411676	0.007211
55	6	0	-2.307142	4.433916	1.235945
56	6	0	-1.194678	4.225901	-0.895174
57	6	0	-1.144394	5.613742	-1.006382
58	6	0	-2.248731	5.821002	1.129640
59	1	0	-2.758393	3.974236	2.112266
60	1	0	-0.758201	3.594600	-1.665893
61	1	0	-0.684065	6.070377	-1.877269
62	1	0	-2.652413	6.441809	1.923708
63	1	0	-1.621320	7.493430	-0.072680
64	6	0	-1.710830	1.471365	2.088481
65	6	0	-1.304695	0.936580	4.807926
66	6	0	-2.673701	0.778180	2.822916
67	6	0	-0.533083	1.886915	2.727893
68	6	0	-0.335740	1.628169	4.079718
69	6	0	-2.468424	0.509933	4.176506
70	1	0	-3.592425	0.447818	2.346100
71	1	0	0.231372	2.411796	2.157860
72	1	0	0.576514	1.963435	4.564965

73	1	0	-3.224904	-0.031965	4.735931
74	1	0	-1.149029	0.729858	5.862575
75	6	0	4.237218	1.357093	-1.958469
76	6	0	2.933129	1.887453	-1.365832
77	6	0	2.413571	2.824174	-2.470173
78	7	0	3.587142	3.169120	-3.260642
79	6	0	4.347778	1.928951	-3.355002
80	1	0	3.148438	2.456652	-0.454940
81	1	0	1.666673	2.278840	-3.086535
82	1	0	1.925309	3.724084	-2.078949
83	1	0	5.376242	2.128013	-3.673512
84	1	0	3.894364	1.230853	-4.093400
85	6	0	3.265811	3.743471	-4.546455
86	1	0	2.660222	3.058924	-5.172178
87	1	0	4.185100	3.982037	-5.090720
88	1	0	2.699771	4.669904	-4.407064
89	6	0	5.105336	0.522757	-1.365990
90	6	0	1.927155	0.768380	-1.054562
91	1	0	2.321614	0.140580	-0.245369
92	1	0	1.848545	0.141098	-1.955429
93	28	0	-0.030541	0.724181	-0.626508
94	1	0	0.859489	1.899211	-0.562399
95	6	0	6.303604	-0.053176	-2.090157
96	1	0	6.317435	-1.143366	-1.982208
97	1	0	7.245890	0.312921	-1.663820
98	1	0	6.304299	0.178536	-3.158563
99	5	0	4.932490	0.082767	0.115051
100	8	0	5.489827	-1.076928	0.608974
101	8	0	4.285715	0.803165	1.095322
102	6	0	4.956679	-1.271590	1.935524
103	6	0	4.595951	0.187248	2.359799
104	6	0	3.724983	-2.164727	1.795014
105	1	0	3.275717	-2.394281	2.766945
106	1	0	4.021550	-3.100773	1.312341
107	1	0	2.962672	-1.690407	1.166095

108	6	0	6.007913	-1.948248	2.800043
109	1	0	5.654854	-2.037769	3.833157
110	1	0	6.946669	-1.390722	2.795461
111	1	0	6.203954	-2.953722	2.416811
112	6	0	3.386862	0.309864	3.273418
113	1	0	3.552894	-0.231087	4.211887
114	1	0	3.212588	1.364352	3.508002
115	6	0	5.786250	0.943992	2.946362
116	1	0	6.045510	0.573885	3.943020
117	1	0	5.527007	2.003421	3.022819
118	1	0	6.663145	0.851624	2.297844
119	1	0	2.490642	-0.086163	2.791304

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Zero-point correction=                0.994591
(Hartree/Particle)

Thermal correction to Energy=          1.052448

Thermal correction to Enthalpy=        1.053392

Thermal correction to Gibbs Free Energy= 0.900231

Sum of electronic and zero-point Energies= -3209.845850
Sum of electronic and thermal Energies= -3209.787992
Sum of electronic and thermal Enthalpies= -3209.787048
Sum of electronic and thermal Free Energies= -3209.940209

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TS_{VIIa-VIIIa}

Imaginary frequency: -104.5637

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	3.106186	3.672808	-2.727340
2	6	0	3.233124	3.816745	-1.648957
3	6	0	2.078156	3.209079	-0.822780
4	6	0	2.800785	2.740156	0.439733
5	6	0	4.272142	3.045356	0.269783
6	7	0	4.434421	3.132887	-1.177675

7	1	0	3.309909	4.906111	-1.455352
8	1	0	4.933421	2.274228	0.685277
9	1	0	4.530646	4.007557	0.761449
10	6	0	5.658895	3.788091	-1.578867
11	1	0	6.523478	3.241662	-1.186236
12	1	0	5.731097	3.805724	-2.670723
13	6	0	2.236473	2.152474	1.496323
14	28	0	0.086651	0.631779	-0.934358
15	5	0	-0.644431	2.352224	-0.538925
16	8	0	-0.917630	2.548912	0.819780
17	6	0	-1.406715	3.881111	1.042176
18	6	0	-1.840468	4.329791	-0.399386
19	8	0	-1.098824	3.453467	-1.261828
20	1	0	1.380457	4.018871	-0.580642
21	6	0	1.286736	2.124396	-1.564121
22	1	0	1.158656	1.999185	1.482048
23	1	0	2.004559	1.384341	-1.950445
24	1	0	0.836483	2.594802	-2.448139
25	6	0	-0.273395	4.708416	1.653380
26	1	0	0.024972	4.243588	2.598123
27	1	0	-0.597514	5.733608	1.859682
28	1	0	0.609254	4.741375	1.012395
29	6	0	-2.548306	3.827958	2.051566
30	1	0	-2.175637	3.417887	2.995115
31	1	0	-3.365428	3.192301	1.710102
32	1	0	-2.939321	4.834305	2.240765
33	6	0	-1.474821	5.767593	-0.744421
34	1	0	-1.983357	6.469527	-0.074281
35	1	0	-1.784763	5.986499	-1.770451
36	1	0	-0.396747	5.931071	-0.671194
37	6	0	-3.325177	4.096525	-0.679855
38	1	0	-3.608960	3.059939	-0.469816
39	1	0	-3.517166	4.280616	-1.740846
40	1	0	-3.956905	4.765464	-0.086725
41	1	0	5.716630	4.830165	-1.209995

42	1	0	4.008474	-1.955822	3.861656
43	6	0	3.056759	-1.867548	3.347739
44	6	0	0.652368	-1.655469	2.052081
45	6	0	1.874916	-1.826626	4.085379
46	6	0	3.031249	-1.772995	1.958338
47	6	0	1.815245	-1.651532	1.279733
48	6	0	0.639832	-1.723910	3.444821
49	1	0	1.921573	-1.882220	5.168074
50	1	0	3.962197	-1.773876	1.400832
51	6	0	-0.719800	-1.769072	4.139050
52	8	0	-0.534675	-1.606272	1.363068
53	6	0	-1.240123	-3.222965	4.060960
54	1	0	-0.557110	-3.895842	4.590193
55	1	0	-1.314780	-3.553471	3.019196
56	1	0	-2.232647	-3.293659	4.518362
57	6	0	-0.631487	-1.342751	5.603781
58	1	0	-0.259463	-0.318045	5.701053
59	1	0	0.031970	-2.011233	6.159368
60	1	0	-1.613613	-1.407443	6.080520
61	6	0	-1.681752	-0.891666	3.341567
62	6	0	-3.479722	0.468368	1.649310
63	6	0	-2.733518	-0.143097	3.872336
64	6	0	-1.559348	-0.906419	1.955422
65	6	0	-2.432567	-0.256154	1.083982
66	6	0	-3.621514	0.528843	3.034877
67	1	0	-2.870487	-0.085380	4.947220
68	1	0	-4.431503	1.108352	3.466731
69	1	0	-4.175072	1.003768	1.009599
70	15	0	1.655456	-1.336004	-0.534230
71	15	0	-1.969436	-0.358812	-0.687281
72	6	0	-3.361341	0.419888	-1.597069
73	6	0	-5.408338	1.546016	-3.132764
74	6	0	-3.060382	1.318853	-2.622747
75	6	0	-4.697527	0.066600	-1.364848
76	6	0	-5.716635	0.639852	-2.116417

77	6	0	-4.082082	1.873941	-3.393319
78	1	0	-2.025723	1.598553	-2.802084
79	1	0	-4.934995	-0.668244	-0.598482
80	1	0	-6.750345	0.371363	-1.921076
81	1	0	-3.837803	2.571535	-4.188773
82	1	0	-6.204644	1.987328	-3.724567
83	6	0	-2.356074	-2.123388	-1.074614
84	6	0	-3.046299	-4.711669	-1.887601
85	6	0	-2.976465	-3.001730	-0.183868
86	6	0	-2.067709	-2.561198	-2.371362
87	6	0	-2.419500	-3.842569	-2.779076
88	6	0	-3.315739	-4.292352	-0.589069
89	1	0	-3.209947	-2.680850	0.827895
90	1	0	-1.567439	-1.890824	-3.068161
91	1	0	-2.187989	-4.169144	-3.788316
92	1	0	-3.798556	-4.966317	0.112648
93	1	0	-3.314656	-5.715425	-2.203552
94	6	0	3.434735	-1.356563	-1.012666
95	6	0	6.171259	-1.255396	-1.608770
96	6	0	4.107245	-0.133942	-1.063361
97	6	0	4.151970	-2.536471	-1.254614
98	6	0	5.511298	-2.483326	-1.548803
99	6	0	5.466417	-0.080776	-1.366334
100	1	0	3.578042	0.790426	-0.867922
101	1	0	3.648923	-3.498159	-1.208582
102	1	0	6.056699	-3.404015	-1.733454
103	1	0	5.951521	0.889384	-1.421900
104	1	0	7.230077	-1.220205	-1.847596
105	6	0	1.123898	-2.958179	-1.224297
106	6	0	0.442737	-5.391535	-2.431415
107	6	0	0.581159	-3.994597	-0.463907
108	6	0	1.289350	-3.141278	-2.603821
109	6	0	0.963547	-4.353222	-3.201746
110	6	0	0.238554	-5.203582	-1.068095
111	1	0	0.434026	-3.869781	0.604899

112	1	0	1.705650	-2.338079	-3.209039
113	1	0	1.116340	-4.487172	-4.268618
114	1	0	-0.186192	-6.001451	-0.466202
115	1	0	0.183177	-6.338204	-2.896145
116	6	0	2.953518	1.725270	2.745108
117	1	0	2.532409	0.793382	3.134613
118	1	0	2.847725	2.480974	3.534795
119	1	0	4.024555	1.570344	2.578072

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Zero-point correction=                0.999049
(Hartree/Particle)

Thermal correction to Energy=         1.056080
Thermal correction to Enthalpy=       1.057024
Thermal correction to Gibbs Free Energy= 0.908862

Sum of electronic and zero-point Energies= -3209.851530
Sum of electronic and thermal Energies= -3209.794500
Sum of electronic and thermal Enthalpies= -3209.793555
Sum of electronic and thermal Free Energies= -3209.941718

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TS_{VIIa-IXa}

Imaginary frequency: -56.6018

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-5.940229	-1.584309	-0.617052
2	6	0	-4.982142	-1.581914	-0.080071
3	6	0	-4.285889	-0.221399	-0.065875
4	6	0	-3.303572	-0.427681	1.063800
5	6	0	-4.080649	-1.241894	2.097008
6	7	0	-5.204136	-1.835555	1.344854
7	1	0	-4.324043	-2.339395	-0.549512
8	1	0	-4.469401	-0.623774	2.921081
9	1	0	-3.450866	-2.017640	2.553090
10	6	0	-5.485431	-3.214690	1.658750

11	1	0	-5.667316	-3.327724	2.732584
12	1	0	-6.388263	-3.536967	1.128158
13	6	0	-2.020229	-0.046181	1.151471
14	6	0	-1.301998	-0.255822	2.483208
15	1	0	-0.213802	-0.384646	2.375912
16	1	0	-1.667007	-1.142800	3.016986
17	1	0	-1.444836	0.616811	3.132436
18	28	0	-0.427607	0.363586	0.134690
19	5	0	-1.626706	1.836415	-0.159619
20	8	0	-2.278320	2.852808	0.529840
21	6	0	-2.593511	3.919291	-0.389447
22	6	0	-2.561166	3.211443	-1.789065
23	8	0	-1.737267	2.055783	-1.538267
24	1	0	-3.787191	0.012982	-1.010877
25	6	0	-5.289269	0.877034	0.320547
26	1	0	-4.758356	1.796411	0.581547
27	1	0	-5.871772	0.559614	1.190186
28	1	0	-5.993801	1.083731	-0.494213
29	6	0	-1.504898	4.979882	-0.231964
30	1	0	-1.467696	5.292111	0.816670
31	1	0	-1.706368	5.860770	-0.850200
32	1	0	-0.526022	4.578576	-0.503361
33	6	0	-3.940643	4.525249	-0.020110
34	1	0	-3.887628	4.938329	0.991529
35	1	0	-4.746731	3.790523	-0.049943
36	1	0	-4.189712	5.339841	-0.709404
37	6	0	-1.929765	4.043982	-2.897448
38	1	0	-2.523488	4.946375	-3.083099
39	1	0	-1.906251	3.456966	-3.821029
40	1	0	-0.910649	4.339833	-2.650976
41	6	0	-3.920850	2.716301	-2.273599
42	1	0	-4.415546	2.109880	-1.517668
43	1	0	-3.767782	2.097042	-3.163583
44	1	0	-4.577632	3.550642	-2.541035
45	1	0	-4.667113	-3.905340	1.372765

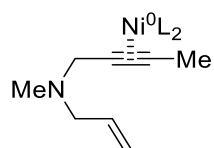
46	1	0	2.426175	-5.116629	-3.423630
47	6	0	2.465940	-4.327297	-2.679928
48	6	0	2.562653	-2.300872	-0.830547
49	6	0	3.699881	-3.869300	-2.220939
50	6	0	1.284020	-3.788559	-2.182669
51	6	0	1.309843	-2.760421	-1.234985
52	6	0	3.767715	-2.849942	-1.274986
53	1	0	4.611347	-4.313714	-2.606591
54	1	0	0.332714	-4.158685	-2.548792
55	6	0	5.046984	-2.321272	-0.634969
56	8	0	2.595738	-1.252624	0.068031
57	6	0	5.167724	-2.927644	0.781751
58	1	0	5.235691	-4.018555	0.718059
59	1	0	4.301039	-2.667968	1.397092
60	1	0	6.067468	-2.545700	1.275320
61	6	0	6.291410	-2.693247	-1.439762
62	1	0	6.255058	-2.280695	-2.453085
63	1	0	6.389614	-3.780404	-1.506885
64	1	0	7.193092	-2.324247	-0.943210
65	6	0	4.874702	-0.812686	-0.501774
66	6	0	4.361119	1.920226	-0.170355
67	6	0	5.888427	0.123255	-0.680248
68	6	0	3.605827	-0.341867	-0.145276
69	6	0	3.304913	1.013257	-0.009456
70	6	0	5.637989	1.482015	-0.496617
71	1	0	6.883913	-0.202587	-0.962927
72	1	0	6.438567	2.202767	-0.626280
73	1	0	4.174524	2.983786	-0.063369
74	15	0	-0.175963	-1.983959	-0.454034
75	15	0	1.562212	1.569173	0.302959
76	6	0	1.683417	3.242139	-0.447123
77	6	0	1.967016	5.699604	-1.756440
78	6	0	1.475383	3.336401	-1.826718
79	6	0	2.029132	4.391147	0.272388
80	6	0	2.161480	5.615174	-0.379355

81	6	0	1.632666	4.556596	-2.480191
82	1	0	1.177164	2.453646	-2.388062
83	1	0	2.193796	4.331777	1.344390
84	1	0	2.421514	6.502400	0.189646
85	1	0	1.474441	4.617537	-3.552944
86	1	0	2.075279	6.653174	-2.263835
87	6	0	1.596805	1.938903	2.105142
88	6	0	1.498179	2.487851	4.846903
89	6	0	2.634789	1.528859	2.944171
90	6	0	0.500911	2.623258	2.650952
91	6	0	0.461235	2.905171	4.012310
92	6	0	2.580499	1.796755	4.312071
93	1	0	3.491098	1.000912	2.534454
94	1	0	-0.326655	2.923174	2.009599
95	1	0	-0.389405	3.439374	4.424871
96	1	0	3.390383	1.468000	4.956133
97	1	0	1.459257	2.699495	5.911044
98	6	0	-1.522533	-2.451369	-1.607102
99	6	0	-3.576116	-2.998804	-3.429834
100	6	0	-2.087485	-1.422327	-2.366824
101	6	0	-2.002143	-3.758855	-1.765837
102	6	0	-3.022252	-4.030958	-2.672324
103	6	0	-3.107981	-1.697143	-3.276688
104	1	0	-1.748749	-0.396262	-2.225352
105	1	0	-1.584488	-4.565174	-1.167855
106	1	0	-3.389401	-5.046546	-2.783776
107	1	0	-3.546084	-0.887633	-3.853192
108	1	0	-4.376576	-3.210297	-4.132336
109	6	0	-0.405919	-3.118757	0.979097
110	6	0	-0.753896	-4.639004	3.311951
111	6	0	0.693577	-3.474860	1.769403
112	6	0	-1.681791	-3.526031	1.378713
113	6	0	-1.853260	-4.284557	2.535039
114	6	0	0.520813	-4.230181	2.925100
115	1	0	1.694127	-3.159143	1.486932

116	1	0	-2.548599	-3.239351	0.789880
117	1	0	-2.852841	-4.592042	2.830119
118	1	0	1.385300	-4.499515	3.524169
119	1	0	-0.888722	-5.227888	4.213986

Zero-point correction=			1.000428		
(Hartree/Particle)					
Thermal correction to Energy=			1.057127		
Thermal correction to Enthalpy=			1.058072		
Thermal correction to Gibbs Free Energy=			0.912417		
Sum of electronic and zero-point Energies=			-3209.845655		
Sum of electronic and thermal Energies=			-3209.788957		
Sum of electronic and thermal Enthalpies=			-3209.788012		
Sum of electronic and thermal Free Energies=			-3209.933667		

Xa



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-5.129940	3.219377	-2.162945
2	6	0	-4.536951	2.416874	-1.736294
3	6	0	-3.042896	0.389487	-0.658436
4	6	0	-5.047616	1.120053	-1.711308
5	6	0	-3.269405	2.691146	-1.230224
6	6	0	-2.486553	1.667377	-0.687721
7	6	0	-4.305336	0.076601	-1.161207
8	1	0	-6.032424	0.928283	-2.124834
9	1	0	-2.878083	3.702293	-1.276650
10	6	0	-4.771626	-1.370147	-1.022698
11	8	0	-2.272292	-0.605475	-0.101071

12	6	0	-5.236869	-1.591095	0.434783
13	1	0	-6.083631	-0.935120	0.662041
14	1	0	-4.429427	-1.374650	1.141593
15	1	0	-5.548678	-2.631510	0.574902
16	6	0	-5.923489	-1.697731	-1.971111
17	1	0	-5.636899	-1.552500	-3.017551
18	1	0	-6.789117	-1.065570	-1.753704
19	1	0	-6.245833	-2.734095	-1.836295
20	6	0	-3.552490	-2.254729	-1.269766
21	6	0	-1.196284	-3.780404	-1.474326
22	6	0	-3.558604	-3.486895	-1.922630
23	6	0	-2.335933	-1.818187	-0.748381
24	6	0	-1.146364	-2.539309	-0.834411
25	6	0	-2.391970	-4.243204	-2.020057
26	1	0	-4.477982	-3.868294	-2.354789
27	1	0	-2.415639	-5.203641	-2.524762
28	1	0	-0.295938	-4.381194	-1.557566
29	15	0	-0.729115	1.852443	-0.149976
30	15	0	0.365246	-1.742871	-0.137723
31	6	0	1.585997	-3.080244	-0.445234
32	6	0	3.424036	-5.093436	-1.077096
33	6	0	2.218166	-3.097607	-1.693901
34	6	0	1.884481	-4.079268	0.483912
35	6	0	2.806351	-5.077008	0.170524
36	6	0	3.125074	-4.104007	-2.012819
37	1	0	2.007547	-2.305840	-2.410962
38	1	0	1.399208	-4.078028	1.456076
39	1	0	3.038348	-5.844170	0.903084
40	1	0	3.608687	-4.108438	-2.984995
41	1	0	4.140575	-5.872415	-1.318990
42	6	0	0.050282	-1.864698	1.671811
43	6	0	-0.316818	-1.950437	4.444906
44	6	0	-0.946370	-2.671587	2.228241
45	6	0	0.858776	-1.095588	2.518143
46	6	0	0.680834	-1.146605	3.897614

47	6	0	-1.131754	-2.709436	3.608715
48	1	0	-1.580338	-3.275065	1.584025
49	1	0	1.617644	-0.444002	2.087819
50	1	0	1.309107	-0.540173	4.542590
51	1	0	-1.911482	-3.336974	4.030108
52	1	0	-0.463316	-1.979899	5.520545
53	6	0	-0.453787	3.619042	-0.564483
54	6	0	-0.020254	6.267054	-1.354089
55	6	0	-0.815025	4.674620	0.278380
56	6	0	0.124112	3.902550	-1.805722
57	6	0	0.333764	5.220136	-2.203157
58	6	0	-0.592951	5.992981	-0.113650
59	1	0	-1.266981	4.465585	1.244421
60	1	0	0.433061	3.079827	-2.447440
61	1	0	0.786889	5.428290	-3.167577
62	1	0	-0.869202	6.807028	0.549590
63	1	0	0.153735	7.295219	-1.656532
64	6	0	-0.846903	1.875995	1.687789
65	6	0	-0.830089	1.843574	4.489117
66	6	0	-1.945604	1.385638	2.395251
67	6	0	0.270419	2.334876	2.399611
68	6	0	0.272141	2.334227	3.789728
69	6	0	-1.931821	1.362632	3.789525
70	1	0	-2.820697	1.021136	1.865615
71	1	0	1.143846	2.689599	1.856528
72	1	0	1.139888	2.705107	4.327536
73	1	0	-2.789449	0.969148	4.327013
74	1	0	-0.824911	1.829418	5.574981
75	28	0	1.049962	0.431988	-0.495798
76	6	0	4.018909	-0.681300	-0.132301
77	1	0	3.701545	-1.336389	0.693745
78	1	0	4.048014	-1.325477	-1.018840
79	6	0	2.971713	0.371707	-0.317745
80	6	0	2.600732	1.592829	-0.373494
81	7	0	5.387819	-0.257654	0.144400

82	6	0	6.146404	0.140114	-1.033885
83	1	0	6.178917	-0.715479	-1.720851
84	1	0	7.177829	0.322727	-0.699818
85	6	0	5.654178	1.350238	-1.789804
86	1	0	5.562089	2.276940	-1.223742
87	6	0	5.360561	1.343535	-3.087337
88	1	0	5.026488	2.236941	-3.606922
89	1	0	5.440717	0.433128	-3.678224
90	6	0	5.487768	0.666423	1.255523
91	1	0	4.994969	0.226012	2.129687
92	1	0	5.020659	1.646677	1.072244
93	1	0	6.543224	0.825695	1.502209
94	1	0	3.066409	3.382612	-1.434511
95	1	0	3.939669	3.216629	0.095424
96	6	0	2.977063	3.032977	-0.398171
97	1	0	2.225627	3.670790	0.079632

Zero-point correction=
(Hartree/Particle)

0.800492

Thermal correction to Energy=

0.849179

Thermal correction to Enthalpy=

0.850123

Thermal correction to Gibbs Free Energy=

0.716666

Sum of electronic and zero-point Energies=

-2798.315608

Sum of electronic and thermal Energies=

-2798.266922

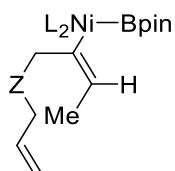
Sum of electronic and thermal Enthalpies=

-2798.265978

Sum of electronic and thermal Free Energies=

-2798.399435

XIIa



Center

Atomic

Atomic

Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	28	0	-0.003103	0.650998	-0.284352
2	5	0	0.086064	-0.949767	-1.575651
3	8	0	0.046145	-0.933761	-2.965653
4	6	0	0.264462	-2.266887	-3.476782
5	6	0	-0.020158	-3.170768	-2.231365
6	8	0	0.175485	-2.267387	-1.130446
7	6	0	-1.462234	-3.669916	-2.159695
8	1	0	-1.657792	-4.439055	-2.914689
9	1	0	-2.172876	-2.852375	-2.300522
10	1	0	-1.633031	-4.101786	-1.167942
11	6	0	0.934832	-4.347138	-2.067009
12	1	0	0.889626	-5.012853	-2.936214
13	1	0	0.650198	-4.925142	-1.182163
14	1	0	1.964677	-4.007331	-1.934956
15	6	0	-0.669992	-2.497136	-4.656766
16	1	0	-0.570721	-3.521394	-5.033579
17	1	0	-0.407120	-1.809405	-5.466796
18	1	0	-1.712167	-2.322349	-4.382277
19	6	0	1.711972	-2.355219	-3.948257
20	1	0	1.916359	-3.324323	-4.415860
21	1	0	2.408206	-2.211439	-3.118181
22	1	0	1.895620	-1.567650	-4.684632
23	6	0	-0.107072	2.120822	1.071072
24	6	0	-0.081254	1.867019	2.392912
25	1	0	0.038639	0.838773	2.746206
26	6	0	-0.195375	2.907722	3.487951
27	1	0	-1.074698	3.552293	3.347295
28	1	0	0.678248	3.576690	3.506300
29	1	0	-0.276374	2.445885	4.476602
30	6	0	-0.313547	3.582261	0.678686
31	1	0	0.364623	4.223886	1.263125
32	1	0	-1.335808	3.881353	0.966369
33	7	0	-0.140622	3.978239	-0.719881

34	6	0	1.229829	3.845813	-1.171536
35	1	0	1.528582	2.787270	-1.277568
36	1	0	1.908881	4.316080	-0.452530
37	1	0	1.352810	4.330856	-2.144688
38	6	0	-1.058098	3.320738	-1.626652
39	1	0	-0.706106	2.299753	-1.900677
40	1	0	-2.015376	3.177445	-1.107364
41	6	0	-1.322683	4.087075	-2.897919
42	1	0	-1.845037	3.527080	-3.674067
43	6	0	-0.986981	5.356097	-3.109897
44	1	0	-1.220432	5.857965	-4.043605
45	1	0	-0.471119	5.924164	-2.341106
46	1	0	4.670048	-1.854182	3.790874
47	6	0	3.720133	-1.759298	3.275601
48	6	0	1.287759	-1.491951	1.988853
49	6	0	2.619693	-2.503809	3.698039
50	6	0	3.601481	-0.904889	2.187179
51	6	0	2.382058	-0.757559	1.514074
52	6	0	1.390992	-2.395112	3.053428
53	1	0	2.730463	-3.182721	4.537083
54	1	0	4.458971	-0.322835	1.859991
55	6	0	0.182167	-3.277288	3.338865
56	8	0	0.084177	-1.302730	1.375200
57	6	0	0.168334	-4.393155	2.266090
58	1	0	1.076191	-5.001019	2.345201
59	1	0	0.125185	-3.959575	1.260582
60	1	0	-0.705929	-5.037904	2.407676
61	6	0	0.237456	-3.912856	4.726562
62	1	0	0.249016	-3.156131	5.517709
63	1	0	1.129325	-4.537573	4.825089
64	1	0	-0.622917	-4.569627	4.881008
65	6	0	-1.074262	-2.441395	3.129909
66	6	0	-3.393887	-1.060116	2.381019
67	6	0	-2.255008	-2.591375	3.851493
68	6	0	-1.073522	-1.545965	2.054592

69	6	0	-2.226825	-0.873732	1.630360
70	6	0	-3.408090	-1.896583	3.490364
71	1	0	-2.284730	-3.262158	4.703668
72	1	0	-4.319319	-2.018817	4.066276
73	1	0	-4.294727	-0.521933	2.099510
74	15	0	2.217811	0.390635	0.086295
75	15	0	-2.198359	0.206327	0.140769
76	6	0	-3.376515	1.544352	0.631722
77	6	0	-5.005756	3.723924	1.320288
78	6	0	-3.315747	2.103345	1.915114
79	6	0	-4.278837	2.080162	-0.293026
80	6	0	-5.084163	3.166063	0.048444
81	6	0	-4.124567	3.182943	2.255527
82	1	0	-2.626134	1.695850	2.646815
83	1	0	-4.357471	1.655269	-1.289592
84	1	0	-5.774551	3.571821	-0.684427
85	1	0	-4.061781	3.603638	3.254782
86	1	0	-5.630040	4.571610	1.584835
87	6	0	-3.216815	-0.689276	-1.104729
88	6	0	-4.751150	-1.848871	-3.140821
89	6	0	-4.170614	-1.665426	-0.802502
90	6	0	-3.031687	-0.308709	-2.439131
91	6	0	-3.807562	-0.871943	-3.450179
92	6	0	-4.925276	-2.248887	-1.817262
93	1	0	-4.316451	-1.990959	0.222441
94	1	0	-2.256682	0.412948	-2.687760
95	1	0	-3.657142	-0.562310	-4.480120
96	1	0	-5.651473	-3.018318	-1.573226
97	1	0	-5.343831	-2.302887	-3.929092
98	6	0	3.277139	1.803955	0.647552
99	6	0	4.678564	4.095727	1.472359
100	6	0	3.104975	2.322504	1.938915
101	6	0	4.181582	2.435666	-0.210729
102	6	0	4.874293	3.574858	0.197709
103	6	0	3.797856	3.458586	2.345157

104	1	0	2.421718	1.838217	2.627666
105	1	0	4.353200	2.049714	-1.209886
106	1	0	5.569154	4.051035	-0.487346
107	1	0	3.649796	3.845074	3.349257
108	1	0	5.215265	4.985027	1.788394
109	6	0	3.276532	-0.310688	-1.242869
110	6	0	4.970353	-1.044170	-3.349404
111	6	0	4.206246	-1.339575	-1.073740
112	6	0	3.171504	0.313268	-2.493471
113	6	0	4.033858	-0.028394	-3.530218
114	6	0	5.038313	-1.712789	-2.129250
115	1	0	4.284823	-1.854061	-0.120856
116	1	0	2.407792	1.071973	-2.652730
117	1	0	3.953399	0.477964	-4.487306
118	1	0	5.752268	-2.518837	-1.990270
119	1	0	5.633155	-1.325035	-4.161999

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Zero-point correction=                0.998082
(Hartree/Particle)

Thermal correction to Energy=         1.056391
Thermal correction to Enthalpy=       1.057335
Thermal correction to Gibbs Free Energy= 0.907816

Sum of electronic and zero-point Energies= -3209.814714
Sum of electronic and thermal Energies= -3209.756406
Sum of electronic and thermal Enthalpies= -3209.755462
Sum of electronic and thermal Free Energies= -3209.904980

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TS_{Xa-XIa}

Imaginary frequency: -956.1779

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Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	28	0	-0.013159	1.023190	1.536136
2	5	0	-1.610305	-0.102086	1.867527

3	8	0	-2.736939	0.266752	2.585730
4	6	0	-3.769960	-0.710801	2.336803
5	6	0	-2.942017	-1.963052	1.914950
6	8	0	-1.771687	-1.365318	1.321651
7	6	0	-2.457929	-2.788815	3.107194
8	1	0	-3.280719	-3.325040	3.590609
9	1	0	-1.973034	-2.145350	3.850507
10	1	0	-1.721572	-3.516805	2.752280
11	6	0	-3.613519	-2.861316	0.889597
12	1	0	-4.542614	-3.280132	1.293560
13	1	0	-2.941220	-3.685498	0.630473
14	1	0	-3.840780	-2.311342	-0.027811
15	6	0	-4.597222	-0.887934	3.600261
16	1	0	-5.332514	-1.689808	3.469358
17	1	0	-5.137316	0.038419	3.817257
18	1	0	-3.966994	-1.126143	4.459715
19	6	0	-4.636379	-0.175528	1.200892
20	1	0	-5.493175	-0.828993	1.005802
21	1	0	-4.050211	-0.081887	0.282402
22	1	0	-5.006974	0.817359	1.473224
23	6	0	1.628856	1.864544	2.267534
24	6	0	1.219086	1.042780	3.157866
25	1	0	-0.127747	0.239965	2.849562
26	6	0	1.476375	0.455102	4.501466
27	1	0	2.313718	0.978689	4.975315
28	1	0	1.738138	-0.605631	4.419037
29	1	0	0.599738	0.535927	5.152090
30	6	0	2.809193	2.783261	2.099462
31	1	0	3.152047	3.118395	3.089062
32	1	0	2.530344	3.674709	1.528009
33	7	0	3.952850	2.169261	1.427977
34	6	0	4.403106	0.970097	2.116784
35	1	0	3.647705	0.162890	2.103703
36	1	0	4.627102	1.209344	3.162347
37	1	0	5.317777	0.601307	1.644295

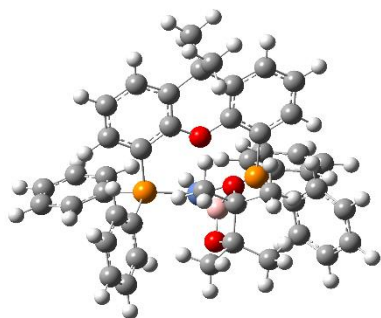
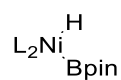
38	6	0	3.695643	1.914100	0.018208
39	1	0	3.075587	1.010727	-0.131330
40	1	0	3.097214	2.743156	-0.379820
41	6	0	4.946822	1.813298	-0.812615
42	1	0	4.788599	1.452182	-1.827882
43	6	0	6.170060	2.147888	-0.409222
44	1	0	7.026404	2.073488	-1.072689
45	1	0	6.340292	2.518666	0.597674
46	1	0	-1.001359	-5.859522	-1.202022
47	6	0	-0.985178	-4.777780	-1.288664
48	6	0	-0.962065	-2.031623	-1.491240
49	6	0	-1.952278	-4.128452	-2.051274
50	6	0	0.013947	-4.043567	-0.654725
51	6	0	0.042960	-2.651990	-0.748102
52	6	0	-1.949263	-2.739124	-2.176866
53	1	0	-2.712776	-4.714516	-2.556322
54	1	0	0.778238	-4.554309	-0.076233
55	6	0	-2.884413	-1.951250	-3.082657
56	8	0	-0.919188	-0.656175	-1.560593
57	6	0	-2.136387	-1.677475	-4.408199
58	1	0	-1.892375	-2.623301	-4.903635
59	1	0	-1.204804	-1.132638	-4.222590
60	1	0	-2.760525	-1.075617	-5.077062
61	6	0	-4.172349	-2.716161	-3.388844
62	1	0	-4.740105	-2.931783	-2.477557
63	1	0	-3.944471	-3.660352	-3.890424
64	1	0	-4.807255	-2.145869	-4.071906
65	6	0	-3.153377	-0.604395	-2.420309
66	6	0	-3.398201	1.992394	-1.403966
67	6	0	-4.352829	0.094706	-2.543178
68	6	0	-2.099225	0.017444	-1.741195
69	6	0	-2.175811	1.328718	-1.249654
70	6	0	-4.478075	1.381646	-2.032705
71	1	0	-5.196926	-0.362720	-3.047536
72	1	0	-5.418994	1.913965	-2.124881

73	1	0	-3.524984	2.989139	-1.000997
74	15	0	1.339241	-1.580118	0.011437
75	15	0	-0.762714	2.059173	-0.291689
76	6	0	-1.447879	3.685072	0.215012
77	6	0	-2.495085	6.124839	1.104894
78	6	0	-1.605233	3.932122	1.581335
79	6	0	-1.825083	4.675761	-0.703274
80	6	0	-2.343723	5.887832	-0.262049
81	6	0	-2.128163	5.147640	2.023876
82	1	0	-1.315797	3.168455	2.299525
83	1	0	-1.709114	4.494867	-1.769569
84	1	0	-2.629937	6.647645	-0.982740
85	1	0	-2.245013	5.326944	3.088025
86	1	0	-2.898148	7.072041	1.449927
87	6	0	0.523191	2.506350	-1.543238
88	6	0	2.690484	3.077945	-3.244037
89	6	0	1.127546	1.494244	-2.302135
90	6	0	1.041388	3.804470	-1.632920
91	6	0	2.107081	4.088551	-2.486540
92	6	0	2.201174	1.776887	-3.141379
93	1	0	0.773929	0.473061	-2.227700
94	1	0	0.630361	4.603732	-1.026338
95	1	0	2.490088	5.102955	-2.542372
96	1	0	2.663626	0.967163	-3.700573
97	1	0	3.531202	3.298479	-3.894751
98	6	0	1.955957	-2.714987	1.326241
99	6	0	2.662997	-4.381108	3.469052
100	6	0	1.252553	-2.660155	2.536857
101	6	0	3.018285	-3.615799	1.202924
102	6	0	3.371539	-4.439495	2.271364
103	6	0	1.596641	-3.492820	3.597911
104	1	0	0.419900	-1.967040	2.632885
105	1	0	3.570697	-3.680486	0.269732
106	1	0	4.199431	-5.133866	2.163354
107	1	0	1.034263	-3.443459	4.526370

108	1	0	2.939772	-5.025200	4.298032
109	6	0	2.642165	-1.713594	-1.293269
110	6	0	4.643558	-1.646870	-3.270794
111	6	0	2.341621	-2.012529	-2.628133
112	6	0	3.963539	-1.373241	-0.970215
113	6	0	4.956488	-1.351621	-1.945147
114	6	0	3.332799	-1.974988	-3.607993
115	1	0	1.328438	-2.286272	-2.910418
116	1	0	4.222318	-1.122621	0.056802
117	1	0	5.970924	-1.082055	-1.666642
118	1	0	3.078111	-2.212151	-4.636877
119	1	0	5.415678	-1.622229	-4.033714

Zero-point correction=	0.992680
(Hartree/Particle)	
Thermal correction to Energy=	1.051511
Thermal correction to Enthalpy=	1.052455
Thermal correction to Gibbs Free Energy=	0.899092
Sum of electronic and zero-point Energies=	-3209.778252
Sum of electronic and thermal Energies=	-3209.719422
Sum of electronic and thermal Enthalpies=	-3209.718478
Sum of electronic and thermal Free Energies=	-3209.871840

XII



Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	1	0	-4.666022	2.427782	-2.864583
2	6	0	-3.690287	2.177687	-2.461949
3	6	0	-1.192925	1.571703	-1.434726
4	6	0	-2.537723	2.518369	-3.160404
5	6	0	-3.583882	1.518407	-1.241285
6	6	0	-2.336182	1.182733	-0.715959
7	6	0	-1.265610	2.232734	-2.661149
8	1	0	-2.628651	3.032370	-4.113669
9	1	0	-4.481886	1.256798	-0.687609
10	6	0	-0.013769	2.644923	-3.430787
11	8	0	0.000413	1.297820	-0.846840
12	6	0	-0.013707	1.946645	-4.804400
13	1	0	-0.897514	2.232213	-5.383418
14	1	0	-0.016614	0.859500	-4.682203
15	1	0	0.871936	2.228982	-5.382248
16	6	0	-0.022565	4.173636	-3.627171
17	1	0	-0.019045	4.685857	-2.660718
18	1	0	-0.912250	4.487221	-4.181640
19	1	0	0.855998	4.497059	-4.193663
20	6	0	1.246506	2.245491	-2.667853
21	6	0	3.579334	1.579415	-1.246933
22	6	0	2.512476	2.557943	-3.165958
23	6	0	1.186946	1.576586	-1.444005
24	6	0	2.339494	1.197131	-0.731516
25	6	0	3.671603	2.247213	-2.463908
26	1	0	2.592771	3.078444	-4.116642
27	1	0	4.640925	2.531893	-2.858892
28	1	0	4.481078	1.356517	-0.682224
29	15	0	-2.185006	0.277243	0.887215
30	15	0	2.200888	0.266884	0.859482
31	6	0	3.346685	1.241987	1.934381
32	6	0	5.026160	2.851115	3.492762
33	6	0	2.843967	2.380084	2.572393

34	6	0	4.696937	0.911254	2.092460
35	6	0	5.530997	1.713104	2.869920
36	6	0	3.681343	3.182925	3.341406
37	1	0	1.787506	2.613909	2.472711
38	1	0	5.102916	0.023623	1.615694
39	1	0	6.576052	1.443758	2.989643
40	1	0	3.278945	4.064542	3.831198
41	1	0	5.676223	3.473456	4.100221
42	6	0	3.190136	-1.267625	0.624042
43	6	0	4.704455	-3.625874	0.578954
44	6	0	4.036774	-1.543828	-0.451535
45	6	0	3.092410	-2.199227	1.665470
46	6	0	3.851208	-3.363424	1.650373
47	6	0	4.786361	-2.721515	-0.475367
48	1	0	4.111715	-0.852110	-1.284442
49	1	0	2.403031	-2.013001	2.485834
50	1	0	3.765833	-4.073351	2.467052
51	1	0	5.436893	-2.925997	-1.320377
52	1	0	5.293812	-4.537473	0.561873
53	6	0	-3.327141	1.253780	1.963935
54	6	0	-5.003318	2.864422	3.525917
55	6	0	-4.700793	0.990578	2.033957
56	6	0	-2.801878	2.325137	2.691629
57	6	0	-3.637350	3.128542	3.463847
58	6	0	-5.532937	1.792434	2.811528
59	1	0	-5.126390	0.153254	1.487403
60	1	0	-1.731345	2.508378	2.655808
61	1	0	-3.216226	3.957076	4.025442
62	1	0	-6.595794	1.575818	2.860226
63	1	0	-5.652134	3.486905	4.134552
64	6	0	-3.184275	-1.249997	0.649478
65	6	0	-4.708092	-3.597857	0.514001
66	6	0	-3.776072	-1.637598	-0.553767
67	6	0	-3.337866	-2.066612	1.777461
68	6	0	-4.098849	-3.229042	1.713014

69	6	0	-4.538223	-2.805717	-0.617585
70	1	0	-3.637479	-1.037368	-1.447574
71	1	0	-2.863377	-1.785147	2.715510
72	1	0	-4.211373	-3.848991	2.597044
73	1	0	-4.995012	-3.096061	-1.559342
74	1	0	-5.302530	-4.504661	0.461620
75	28	0	0.005099	0.142009	1.303903
76	1	0	0.025369	1.454746	2.192943
77	5	0	-0.042297	-1.484387	0.111011
78	8	0	-0.465345	-1.449789	-1.213638
79	8	0	0.362798	-2.758935	0.454545
80	6	0	-0.101494	-2.689212	-1.849830
81	6	0	0.087721	-3.660214	-0.635005
82	6	0	1.260942	-4.619989	-0.770229
83	1	0	2.205603	-4.079056	-0.870138
84	1	0	1.128850	-5.276299	-1.638219
85	1	0	1.324114	-5.244151	0.126538
86	6	0	-1.185221	-4.418427	-0.271987
87	1	0	-2.022284	-3.726073	-0.148927
88	1	0	-1.028630	-4.934552	0.679978
89	1	0	-1.446546	-5.160577	-1.033810
90	6	0	1.192449	-2.419159	-2.616515
91	1	0	1.019265	-1.596754	-3.317630
92	1	0	1.524021	-3.296937	-3.180750
93	1	0	1.990226	-2.120753	-1.930494
94	6	0	-1.202886	-3.090039	-2.820783
95	1	0	-1.283448	-2.334849	-3.609221
96	1	0	-2.169360	-3.165589	-2.317671
97	1	0	-0.972758	-4.053080	-3.290425

Zero-point correction= 0.795102
(Hartree/Particle)

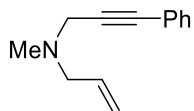
Thermal correction to Energy= 0.842913

Thermal correction to Enthalpy= 0.843857

Thermal correction to Gibbs Free Energy= 0.713308

Sum of electronic and zero-point Energies=	-2842.801724
Sum of electronic and thermal Energies=	-2842.753913
Sum of electronic and thermal Enthalpies=	-2842.752969
Sum of electronic and thermal Free Energies=	-2842.883518

Enyne-Ph

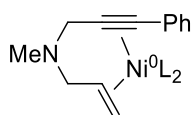


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-2.983706	-0.510363	-0.430397
2	6	0	-4.248585	-1.167535	-0.728673
3	1	0	-4.793415	-1.481175	0.181219
4	1	0	-4.069016	-2.051282	-1.347090
5	1	0	-4.889760	-0.482000	-1.289545
6	6	0	-3.251741	0.718094	0.324349
7	1	0	-3.774741	0.470367	1.271382
8	1	0	-3.942016	1.320213	-0.276712
9	6	0	-2.112277	-1.433210	0.295794
10	1	0	-2.405465	-1.516476	1.360580
11	1	0	-2.244200	-2.430799	-0.137791
12	6	0	-0.687545	-1.088010	0.202140
13	6	0	0.487418	-0.815401	0.125381
14	6	0	-2.040159	1.551327	0.644424
15	1	0	-1.342033	1.154966	1.378146
16	6	0	-1.819160	2.748568	0.108842
17	1	0	-0.954685	3.345498	0.383418
18	1	0	-2.498867	3.174436	-0.625428
19	6	0	1.865525	-0.430926	0.020558
20	6	0	4.542298	0.345932	-0.192738
21	6	0	2.193951	0.880807	-0.351272
22	6	0	2.891034	-1.348513	0.285636

23	6	0	4.221176	-0.958318	0.178677
24	6	0	3.526097	1.262989	-0.457113
25	1	0	1.393613	1.585689	-0.554961
26	1	0	2.634203	-2.363308	0.571768
27	1	0	5.009737	-1.675535	0.383856
28	1	0	3.772606	2.279930	-0.746021
29	1	0	5.581791	0.647188	-0.276065

Zero-point correction=			0.249187		
(Hartree/Particle)					
Thermal correction to Energy=			0.262944		
Thermal correction to Enthalpy=			0.263888		
Thermal correction to Gibbs Free Energy=			0.205940		
Sum of electronic and zero-point Energies=			-558.551173		
Sum of electronic and thermal Energies=			-558.537416		
Sum of electronic and thermal Enthalpies=			-558.536472		
Sum of electronic and thermal Free Energies=			-558.594420		

IIIb



Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	28	0	-0.072101	1.635475	-0.863502
2	6	0	1.260479	2.256519	-3.700107
3	1	0	1.858476	1.616642	-4.361382
4	1	0	0.499825	2.753607	-4.338172
5	6	0	0.540862	1.432002	-2.701712
6	6	0	-0.228925	0.457725	-2.437149
7	7	0	2.150099	3.254441	-3.111556
8	6	0	1.487425	4.026106	-2.065612
9	1	0	0.500483	4.412566	-2.389452

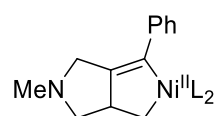
10	1	0	2.125925	4.897575	-1.868022
11	6	0	1.360648	3.246482	-0.787395
12	1	0	2.281206	2.743563	-0.494594
13	6	0	0.384266	3.419932	0.163776
14	1	0	0.563711	3.112637	1.189894
15	1	0	-0.451868	4.098463	-0.005557
16	6	0	2.672339	4.115058	-4.157510
17	1	0	3.182071	3.506586	-4.911113
18	1	0	3.395585	4.818502	-3.735907
19	1	0	1.878955	4.693412	-4.667845
20	1	0	-5.439652	-2.209916	-0.424236
21	6	0	-4.383229	-2.076606	-0.213729
22	6	0	-1.709330	-1.747216	0.317970
23	6	0	-3.520786	-3.167475	-0.287297
24	6	0	-3.897682	-0.813873	0.113498
25	6	0	-2.539216	-0.625092	0.378632
26	6	0	-2.161439	-3.024041	-0.011973
27	1	0	-3.916595	-4.140430	-0.560009
28	1	0	-4.575011	0.033777	0.139334
29	6	0	-1.159438	-4.171545	0.048394
30	8	0	-0.386458	-1.542332	0.630458
31	6	0	-1.022822	-4.599886	1.528231
32	1	0	-1.985367	-4.958276	1.908403
33	1	0	-0.696605	-3.757770	2.148447
34	1	0	-0.283256	-5.402554	1.620661
35	6	0	-1.608041	-5.374756	-0.780378
36	1	0	-1.731548	-5.105061	-1.833899
37	1	0	-2.556232	-5.767725	-0.402930
38	1	0	-0.878903	-6.186134	-0.702389
39	6	0	0.196374	-3.633699	-0.395199
40	6	0	2.753452	-2.551801	-0.858830
41	6	0	1.163784	-4.362717	-1.086283
42	6	0	0.537292	-2.340706	-0.002785
43	6	0	1.804580	-1.783314	-0.181195
44	6	0	2.424973	-3.821850	-1.329801

45	1	0	0.938524	-5.364933	-1.436126
46	1	0	3.165750	-4.404733	-1.867909
47	1	0	3.749528	-2.151809	-1.022726
48	15	0	-1.739819	1.018051	0.601427
49	15	0	2.054900	-0.082111	0.474169
50	6	0	3.815138	0.188180	0.008288
51	6	0	6.427326	0.660693	-0.882362
52	6	0	4.043815	0.793431	-1.234528
53	6	0	4.908982	-0.174181	0.801818
54	6	0	6.207778	0.063384	0.358064
55	6	0	5.343516	1.024498	-1.678775
56	1	0	3.199376	1.099488	-1.850481
57	1	0	4.743960	-0.642024	1.768857
58	1	0	7.051073	-0.219607	0.981056
59	1	0	5.504755	1.499447	-2.641964
60	1	0	7.441286	0.845870	-1.224168
61	6	0	2.183097	-0.395935	2.285165
62	6	0	2.383375	-0.649019	5.070792
63	6	0	2.126310	-1.655226	2.888428
64	6	0	2.321809	0.736472	3.098418
65	6	0	2.435120	0.611928	4.478367
66	6	0	2.220144	-1.779093	4.274308
67	1	0	2.020788	-2.546909	2.275556
68	1	0	2.343424	1.725294	2.642914
69	1	0	2.543430	1.500509	5.093297
70	1	0	2.175113	-2.764303	4.729743
71	1	0	2.461049	-0.748511	6.149522
72	6	0	-3.163633	2.163713	0.406657
73	6	0	-5.307274	3.904888	-0.044919
74	6	0	-4.148000	2.343262	1.386329
75	6	0	-3.263904	2.867868	-0.797749
76	6	0	-4.333109	3.732764	-1.024612
77	6	0	-5.213392	3.209916	1.160871
78	1	0	-4.075120	1.804919	2.328052
79	1	0	-2.492439	2.737689	-1.555037

80	1	0	-4.400100	4.275195	-1.962679
81	1	0	-5.971229	3.344725	1.926450
82	1	0	-6.137391	4.583167	-0.217161
83	6	0	-1.421268	1.103051	2.413737
84	6	0	-0.811858	1.347006	5.140641
85	6	0	-1.240975	-0.034781	3.205969
86	6	0	-1.288807	2.365896	3.006988
87	6	0	-0.988679	2.487301	4.360632
88	6	0	-0.939298	0.088748	4.559912
89	1	0	-1.336064	-1.024656	2.772645
90	1	0	-1.446068	3.262483	2.411692
91	1	0	-0.897473	3.473853	4.805052
92	1	0	-0.792997	-0.805443	5.158158
93	1	0	-0.572396	1.438883	6.195962
94	1	0	-0.347118	-3.925705	-3.909258
95	6	0	-0.910078	-3.033873	-3.646401
96	6	0	-2.332942	-0.754607	-2.930646
97	6	0	-2.300072	-3.029053	-3.740872
98	6	0	-0.228873	-1.900549	-3.211582
99	6	0	-0.930920	-0.739630	-2.857977
100	6	0	-3.008198	-1.883086	-3.377749
101	1	0	-2.829364	-3.913493	-4.084170
102	1	0	0.854781	-1.911784	-3.124043
103	1	0	-4.093111	-1.873998	-3.429170
104	1	0	-2.883722	0.132836	-2.628495

Zero-point correction=				0.854146	
(Hartree/Particle)					
Thermal correction to Energy=				0.905152	
Thermal correction to Enthalpy=				0.906096	
Thermal correction to Gibbs Free Energy=				0.769582	
Sum of electronic and zero-point Energies=				-2989.945098	
Sum of electronic and thermal Energies=				-2989.894092	
Sum of electronic and thermal Enthalpies=				-2989.893148	
Sum of electronic and thermal Free Energies=				-2990.029662	

IIIb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-6.457289	0.380736	-0.343273
2	6	0	-5.440934	0.057252	-0.542978
3	6	0	-2.871141	-0.776930	-1.019946
4	6	0	-5.217054	-1.151070	-1.205119
5	6	0	-4.372388	0.848363	-0.137527
6	6	0	-3.053292	0.441729	-0.374836
7	6	0	-3.921066	-1.587982	-1.460284
8	1	0	-6.065107	-1.752839	-1.515251
9	1	0	-4.559781	1.778325	0.391704
10	6	0	-3.537582	-2.866920	-2.202209
11	8	0	-1.576130	-1.211067	-1.204432
12	6	0	-4.705080	-3.846583	-2.302882
13	1	0	-5.533290	-3.394019	-2.855555
14	1	0	-5.067030	-4.148574	-1.314745
15	1	0	-4.404870	-4.741903	-2.854772
16	6	0	-3.073212	-2.489974	-3.626779
17	1	0	-2.234582	-1.789060	-3.597575
18	1	0	-3.896990	-2.021998	-4.175083
19	1	0	-2.756813	-3.389107	-4.165330
20	6	0	-2.357784	-3.456063	-1.435865
21	6	0	-0.157532	-4.296759	0.095585
22	6	0	-2.168687	-4.804817	-1.147773
23	6	0	-1.402618	-2.554957	-0.958660
24	6	0	-0.315512	-2.931229	-0.172776
25	6	0	-1.067245	-5.223971	-0.401167
26	1	0	-2.888077	-5.539152	-1.495106

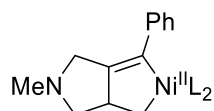
27	1	0	-0.933612	-6.278467	-0.183332
28	1	0	0.668120	-4.629435	0.716122
29	15	0	-1.565188	1.462464	0.030338
30	15	0	0.667266	-1.587785	0.612128
31	6	0	2.199683	-2.480021	1.104598
32	6	0	4.596909	-3.778938	1.755253
33	6	0	2.823731	-3.327878	0.182248
34	6	0	2.800541	-2.277455	2.350259
35	6	0	3.994911	-2.920260	2.669682
36	6	0	4.005992	-3.981276	0.510266
37	1	0	2.387559	-3.478562	-0.800713
38	1	0	2.336973	-1.627501	3.085150
39	1	0	4.447530	-2.754683	3.642597
40	1	0	4.474408	-4.634119	-0.219749
41	1	0	5.523505	-4.284860	2.008609
42	6	0	-0.217883	-1.373414	2.220692
43	6	0	-1.457707	-0.914679	4.693940
44	6	0	-1.265662	-2.193261	2.649866
45	6	0	0.178952	-0.298875	3.032047
46	6	0	-0.424482	-0.082272	4.267373
47	6	0	-1.884617	-1.959282	3.877999
48	1	0	-1.600414	-3.020950	2.031682
49	1	0	0.964055	0.375293	2.692457
50	1	0	-0.103141	0.751690	4.883393
51	1	0	-2.697527	-2.603508	4.198898
52	1	0	-1.935530	-0.742159	5.653630
53	6	0	-1.622006	2.640958	-1.385876
54	6	0	-1.668520	4.302609	-3.638659
55	6	0	-2.727735	3.461891	-1.639717
56	6	0	-0.545522	2.655963	-2.277510
57	6	0	-0.571146	3.481841	-3.400958
58	6	0	-2.747586	4.293185	-2.754884
59	1	0	-3.577038	3.456364	-0.961497
60	1	0	0.325667	2.031376	-2.088186
61	1	0	0.273909	3.484729	-4.082334

62	1	0	-3.607241	4.930605	-2.937728
63	1	0	-1.686075	4.949510	-4.510321
64	6	0	-2.205855	2.394403	1.473190
65	6	0	-3.070575	3.662360	3.814649
66	6	0	-2.650380	1.641210	2.566500
67	6	0	-2.195706	3.788766	1.565868
68	6	0	-2.627950	4.417878	2.732533
69	6	0	-3.080256	2.271012	3.729276
70	1	0	-2.660078	0.553905	2.508897
71	1	0	-1.854052	4.387971	0.726828
72	1	0	-2.616432	5.501698	2.792395
73	1	0	-3.415002	1.671043	4.570446
74	1	0	-3.405115	4.155222	4.722342
75	28	0	0.780506	0.811360	0.049677
76	1	0	1.528673	2.531707	1.605198
77	6	0	1.129806	2.693312	0.590838
78	1	0	0.272346	3.370780	0.679068
79	6	0	2.211049	3.259650	-0.310802
80	6	0	3.238247	4.285522	0.175891
81	7	0	4.301904	4.142598	-0.822304
82	6	0	4.468037	2.698501	-1.051968
83	6	0	3.103810	2.126207	-0.712594
84	1	0	1.746798	3.684162	-1.215616
85	1	0	3.588937	4.012202	1.192934
86	1	0	2.879439	5.320590	0.202169
87	1	0	5.239334	2.275998	-0.381182
88	1	0	4.796672	2.503422	-2.081120
89	6	0	5.532244	4.808428	-0.465954
90	1	0	6.269160	4.687813	-1.267084
91	1	0	5.974746	4.410718	0.468213
92	1	0	5.350287	5.879511	-0.328336
93	6	0	2.637935	0.870654	-0.608008
94	6	0	3.488277	-0.248243	-1.072760
95	6	0	5.184573	-2.250785	-2.110675
96	6	0	3.117139	-1.003233	-2.196389

97	6	0	4.712345	-0.553899	-0.456617
98	6	0	5.551952	-1.535797	-0.970873
99	6	0	3.958178	-1.985550	-2.716181
100	1	0	2.162565	-0.790179	-2.674625
101	1	0	5.000704	-0.003176	0.435168
102	1	0	6.495587	-1.750013	-0.476051
103	1	0	3.656772	-2.542272	-3.599683
104	1	0	5.844135	-3.012671	-2.515980

Zero-point correction=		0.857302
(Hartree/Particle)		
Thermal correction to Energy=		0.906957
Thermal correction to Enthalpy=		0.907901
Thermal correction to Gibbs Free Energy=		0.774533
Sum of electronic and zero-point Energies=		-2989.941542
Sum of electronic and thermal Energies=		-2989.891886
Sum of electronic and thermal Enthalpies=		-2989.890942
Sum of electronic and thermal Free Energies=		-2990.024311

IIIb-HBpin



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	28	0	-0.916351	-0.483357	0.710394
2	1	0	1.604082	-2.905362	-4.782915
3	6	0	1.717664	-2.175980	-3.987440
4	6	0	2.005519	-0.338463	-1.964698
5	6	0	2.978691	-1.932126	-3.447363
6	6	0	0.601429	-1.493242	-3.512595
7	6	0	0.726405	-0.563574	-2.478075
8	6	0	3.147268	-0.992867	-2.429538
9	1	0	3.837070	-2.475338	-3.829685

10	1	0	-0.377982	-1.701440	-3.930723
11	6	0	4.484856	-0.578600	-1.827109
12	8	0	2.113556	0.585639	-0.948028
13	6	0	4.900408	0.766010	-2.468769
14	1	0	5.036351	0.641227	-3.548227
15	1	0	4.138265	1.533710	-2.300170
16	1	0	5.842218	1.114015	-2.031733
17	6	0	5.585816	-1.606888	-2.081359
18	1	0	5.345019	-2.580643	-1.642424
19	1	0	5.745958	-1.737399	-3.155309
20	1	0	6.533209	-1.259566	-1.659679
21	6	0	4.246725	-0.332581	-0.341534
22	6	0	3.704440	0.428005	2.310199
23	6	0	5.147389	-0.630361	0.681527
24	6	0	3.065203	0.314711	0.015382
25	6	0	2.765166	0.717855	1.318458
26	6	0	4.877046	-0.255139	1.995061
27	1	0	6.073065	-1.149314	0.454429
28	1	0	5.591636	-0.485563	2.778607
29	1	0	3.508448	0.723667	3.336257
30	15	0	-0.707254	0.247843	-1.653054
31	15	0	1.110161	1.478225	1.593249
32	6	0	1.203127	1.869649	3.385983
33	6	0	1.296500	2.277715	6.153613
34	6	0	0.914289	0.821133	4.269716
35	6	0	1.530715	3.125931	3.902839
36	6	0	1.571944	3.327849	5.281409
37	6	0	0.970768	1.021157	5.645780
38	1	0	0.648997	-0.157167	3.873280
39	1	0	1.752731	3.948719	3.229206
40	1	0	1.823520	4.308686	5.673712
41	1	0	0.750101	0.199388	6.320081
42	1	0	1.331027	2.438743	7.226736
43	6	0	1.323975	3.122449	0.803765
44	6	0	1.482882	5.685838	-0.307071

45	6	0	2.569538	3.709229	0.555929
46	6	0	0.160963	3.823675	0.468354
47	6	0	0.239465	5.104502	-0.070635
48	6	0	2.647041	4.983096	-0.002679
49	1	0	3.480334	3.171578	0.807313
50	1	0	-0.811513	3.359270	0.613135
51	1	0	-0.671654	5.635576	-0.328101
52	1	0	3.618428	5.430677	-0.191177
53	1	0	1.546263	6.680782	-0.737831
54	6	0	-2.121068	-0.519627	-2.536640
55	6	0	-4.302116	-1.794140	-3.736515
56	6	0	-2.582949	-1.746682	-2.042067
57	6	0	-2.743621	0.048101	-3.650869
58	6	0	-3.835582	-0.583139	-4.242642
59	6	0	-3.666433	-2.381469	-2.643389
60	1	0	-2.095030	-2.198346	-1.181435
61	1	0	-2.385651	0.991100	-4.052133
62	1	0	-4.320630	-0.126812	-5.100035
63	1	0	-4.023199	-3.327558	-2.247712
64	1	0	-5.156922	-2.281742	-4.195320
65	6	0	-0.651125	1.967589	-2.298976
66	6	0	-0.669817	4.617261	-3.211373
67	6	0	0.506368	2.540161	-2.834247
68	6	0	-1.815188	2.741753	-2.214041
69	6	0	-1.825607	4.054476	-2.674608
70	6	0	0.495006	3.858636	-3.283817
71	1	0	1.421691	1.963346	-2.913694
72	1	0	-2.727155	2.309507	-1.815845
73	1	0	-2.743633	4.631649	-2.607986
74	1	0	1.403148	4.290760	-3.692910
75	1	0	-0.674822	5.643778	-3.566144
76	7	0	-4.813740	-2.689086	2.666362
77	6	0	-4.888602	-1.440545	1.894804
78	6	0	-3.459395	-1.223249	1.444098
79	6	0	-2.586250	-2.280637	2.063449

80	6	0	-3.464979	-2.738787	3.234425
81	1	0	-5.220591	-0.590867	2.524679
82	1	0	-5.614162	-1.540639	1.077937
83	1	0	-3.353910	-2.026593	4.078566
84	1	0	-3.245901	-3.746473	3.606229
85	6	0	-5.864074	-2.814134	3.649853
86	1	0	-6.842153	-2.787439	3.157719
87	1	0	-5.836614	-2.002433	4.402429
88	1	0	-5.771654	-3.770770	4.174662
89	6	0	-2.844240	-0.208295	0.827663
90	6	0	-3.567976	0.973788	0.328837
91	6	0	-4.915047	3.275837	-0.592012
92	6	0	-4.553217	0.884366	-0.668538
93	6	0	-3.276623	2.244619	0.852079
94	6	0	-3.942298	3.381360	0.403439
95	6	0	-5.217021	2.022359	-1.123623
96	1	0	-4.778866	-0.089513	-1.097806
97	1	0	-2.521761	2.319883	1.632431
98	1	0	-3.701098	4.352244	0.828655
99	1	0	-5.969641	1.928277	-1.901668
100	1	0	-5.433215	4.161545	-0.947769
101	1	0	-2.473265	-3.129831	1.370352
102	6	0	-1.238082	-1.609573	2.316530
103	1	0	-0.439084	-2.315239	2.591913
104	1	0	-1.349185	-0.891393	3.140229
105	1	0	0.810502	-1.027838	0.515337
106	5	0	0.939778	-2.220224	0.475970
107	8	0	1.819057	-2.852574	1.299908
108	6	0	2.062704	-4.153421	0.707897
109	6	0	0.785191	-4.370956	-0.175026
110	8	0	0.385832	-3.010432	-0.484183
111	6	0	2.250035	-5.172826	1.818292
112	1	0	3.157607	-4.936005	2.380489
113	1	0	2.357357	-6.178433	1.398175
114	1	0	1.405600	-5.166690	2.510245

115	6	0	3.336256	-4.014499	-0.121542
116	1	0	4.140856	-3.649904	0.524526
117	1	0	3.187664	-3.287655	-0.927387
118	1	0	3.637309	-4.971147	-0.559881
119	6	0	-0.367496	-5.008060	0.594117
120	1	0	-0.553577	-4.479869	1.534933
121	1	0	-0.163473	-6.060333	0.813529
122	1	0	-1.274801	-4.948368	-0.014307
123	6	0	1.033283	-5.105288	-1.482168
124	1	0	1.726680	-4.551432	-2.119709
125	1	0	0.088180	-5.216390	-2.021826
126	1	0	1.440152	-6.103772	-1.289418

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Zero-point correction=                1.052588
(Hartree/Particle)

Thermal correction to Energy=          1.113320

Thermal correction to Enthalpy=        1.114265

Thermal correction to Gibbs Free Energy= 0.956529

Sum of electronic and zero-point Energies= -3401.452251
Sum of electronic and thermal Energies=    -3401.391519
Sum of electronic and thermal Enthalpies=   -3401.390575
Sum of electronic and thermal Free Energies= -3401.548310

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TS_{nb-nb}

imaginary frequencies = -152.6732 cm⁻¹

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	28	0	-0.153588	-1.433476	-0.280921
2	1	0	-1.016372	-3.456736	1.156058
3	6	0	-0.260252	-3.263058	0.391808
4	1	0	0.695129	-3.745017	0.598213
5	6	0	-0.733250	-3.404010	-1.006931
6	6	0	-2.020477	-4.164519	-1.256689

7	7	0	-2.354991	-3.978031	-2.657449
8	6	0	-2.337053	-2.543745	-2.885432
9	6	0	-1.241476	-1.924162	-2.056364
10	1	0	0.047328	-3.782147	-1.671756
11	1	0	-2.816363	-3.791643	-0.578943
12	1	0	-1.876927	-5.231317	-1.053034
13	1	0	-3.304436	-2.092050	-2.576065
14	1	0	-2.203942	-2.315842	-3.949584
15	1	0	-3.809948	-4.416636	-4.090792
16	6	0	-0.755909	-0.710935	-1.982275
17	6	0	-3.619079	-4.576606	-3.025164
18	1	0	-3.587896	-5.654081	-2.838277
19	1	0	-4.467018	-4.148270	-2.455470
20	1	0	4.327823	2.449622	-3.104145
21	6	0	3.545853	2.303591	-2.366076
22	6	0	1.558276	1.939007	-0.504970
23	6	0	2.646992	3.334582	-2.097405
24	6	0	3.445565	1.086863	-1.697125
25	6	0	2.432417	0.879682	-0.756356
26	6	0	1.638192	3.173797	-1.149417
27	1	0	2.738121	4.271482	-2.637286
28	1	0	4.141082	0.285121	-1.925405
29	6	0	0.650535	4.256375	-0.727246
30	8	0	0.572331	1.715533	0.426126
31	6	0	1.167440	4.879988	0.589948
32	1	0	2.145700	5.344986	0.427905
33	1	0	1.269926	4.117344	1.368861
34	1	0	0.466716	5.643430	0.944333
35	6	0	0.511192	5.354781	-1.780234
36	1	0	0.138645	4.949813	-2.726253
37	1	0	1.473658	5.843804	-1.954999
38	1	0	-0.177638	6.129606	-1.432299
39	6	0	-0.680822	3.574561	-0.427264
40	6	0	-3.014954	2.246064	0.419585
41	6	0	-1.939601	4.139373	-0.634919

42	6	0	-0.639598	2.327137	0.190251
43	6	0	-1.774409	1.637024	0.619753
44	6	0	-3.094181	3.485411	-0.210714
45	1	0	-2.025599	5.102738	-1.126904
46	1	0	-4.063426	3.946441	-0.373047
47	1	0	-3.920405	1.739877	0.742180
48	15	0	2.046192	-0.749509	0.002658
49	15	0	-1.498392	-0.050294	1.284177
50	6	0	-3.216642	-0.596168	1.626240
51	6	0	-5.841587	-1.509051	1.951517
52	6	0	-3.880728	-1.241844	0.575707
53	6	0	-3.878799	-0.415112	2.843133
54	6	0	-5.185314	-0.873552	3.003938
55	6	0	-5.188466	-1.690932	0.733443
56	1	0	-3.357735	-1.393943	-0.366943
57	1	0	-3.371157	0.080630	3.666262
58	1	0	-5.691305	-0.733713	3.954413
59	1	0	-5.691474	-2.191174	-0.089155
60	1	0	-6.858107	-1.867164	2.082369
61	6	0	-0.814383	0.280039	2.953411
62	6	0	0.271764	0.629847	5.505558
63	6	0	-0.907086	1.518189	3.595257
64	6	0	-0.160327	-0.778310	3.594651
65	6	0	0.369180	-0.606601	4.870206
66	6	0	-0.361146	1.692881	4.865474
67	1	0	-1.407850	2.346389	3.100439
68	1	0	-0.055515	-1.731922	3.080116
69	1	0	0.876853	-1.432291	5.358750
70	1	0	-0.435002	2.659010	5.355917
71	1	0	0.697083	0.766668	6.495420
72	6	0	3.225113	-1.855011	-0.864295
73	6	0	4.909850	-3.513181	-2.356961
74	6	0	4.549946	-2.056448	-0.464232
75	6	0	2.752142	-2.489807	-2.018659
76	6	0	3.593007	-3.311942	-2.764640

77	6	0	5.386864	-2.885902	-1.207280
78	1	0	4.925930	-1.566384	0.429942
79	1	0	1.722388	-2.325121	-2.333140
80	1	0	3.217590	-3.798249	-3.659747
81	1	0	6.413388	-3.040511	-0.889153
82	1	0	5.564183	-4.159082	-2.934376
83	6	0	2.730211	-0.645110	1.699848
84	6	0	3.692627	-0.605074	4.327833
85	6	0	2.991562	0.569429	2.336661
86	6	0	2.928199	-1.841195	2.402551
87	6	0	3.420585	-1.821689	3.702629
88	6	0	3.465825	0.587159	3.647100
89	1	0	2.831075	1.506407	1.811277
90	1	0	2.708502	-2.791992	1.921505
91	1	0	3.587163	-2.756393	4.229877
92	1	0	3.661031	1.538123	4.133378
93	1	0	4.070299	-0.588101	5.345787
94	6	0	-1.005766	0.515699	-2.728492
95	6	0	-1.491334	2.930737	-4.092660
96	6	0	0.036143	1.200075	-3.372283
97	6	0	-2.293669	1.075752	-2.769727
98	6	0	-2.531139	2.271480	-3.437869
99	6	0	-0.208498	2.387065	-4.056084
100	1	0	1.046604	0.800733	-3.317305
101	1	0	-3.104682	0.573257	-2.247388
102	1	0	-3.532288	2.693785	-3.441597
103	1	0	0.615084	2.897456	-4.548984
104	1	0	-1.677688	3.863634	-4.616969

Zero-point correction=
(Hartree/Particle)

0.854240

Thermal correction to Energy=

0.904204

Thermal correction to Enthalpy=

0.905149

Thermal correction to Gibbs Free Energy=

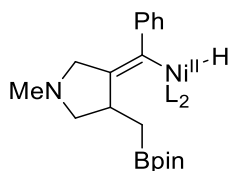
0.769915

Sum of electronic and zero-point Energies=

-2989.920054

Sum of electronic and thermal Energies=	-2989.870090
Sum of electronic and thermal Enthalpies=	-2989.869145
Sum of electronic and thermal Free Energies=	-2990.004379

IVb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-5.913723	-1.886142	0.718845
2	6	0	-4.907527	-1.887251	0.312282
3	6	0	-2.364671	-1.895274	-0.715060
4	6	0	-4.711439	-2.121956	-1.047656
5	6	0	-3.825445	-1.638062	1.151605
6	6	0	-2.521706	-1.622749	0.642871
7	6	0	-3.426743	-2.133679	-1.587524
8	1	0	-5.570395	-2.291598	-1.688817
9	1	0	-3.997953	-1.425743	2.201848
10	6	0	-3.082690	-2.397540	-3.049513
11	8	0	-1.077098	-1.884135	-1.200061
12	6	0	-2.588690	-3.856632	-3.177359
13	1	0	-3.386065	-4.549456	-2.888850
14	1	0	-1.723259	-4.035353	-2.530747
15	1	0	-2.297082	-4.063950	-4.212228
16	6	0	-4.285245	-2.190597	-3.968123
17	1	0	-4.671569	-1.168255	-3.898789
18	1	0	-5.088092	-2.886994	-3.710219
19	1	0	-4.012107	-2.393030	-5.007388
20	6	0	-1.920209	-1.474226	-3.403766
21	6	0	0.418303	0.009579	-3.904652
22	6	0	-1.729625	-0.841170	-4.631685

23	6	0	-0.926904	-1.304985	-2.440448
24	6	0	0.248577	-0.586936	-2.652305
25	6	0	-0.572160	-0.104974	-4.877408
26	1	0	-2.481200	-0.928777	-5.409495
27	1	0	-0.435171	0.374601	-5.840941
28	1	0	1.320887	0.573789	-4.115489
29	15	0	-1.043930	-1.062948	1.591230
30	15	0	1.420870	-0.455011	-1.241277
31	6	0	2.842013	0.398320	-2.033919
32	6	0	5.005231	1.810629	-3.119262
33	6	0	2.778681	1.789374	-2.188475
34	6	0	3.995606	-0.277652	-2.440642
35	6	0	5.072292	0.426825	-2.976201
36	6	0	3.850920	2.490615	-2.733041
37	1	0	1.901380	2.335854	-1.862723
38	1	0	4.067202	-1.354583	-2.322748
39	1	0	5.967054	-0.109847	-3.276707
40	1	0	3.785533	3.570001	-2.832318
41	1	0	5.848899	2.357200	-3.529920
42	6	0	2.042586	-2.168879	-1.039451
43	6	0	3.150863	-4.703092	-0.634674
44	6	0	1.736700	-3.217329	-1.909692
45	6	0	2.899783	-2.400415	0.043900
46	6	0	3.459586	-3.659360	0.235650
47	6	0	2.284328	-4.482117	-1.701665
48	1	0	1.080135	-3.050205	-2.759432
49	1	0	3.141148	-1.592557	0.732583
50	1	0	4.127553	-3.823025	1.076115
51	1	0	2.040210	-5.292195	-2.382553
52	1	0	3.581653	-5.687870	-0.478980
53	6	0	-1.828441	-0.601120	3.182127
54	6	0	-3.134286	0.190123	5.520928
55	6	0	-2.175921	-1.549052	4.149516
56	6	0	-2.138535	0.746030	3.391544
57	6	0	-2.796040	1.136728	4.556376

58	6	0	-2.822666	-1.153108	5.317793
59	1	0	-1.938469	-2.597685	3.989088
60	1	0	-1.863392	1.485195	2.641236
61	1	0	-3.032234	2.184944	4.714821
62	1	0	-3.082142	-1.893084	6.068840
63	1	0	-3.636657	0.498403	6.432882
64	6	0	-0.132796	-2.600284	2.007840
65	6	0	1.447817	-4.814095	2.652769
66	6	0	-0.272718	-3.793719	1.296943
67	6	0	0.818855	-2.517769	3.033104
68	6	0	1.599447	-3.621803	3.358365
69	6	0	0.518173	-4.894868	1.619864
70	1	0	-0.997471	-3.870613	0.491426
71	1	0	0.937141	-1.585386	3.580449
72	1	0	2.329457	-3.547451	4.158938
73	1	0	0.408345	-5.817612	1.058102
74	1	0	2.060839	-5.675438	2.900985
75	6	0	-3.844538	2.802021	-1.108519
76	8	0	-2.545606	3.263442	-1.536520
77	5	0	-1.703547	3.144220	-0.456487
78	8	0	-2.388487	2.918109	0.717050
79	6	0	-3.796297	3.070892	0.429212
80	6	0	-4.590071	2.083869	1.268961
81	1	0	-4.519037	2.352915	2.327315
82	1	0	-4.210633	1.065721	1.150931
83	1	0	-5.646964	2.102043	0.979693
84	6	0	-4.169784	4.506666	0.791875
85	1	0	-3.617278	5.221640	0.173835
86	1	0	-3.909688	4.684624	1.838982
87	1	0	-5.241494	4.686145	0.663505
88	6	0	-3.911114	1.311316	-1.438106
89	1	0	-3.153581	0.753907	-0.874506
90	1	0	-3.707122	1.172897	-2.504973
91	1	0	-4.891736	0.883516	-1.206712
92	6	0	-4.920120	3.568726	-1.859237

93	1	0	-4.788322	4.647490	-1.752670
94	1	0	-5.914131	3.295483	-1.488903
95	1	0	-4.871206	3.320493	-2.923285
96	6	0	-0.142883	3.129570	-0.567686
97	1	0	0.198092	3.692221	-1.446296
98	1	0	0.079839	2.070848	-0.786172
99	6	0	0.633238	3.553087	0.691428
100	1	0	0.023034	3.303613	1.568521
101	6	0	2.005718	2.897263	0.861473
102	6	0	3.046808	3.996975	0.758664
103	1	0	3.933972	3.713618	0.181891
104	1	0	3.390310	4.319662	1.764880
105	7	0	2.322716	5.074724	0.083521
106	6	0	0.989384	5.046361	0.679222
107	1	0	0.293739	5.660820	0.094739
108	1	0	1.013044	5.446244	1.712704
109	6	0	2.973583	6.359760	0.202722
110	1	0	3.968978	6.315813	-0.251075
111	1	0	3.089686	6.675011	1.257671
112	1	0	2.390946	7.124325	-0.321361
113	6	0	2.167834	1.594139	1.108509
114	28	0	0.689768	0.367583	0.935784
115	1	0	0.556819	0.877570	2.332201
116	1	0	2.655496	0.130587	3.265170
117	6	0	3.529689	0.167665	2.621222
118	6	0	5.732799	0.240643	0.941496
119	6	0	3.455862	0.946460	1.450231
120	6	0	4.672357	-0.555560	2.945593
121	6	0	5.779519	-0.535651	2.096729
122	6	0	4.593329	0.979811	0.627284
123	1	0	4.693622	-1.148373	3.856261
124	1	0	6.666632	-1.114377	2.335988
125	1	0	4.576693	1.567433	-0.285402
126	1	0	6.586793	0.269343	0.269861

Zero-point correction=	1.050986
(Hartree/Particle)	
Thermal correction to Energy=	1.111310
Thermal correction to Enthalpy=	1.112255
Thermal correction to Gibbs Free Energy=	0.957667
Sum of electronic and zero-point Energies=	-3401.485172
Sum of electronic and thermal Energies=	-3401.424847
Sum of electronic and thermal Enthalpies=	-3401.423903
Sum of electronic and thermal Free Energies=	-3401.578491

TS_{mb-ivb}

imaginary frequencies = -98.6048 cm⁻¹

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	28	0	-0.912765	-0.383779	0.643904
2	1	0	0.883182	-3.107750	-4.846116
3	6	0	1.151592	-2.420304	-4.050412
4	6	0	1.834525	-0.687423	-2.030371
5	6	0	2.447122	-2.428437	-3.537412
6	6	0	0.197156	-1.539355	-3.547835
7	6	0	0.525427	-0.659867	-2.515001
8	6	0	2.817145	-1.546998	-2.521266
9	1	0	3.174771	-3.127467	-3.936847
10	1	0	-0.813518	-1.551017	-3.942925
11	6	0	4.218780	-1.413271	-1.935820
12	8	0	2.136668	0.192679	-1.015615
13	6	0	4.891404	-0.180265	-2.583179
14	1	0	4.977754	-0.323376	-3.665415
15	1	0	4.308480	0.727602	-2.396090
16	1	0	5.892674	-0.038425	-2.163305
17	6	0	5.080808	-2.646052	-2.203965
18	1	0	4.645427	-3.550077	-1.765291
19	1	0	5.200866	-2.801355	-3.279989

20	1	0	6.083219	-2.505716	-1.790293
21	6	0	4.058358	-1.126757	-0.446006
22	6	0	3.719981	-0.281801	2.215174
23	6	0	4.904809	-1.591929	0.561150
24	6	0	3.031041	-0.264619	-0.067763
25	6	0	2.838836	0.187953	1.239388
26	6	0	4.733402	-1.177303	1.879535
27	1	0	5.709932	-2.277684	0.317896
28	1	0	5.403723	-1.544553	2.649849
29	1	0	3.603414	0.043766	3.244347
30	15	0	-0.691259	0.410656	-1.645922
31	15	0	1.391488	1.290113	1.538162
32	6	0	1.579280	1.623518	3.336168
33	6	0	1.760371	1.965908	6.108422
34	6	0	1.045848	0.664652	4.207913
35	6	0	2.198906	2.757790	3.867844
36	6	0	2.283479	2.928641	5.248534
37	6	0	1.144439	0.829827	5.586180
38	1	0	0.558369	-0.218487	3.799199
39	1	0	2.613460	3.510749	3.203561
40	1	0	2.761318	3.816083	5.652523
41	1	0	0.732120	0.077664	6.251598
42	1	0	1.828624	2.102224	7.183405
43	6	0	1.973996	2.860710	0.780469
44	6	0	2.715851	5.348918	-0.265922
45	6	0	3.315725	3.137014	0.496290
46	6	0	1.007173	3.836698	0.516652
47	6	0	1.377417	5.078694	0.008987
48	6	0	3.682388	4.373294	-0.030402
49	1	0	4.077738	2.387474	0.693182
50	1	0	-0.043277	3.617925	0.694249
51	1	0	0.615589	5.826807	-0.187748
52	1	0	4.726440	4.577757	-0.248511
53	1	0	3.005339	6.314334	-0.670409
54	6	0	-2.258580	-0.002864	-2.502366

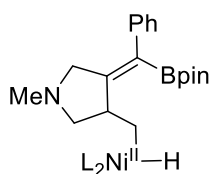
55	6	0	-4.714341	-0.722067	-3.628475
56	6	0	-2.934793	-1.146062	-2.054284
57	6	0	-2.809023	0.759283	-3.535488
58	6	0	-4.036979	0.403660	-4.090345
59	6	0	-4.154967	-1.504808	-2.619034
60	1	0	-2.504217	-1.752429	-1.260038
61	1	0	-2.289984	1.640635	-3.899611
62	1	0	-4.463672	1.009487	-4.883892
63	1	0	-4.675303	-2.387205	-2.258877
64	1	0	-5.674679	-0.992672	-4.057149
65	6	0	-0.287419	2.105518	-2.224254
66	6	0	0.218195	4.729680	-3.061928
67	6	0	0.918491	2.426408	-2.853665
68	6	0	-1.232921	3.116129	-2.007023
69	6	0	-0.984601	4.416704	-2.432553
70	6	0	1.169725	3.733892	-3.264075
71	1	0	1.664015	1.660393	-3.039628
72	1	0	-2.179957	2.883291	-1.531489
73	1	0	-1.737240	5.181825	-2.264383
74	1	0	2.112383	3.970045	-3.748150
75	1	0	0.416658	5.746539	-3.388029
76	7	0	-5.164123	-1.986631	2.399505
77	6	0	-4.976372	-0.652762	1.812706
78	6	0	-3.525110	-0.659328	1.378855
79	6	0	-2.893847	-1.948609	1.833536
80	6	0	-3.863055	-2.383074	2.938979
81	1	0	-5.144528	0.149098	2.559175
82	1	0	-5.692612	-0.492084	0.997470
83	1	0	-3.626195	-1.836531	3.875563
84	1	0	-3.851471	-3.457338	3.158013
85	6	0	-6.237762	-2.038083	3.364521
86	1	0	-7.181903	-1.754504	2.887538
87	1	0	-6.068387	-1.357277	4.220982
88	1	0	-6.342927	-3.056562	3.752258
89	6	0	-2.723515	0.287700	0.881794

90	6	0	-3.199292	1.632850	0.520201
91	6	0	-4.060941	4.229360	-0.164618
92	6	0	-4.218260	1.829663	-0.426754
93	6	0	-2.621430	2.768213	1.111980
94	6	0	-3.049080	4.050637	0.780372
95	6	0	-4.642517	3.113211	-0.765700
96	1	0	-4.657560	0.960417	-0.911617
97	1	0	-1.832929	2.622732	1.848255
98	1	0	-2.589432	4.913223	1.255888
99	1	0	-5.424560	3.241936	-1.508785
100	1	0	-4.391827	5.228996	-0.430217
101	1	0	-2.943353	-2.695686	1.025047
102	6	0	-1.439313	-1.642632	2.173734
103	1	0	-0.891754	-2.525096	2.523547
104	1	0	-1.408932	-0.912488	2.993017
105	1	0	0.571518	-1.166007	0.417920
106	5	0	0.241347	-2.337657	0.612277
107	8	0	1.099111	-3.109784	1.363289
108	6	0	1.157231	-4.406949	0.733407
109	6	0	-0.171222	-4.454234	-0.099339
110	8	0	-0.429252	-3.055393	-0.353030
111	6	0	1.269313	-5.474097	1.810548
112	1	0	2.222140	-5.361002	2.335295
113	1	0	1.238661	-6.474672	1.365691
114	1	0	0.463025	-5.387796	2.541882
115	6	0	2.406209	-4.403076	-0.145082
116	1	0	3.271796	-4.162802	0.479821
117	1	0	2.323259	-3.633837	-0.920397
118	1	0	2.569460	-5.373968	-0.623947
119	6	0	-1.353335	-5.016024	0.687346
120	1	0	-1.464761	-4.519683	1.656211
121	1	0	-1.238535	-6.091271	0.856058
122	1	0	-2.270247	-4.850517	0.113929
123	6	0	-0.052897	-5.161025	-1.441338
124	1	0	0.681273	-4.668557	-2.083384

125	1	0	-1.021163	-5.135989	-1.950179
126	1	0	0.235100	-6.208870	-1.302711

Zero-point correction=				1.052018	
(Hartree/Particle)					
Thermal correction to Energy=				1.111868	
Thermal correction to Enthalpy=				1.112812	
Thermal correction to Gibbs Free Energy=				0.957935	
Sum of electronic and zero-point Energies=				-3401.450747	
Sum of electronic and thermal Energies=				-3401.390898	
Sum of electronic and thermal Enthalpies=				-3401.389954	
Sum of electronic and thermal Free Energies=				-3401.544831	

Vb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-7.164474	2.345437	-1.853751
2	6	0	-6.409136	1.644597	-1.513677
3	6	0	-4.497897	-0.126167	-0.665109
4	6	0	-6.654833	0.274839	-1.587584
5	6	0	-5.199588	2.123363	-1.018007
6	6	0	-4.208743	1.235169	-0.586017
7	6	0	-5.697851	-0.641243	-1.155399
8	1	0	-7.600582	-0.076938	-1.986415
9	1	0	-5.017745	3.192281	-0.986261
10	6	0	-5.869611	-2.157087	-1.131365
11	8	0	-3.515888	-0.990253	-0.234704
12	6	0	-6.205391	-2.583070	0.316408

13	1	0	-7.147059	-2.123332	0.634021
14	1	0	-5.416077	-2.274688	1.009656
15	1	0	-6.307472	-3.671910	0.371870
16	6	0	-6.985555	-2.626465	-2.063052
17	1	0	-6.788033	-2.345092	-3.102290
18	1	0	-7.943245	-2.195118	-1.758528
19	1	0	-7.095953	-3.713106	-2.008525
20	6	0	-4.517901	-2.762225	-1.497603
21	6	0	-1.928546	-3.792700	-1.896561
22	6	0	-4.320855	-3.918660	-2.251120
23	6	0	-3.383568	-2.139314	-0.980848
24	6	0	-2.086020	-2.613970	-1.163954
25	6	0	-3.039139	-4.430908	-2.444188
26	1	0	-5.170874	-4.433391	-2.686817
27	1	0	-2.905006	-5.339749	-3.021696
28	1	0	-0.936860	-4.206670	-2.047159
29	15	0	-2.508316	1.725855	-0.063484
30	15	0	-0.732807	-1.615732	-0.417947
31	6	0	0.738780	-2.639459	-0.808929
32	6	0	3.060738	-4.044550	-1.499146
33	6	0	1.201286	-2.645712	-2.132102
34	6	0	1.451919	-3.344027	0.162246
35	6	0	2.611354	-4.039134	-0.182700
36	6	0	2.349245	-3.349416	-2.477344
37	1	0	0.663025	-2.086405	-2.895283
38	1	0	1.112356	-3.346326	1.194169
39	1	0	3.161295	-4.576917	0.583799
40	1	0	2.697422	-3.343502	-3.505347
41	1	0	3.964686	-4.583908	-1.764681
42	6	0	-0.989663	-1.919414	1.373536
43	6	0	-1.232926	-2.314721	4.130094
44	6	0	-1.694508	-3.020943	1.867745
45	6	0	-0.415342	-1.013271	2.270915
46	6	0	-0.528236	-1.216567	3.644179
47	6	0	-1.819949	-3.213301	3.241078

48	1	0	-2.142503	-3.732529	1.179085
49	1	0	0.113802	-0.141355	1.888237
50	1	0	-0.083673	-0.504074	4.332643
51	1	0	-2.371841	-4.069700	3.616676
52	1	0	-1.331016	-2.467465	5.200723
53	6	0	-2.588010	3.537420	-0.330425
54	6	0	-2.755866	6.270166	-0.888880
55	6	0	-3.255099	4.396364	0.548325
56	6	0	-2.001427	4.058252	-1.486819
57	6	0	-2.091201	5.418909	-1.768998
58	6	0	-3.335227	5.758852	0.270879
59	1	0	-3.709546	3.998447	1.452289
60	1	0	-1.455160	3.394037	-2.152226
61	1	0	-1.632036	5.815755	-2.669049
62	1	0	-3.848794	6.421230	0.961019
63	1	0	-2.817010	7.332791	-1.102949
64	6	0	-2.548267	1.587426	1.768615
65	6	0	-2.426949	1.383805	4.556262
66	6	0	-3.493195	0.828089	2.460479
67	6	0	-1.526488	2.230393	2.483240
68	6	0	-1.473840	2.136125	3.869851
69	6	0	-3.428126	0.724835	3.849378
70	1	0	-4.289933	0.321712	1.923455
71	1	0	-0.775444	2.805344	1.946069
72	1	0	-0.684949	2.647741	4.413552
73	1	0	-4.167234	0.130614	4.378060
74	1	0	-2.383502	1.306252	5.638650
75	6	0	3.854454	1.253080	-1.505771
76	6	0	2.445833	1.719256	-1.148414
77	6	0	1.995065	2.453083	-2.426203
78	7	0	3.216153	2.711308	-3.183799
79	6	0	4.030707	1.519714	-2.982237
80	1	0	2.483595	2.406450	-0.299281
81	1	0	1.312210	1.791494	-3.000124
82	1	0	1.454895	3.383203	-2.219585

83	1	0	5.064046	1.680770	-3.299583
84	1	0	3.633180	0.653667	-3.558779
85	6	0	2.972333	3.008628	-4.575815
86	1	0	2.449104	2.181185	-5.094597
87	1	0	3.919475	3.192886	-5.093011
88	1	0	2.354848	3.908633	-4.659725
89	6	0	4.734845	0.656928	-0.681166
90	6	0	1.522828	0.539652	-0.824646
91	1	0	1.877368	0.034736	0.088617
92	1	0	1.628527	-0.193276	-1.639134
93	28	0	-0.403964	0.791424	-0.621013
94	1	0	-0.012589	2.227528	-0.450413
95	5	0	4.423563	0.453686	0.830761
96	8	0	4.982113	-0.555516	1.585246
97	8	0	3.620530	1.278886	1.586319
98	6	0	4.310461	-0.552694	2.860957
99	6	0	3.817209	0.924298	2.967613
100	6	0	3.157876	-1.549942	2.757449
101	1	0	2.612630	-1.643012	3.702491
102	1	0	3.562603	-2.529421	2.485093
103	1	0	2.452106	-1.247496	1.975921
104	6	0	5.290835	-0.979131	3.941375
105	1	0	4.829144	-0.897808	4.931499
106	1	0	6.194054	-0.366276	3.922299
107	1	0	5.580384	-2.021790	3.782363
108	6	0	2.504223	1.109770	3.711219
109	1	0	2.582676	0.734801	4.738069
110	1	0	2.250245	2.173283	3.748326
111	6	0	4.884177	1.864994	3.525441
112	1	0	5.042863	1.701316	4.595820
113	1	0	4.556591	2.897058	3.373818
114	1	0	5.836653	1.727307	3.004082
115	1	0	1.694304	0.584532	3.201252
116	1	0	7.735984	-2.800574	-1.539574
117	6	0	7.540511	-1.732760	-1.581517

118	6	0	7.030488	0.996248	-1.674303
119	6	0	6.321903	-1.235430	-1.127659
120	6	0	8.508537	-0.867230	-2.087548
121	6	0	8.249787	0.500846	-2.129949
122	6	0	6.043293	0.136008	-1.178436
123	1	0	5.569222	-1.908665	-0.726848
124	1	0	9.458915	-1.255255	-2.441412
125	1	0	9.000652	1.186039	-2.512664
126	1	0	6.834260	2.065392	-1.692951

Zero-point correction=			1.050147		
(Hartree/Particle)					
Thermal correction to Energy=			1.111073		
Thermal correction to Enthalpy=			1.112017		
Thermal correction to Gibbs Free Energy=			0.951378		
Sum of electronic and zero-point Energies=			-3401.463916		
Sum of electronic and thermal Energies=			-3401.402990		
Sum of electronic and thermal Enthalpies=			-3401.402046		
Sum of electronic and thermal Free Energies=			-3401.562685		

TS_{mb-vb}

Imaginary frequencies = -158.8413 cm⁻¹

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	28	0	-0.507276	0.555956	0.274984
2	1	0	-1.446799	2.743394	0.789078
3	6	0	-1.077971	1.994479	1.496219
4	1	0	-0.332587	2.460168	2.151098
5	6	0	-2.196144	1.376771	2.293125
6	6	0	-3.264282	2.236624	2.972066
7	7	0	-4.269151	1.233436	3.319633
8	6	0	-4.358349	0.305409	2.184153
9	6	0	-3.035967	0.469016	1.445610

10	1	0	-1.768291	0.744329	3.092809
11	1	0	-3.650020	2.987139	2.252837
12	1	0	-2.919647	2.762795	3.869321
13	1	0	-5.179824	0.575473	1.492199
14	1	0	-4.561248	-0.714857	2.531155
15	1	0	-6.228313	0.982056	3.999682
16	6	0	-2.687468	-0.043901	0.241082
17	6	0	-5.545356	1.786883	3.708461
18	1	0	-5.415140	2.452196	4.568332
19	1	0	-6.023118	2.363423	2.893242
20	1	0	-0.794350	0.278937	-1.594885
21	5	0	-1.917168	0.805292	-1.511990
22	8	0	-2.823245	0.403556	-2.520952
23	6	0	-3.204667	1.574870	-3.252906
24	6	0	-3.030851	2.704183	-2.193043
25	8	0	-1.911668	2.226457	-1.449709
26	6	0	-4.618763	1.417505	-3.795063
27	1	0	-4.661359	0.547822	-4.457900
28	1	0	-4.901848	2.304141	-4.373319
29	1	0	-5.355805	1.280260	-3.001454
30	6	0	-2.222192	1.722244	-4.418188
31	1	0	-2.243828	0.804941	-5.013458
32	1	0	-1.203491	1.864524	-4.043545
33	1	0	-2.482075	2.565343	-5.066271
34	6	0	-4.226782	2.829138	-1.246313
35	1	0	-4.511974	1.855395	-0.836639
36	1	0	-5.092686	3.279231	-1.743063
37	1	0	-3.935730	3.467743	-0.405780
38	6	0	-2.684893	4.071611	-2.767515
39	1	0	-1.736703	4.044054	-3.310684
40	1	0	-2.593798	4.795702	-1.950941
41	1	0	-3.470343	4.421542	-3.446798
42	1	0	3.137718	-5.237503	-2.691184
43	6	0	3.110217	-4.267785	-2.204936
44	6	0	3.042821	-1.822841	-0.966225

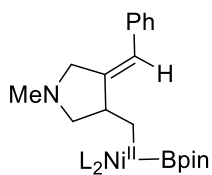
45	6	0	4.182057	-3.389546	-2.352699
46	6	0	1.993255	-3.902124	-1.460438
47	6	0	1.932423	-2.652164	-0.832143
48	6	0	4.166320	-2.144306	-1.730303
49	1	0	5.031351	-3.681241	-2.961632
50	1	0	1.151233	-4.582117	-1.390269
51	6	0	5.282634	-1.108868	-1.800075
52	8	0	2.989119	-0.605379	-0.325875
53	6	0	6.094863	-1.171489	-0.485862
54	1	0	6.556996	-2.158274	-0.378497
55	1	0	5.454046	-0.990980	0.383179
56	1	0	6.883710	-0.411859	-0.498162
57	6	0	6.221690	-1.349338	-2.980546
58	1	0	5.687236	-1.313063	-3.935192
59	1	0	6.708108	-2.324381	-2.887946
60	1	0	7.016569	-0.598116	-2.994807
61	6	0	4.606013	0.256151	-1.867845
62	6	0	3.329268	2.752218	-1.640583
63	6	0	5.045054	1.348699	-2.613803
64	6	0	3.491864	0.446974	-1.052700
65	6	0	2.847206	1.671095	-0.897299
66	6	0	4.406233	2.582563	-2.507246
67	1	0	5.896612	1.245143	-3.278305
68	1	0	4.761181	3.425253	-3.091258
69	1	0	2.864992	3.727711	-1.543508
70	15	0	0.438704	-1.987805	0.035141
71	15	0	1.500033	1.762883	0.356972
72	6	0	1.283748	3.583892	0.416800
73	6	0	0.998079	6.360093	0.301606
74	6	0	0.435535	4.164370	-0.534048
75	6	0	1.976273	4.397797	1.314735
76	6	0	1.827243	5.782882	1.259308
77	6	0	0.303237	5.548866	-0.594168
78	1	0	-0.141416	3.530236	-1.204418
79	1	0	2.630460	3.957345	2.061135

80	1	0	2.364344	6.409422	1.964737
81	1	0	-0.352578	5.993163	-1.337201
82	1	0	0.888144	7.439293	0.256802
83	6	0	2.420362	1.322145	1.883929
84	6	0	3.773623	0.525297	4.198082
85	6	0	3.791802	1.569619	2.021418
86	6	0	1.736921	0.671554	2.914583
87	6	0	2.411133	0.274055	4.067201
88	6	0	4.462859	1.175896	3.175156
89	1	0	4.338615	2.062536	1.221120
90	1	0	0.675635	0.464163	2.811251
91	1	0	1.869034	-0.243614	4.852107
92	1	0	5.526293	1.371682	3.272871
93	1	0	4.302094	0.211930	5.093285
94	6	0	-0.778352	-3.228986	-0.543926
95	6	0	-2.529676	-5.099203	-1.651491
96	6	0	-1.482077	-2.928140	-1.714525
97	6	0	-0.969367	-4.466018	0.078405
98	6	0	-1.842564	-5.398477	-0.476204
99	6	0	-2.352784	-3.862772	-2.267414
100	1	0	-1.369046	-1.951989	-2.181584
101	1	0	-0.429837	-4.702668	0.992345
102	1	0	-1.988081	-6.358507	0.010330
103	1	0	-2.909747	-3.612828	-3.164628
104	1	0	-3.218278	-5.823661	-2.076035
105	6	0	0.729264	-2.458615	1.788244
106	6	0	1.039106	-3.051476	4.507721
107	6	0	1.863828	-3.136664	2.237112
108	6	0	-0.243050	-2.065122	2.718773
109	6	0	-0.096514	-2.370099	4.067778
110	6	0	2.019545	-3.424767	3.593253
111	1	0	2.628531	-3.444806	1.529262
112	1	0	-1.113288	-1.502041	2.381797
113	1	0	-0.861563	-2.064166	4.775402
114	1	0	2.908316	-3.948851	3.931620

115	1	0	1.160940	-3.282899	5.561637
116	6	0	-3.629042	-1.167455	-0.127178
117	6	0	-5.498401	-3.269654	-0.503648
118	6	0	-4.684066	-1.055717	-1.041123
119	6	0	-3.563793	-2.361043	0.614016
120	6	0	-4.471694	-3.396559	0.430676
121	6	0	-5.600369	-2.089877	-1.231258
122	1	0	-4.792854	-0.146721	-1.611531
123	1	0	-2.779068	-2.474279	1.356784
124	1	0	-4.375335	-4.304793	1.019183
125	1	0	-6.404730	-1.959876	-1.950439
126	1	0	-6.212687	-4.074255	-0.652480

Zero-point correction=	1.051617
(Hartree/Particle)	
Thermal correction to Energy=	1.111411
Thermal correction to Enthalpy=	1.112356
Thermal correction to Gibbs Free Energy=	0.956674
Sum of electronic and zero-point Energies=	-3401.417866
Sum of electronic and thermal Energies=	-3401.358072
Sum of electronic and thermal Enthalpies=	-3401.357128
Sum of electronic and thermal Free Energies=	-3401.512809

VIIb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.488764	0.315545	4.703989
2	6	0	2.883533	-0.351100	3.930150
3	6	0	1.800111	-0.828153	2.950581

4	6	0	2.672990	-1.226354	1.760718
5	6	0	3.968065	-0.450045	1.862389
6	7	0	3.804027	0.373793	3.057816
7	1	0	3.389699	-1.207541	4.421142
8	1	0	4.172123	0.184539	0.988407
9	1	0	4.816149	-1.159036	1.961025
10	6	0	5.052853	0.744945	3.680662
11	1	0	5.665934	1.317097	2.975991
12	1	0	4.855435	1.376097	4.552955
13	6	0	2.347060	-2.202371	0.896927
14	28	0	0.227759	-0.087279	0.697785
15	5	0	-0.076649	-0.650604	-1.257619
16	8	0	-0.956089	-0.128774	-2.191511
17	6	0	-1.042424	-1.011403	-3.321099
18	6	0	0.308047	-1.790988	-3.236373
19	8	0	0.614313	-1.720370	-1.828140
20	1	0	1.287423	-1.721437	3.329517
21	6	0	0.774579	0.266687	2.607627
22	1	0	1.385299	-2.690185	1.067685
23	1	0	1.265078	1.236786	2.718312
24	1	0	-0.036987	0.241405	3.343639
25	6	0	-1.231132	-0.168691	-4.573823
26	1	0	-2.190746	0.354749	-4.510013
27	1	0	-1.237106	-0.795700	-5.472350
28	1	0	-0.443911	0.582482	-4.668904
29	6	0	-2.265350	-1.899203	-3.095448
30	1	0	-3.141881	-1.257724	-2.955391
31	1	0	-2.146912	-2.505097	-2.190028
32	1	0	-2.445235	-2.566385	-3.944980
33	6	0	1.452463	-1.098475	-3.972120
34	1	0	1.342770	-1.179138	-5.058660
35	1	0	2.393030	-1.576795	-3.673929
36	1	0	1.506216	-0.039397	-3.699426
37	6	0	0.227563	-3.252926	-3.649140
38	1	0	-0.478507	-3.804155	-3.021610

39	1	0	1.214225	-3.713707	-3.543693
40	1	0	-0.089601	-3.343209	-4.694368
41	1	0	5.638861	-0.132984	4.013334
42	1	0	-0.453090	4.569334	-4.053392
43	6	0	-0.769718	3.953254	-3.218170
44	6	0	-1.572672	2.349443	-1.115998
45	6	0	-2.122550	3.698188	-3.014892
46	6	0	0.174966	3.429034	-2.342614
47	6	0	-0.208622	2.614979	-1.274433
48	6	0	-2.545448	2.906130	-1.949447
49	1	0	-2.852640	4.125188	-3.694087
50	1	0	1.227344	3.637575	-2.505189
51	6	0	-4.001581	2.647617	-1.589751
52	8	0	-1.963946	1.505502	-0.095513
53	6	0	-4.369534	3.547040	-0.387043
54	1	0	-4.269591	4.602018	-0.663594
55	1	0	-3.713088	3.348742	0.465982
56	1	0	-5.403936	3.358425	-0.080426
57	6	0	-4.948833	2.960717	-2.747078
58	1	0	-4.728238	2.346232	-3.626207
59	1	0	-4.871431	4.014606	-3.028259
60	1	0	-5.987185	2.789253	-2.450558
61	6	0	-4.094341	1.195484	-1.140673
62	6	0	-4.193590	-1.387905	-0.075063
63	6	0	-5.178451	0.361550	-1.403063
64	6	0	-3.048276	0.696589	-0.355949
65	6	0	-3.074828	-0.591787	0.192487
66	6	0	-5.232107	-0.924289	-0.872428
67	1	0	-5.996631	0.716569	-2.020438
68	1	0	-6.083629	-1.563636	-1.081241
69	1	0	-4.240777	-2.395634	0.324535
70	15	0	1.004387	1.887195	-0.096884
71	15	0	-1.668808	-1.218471	1.213504
72	6	0	-1.833982	-3.048152	1.050228
73	6	0	-2.062289	-5.822689	0.696411

74	6	0	-1.035360	-3.713881	0.113160
75	6	0	-2.742373	-3.793237	1.814393
76	6	0	-2.854551	-5.169587	1.638278
77	6	0	-1.154925	-5.091976	-0.065358
78	1	0	-0.319787	-3.154117	-0.484518
79	1	0	-3.364629	-3.296963	2.553418
80	1	0	-3.562594	-5.732277	2.238879
81	1	0	-0.530491	-5.592885	-0.800511
82	1	0	-2.150688	-6.896226	0.560721
83	6	0	-2.305747	-0.944770	2.918812
84	6	0	-3.060682	-0.420022	5.565929
85	6	0	-3.250307	0.042677	3.202458
86	6	0	-1.734344	-1.661383	3.978419
87	6	0	-2.114159	-1.406869	5.291219
88	6	0	-3.624093	0.304080	4.520439
89	1	0	-3.702594	0.612150	2.395199
90	1	0	-0.990757	-2.428754	3.773609
91	1	0	-1.665454	-1.973533	6.101364
92	1	0	-4.361335	1.074402	4.725114
93	1	0	-3.353541	-0.216405	6.591247
94	6	0	2.594612	1.930581	-1.013542
95	6	0	4.990540	1.904029	-2.461230
96	6	0	3.086002	0.733623	-1.542930
97	6	0	3.331260	3.110087	-1.190666
98	6	0	4.520648	3.096892	-1.911527
99	6	0	4.275024	0.725739	-2.273925
100	1	0	2.541707	-0.196420	-1.381362
101	1	0	2.973339	4.040302	-0.757371
102	1	0	5.081105	4.017336	-2.043717
103	1	0	4.639615	-0.210868	-2.686118
104	1	0	5.917049	1.894876	-3.027255
105	6	0	1.234957	3.289039	1.077888
106	6	0	1.636163	5.329870	2.955252
107	6	0	0.327543	4.345676	1.178553
108	6	0	2.343915	3.258938	1.935099

109	6	0	2.543954	4.275350	2.862533
110	6	0	0.527516	5.360056	2.115374
111	1	0	-0.537983	4.387484	0.523476
112	1	0	3.038196	2.420525	1.903490
113	1	0	3.406856	4.237096	3.520871
114	1	0	-0.185612	6.176116	2.182674
115	1	0	1.790794	6.120751	3.682856
116	6	0	3.116556	-2.788493	-0.210776
117	6	0	4.467712	-4.068294	-2.337260
118	6	0	2.614119	-3.960840	-0.798545
119	6	0	4.322207	-2.276736	-0.714603
120	6	0	4.984778	-2.908593	-1.765848
121	6	0	3.275916	-4.595954	-1.840890
122	1	0	1.681130	-4.371592	-0.420971
123	1	0	4.744072	-1.365691	-0.307278
124	1	0	5.916007	-2.489174	-2.137163
125	1	0	2.859678	-5.502845	-2.270684
126	1	0	4.988298	-4.558380	-3.154001

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Zero-point correction=                1.055081
(Hartree/Particle)

Thermal correction to Energy=          1.115077

Thermal correction to Enthalpy=        1.116022

Thermal correction to Gibbs Free Energy= 0.961697

Sum of electronic and zero-point Energies= -3401.459863
Sum of electronic and thermal Energies=    -3401.399867
Sum of electronic and thermal Enthalpies=   -3401.398923
Sum of electronic and thermal Free Energies= -3401.553248

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TS_{mb-vib}

Imaginary frequency: -1128.8246

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Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type        X           Y           Z
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1	1	0	-3.277754	-4.412063	-0.138140
2	6	0	-3.730387	-3.475885	0.207113
3	6	0	-2.723086	-2.302283	0.245797
4	6	0	-3.472602	-1.173678	-0.406097
5	6	0	-4.918463	-1.601453	-0.501007
6	7	0	-4.773936	-3.039474	-0.724008
7	1	0	-4.158224	-3.655992	1.214146
8	1	0	-5.473329	-1.124033	-1.314793
9	1	0	-5.456740	-1.395425	0.450853
10	6	0	-6.010660	-3.772578	-0.585141
11	1	0	-6.743165	-3.412144	-1.314458
12	1	0	-5.833597	-4.836204	-0.773607
13	6	0	-2.867352	-0.088419	-0.911503
14	28	0	-0.753126	-0.615379	-0.698036
15	5	0	-0.359783	1.504709	-1.047030
16	8	0	-0.089121	2.321907	0.025681
17	6	0	-0.044011	3.682087	-0.457103
18	6	0	0.287075	3.495732	-1.978264
19	8	0	-0.193768	2.154493	-2.244366
20	1	0	-2.563617	-2.018024	1.295660
21	6	0	-1.355789	-2.472731	-0.415445
22	1	0	-1.580182	0.678034	-0.972199
23	1	0	-1.486409	-2.963204	-1.393218
24	1	0	-0.699721	-3.093330	0.208453
25	6	0	1.003573	4.438462	0.344277
26	1	0	0.708946	4.452895	1.398441
27	1	0	1.093694	5.471409	-0.009512
28	1	0	1.979839	3.950722	0.276773
29	6	0	-1.436443	4.263615	-0.209692
30	1	0	-1.659725	4.187871	0.859080
31	1	0	-2.200118	3.698604	-0.758625
32	1	0	-1.495112	5.315587	-0.505962
33	6	0	1.781492	3.504311	-2.269273
34	1	0	2.203677	4.508089	-2.154215
35	1	0	1.947475	3.167975	-3.296854

36	1	0	2.309570	2.822763	-1.599094
37	6	0	-0.443769	4.452729	-2.907712
38	1	0	-1.526549	4.336276	-2.820829
39	1	0	-0.156739	4.243933	-3.942698
40	1	0	-0.176977	5.490651	-2.680341
41	1	0	-6.449434	-3.670060	0.426650
42	1	0	5.073408	1.637653	-3.260979
43	6	0	4.496630	1.340917	-2.391169
44	6	0	3.020913	0.615303	-0.186749
45	6	0	4.798179	1.881722	-1.143648
46	6	0	3.467715	0.411982	-2.527822
47	6	0	2.710185	0.032547	-1.418528
48	6	0	4.071085	1.516525	-0.008984
49	1	0	5.616559	2.588570	-1.056078
50	1	0	3.247573	-0.013979	-3.501573
51	6	0	4.415522	1.928248	1.417686
52	8	0	2.275279	0.198355	0.885736
53	6	0	5.269013	0.798449	2.038091
54	1	0	6.199193	0.672823	1.473589
55	1	0	4.724215	-0.151914	2.027630
56	1	0	5.513478	1.040502	3.077581
57	6	0	5.209191	3.234243	1.461085
58	1	0	4.641129	4.064082	1.027391
59	1	0	6.150436	3.130263	0.914479
60	1	0	5.472075	3.489492	2.490909
61	6	0	3.113692	2.017034	2.206279
62	6	0	0.721534	1.923436	3.672468
63	6	0	2.882145	2.917674	3.245518
64	6	0	2.107368	1.093582	1.922519
65	6	0	0.907374	1.009872	2.631876
66	6	0	1.697006	2.870248	3.973779
67	1	0	3.630047	3.663168	3.494168
68	1	0	1.531558	3.577209	4.780446
69	1	0	-0.204398	1.912232	4.237905
70	15	0	1.343194	-1.196721	-1.443439

71	15	0	-0.395380	-0.146248	2.002682
72	6	0	-1.863426	0.494603	2.902261
73	6	0	-4.085683	1.699122	4.114969
74	6	0	-2.685527	1.366534	2.178165
75	6	0	-2.165759	0.238471	4.245864
76	6	0	-3.273968	0.831882	4.845424
77	6	0	-3.786639	1.970512	2.782287
78	1	0	-2.451339	1.583665	1.139273
79	1	0	-1.527394	-0.421208	4.827983
80	1	0	-3.499400	0.623114	5.886903
81	1	0	-4.407914	2.649454	2.204671
82	1	0	-4.946323	2.163617	4.586612
83	6	0	0.008679	-1.742810	2.831926
84	6	0	0.627131	-4.340328	3.717595
85	6	0	-0.992161	-2.592983	3.320513
86	6	0	1.325605	-2.220717	2.792774
87	6	0	1.630664	-3.505321	3.232179
88	6	0	-0.684697	-3.877805	3.762182
89	1	0	-2.023208	-2.255139	3.362235
90	1	0	2.122423	-1.595216	2.400708
91	1	0	2.657353	-3.855237	3.184864
92	1	0	-1.477265	-4.517391	4.139103
93	1	0	0.865691	-5.343834	4.056316
94	6	0	1.215176	-1.623974	-3.219043
95	6	0	0.946816	-2.184623	-5.941819
96	6	0	0.138413	-1.103518	-3.942501
97	6	0	2.155302	-2.432912	-3.867696
98	6	0	2.020806	-2.710749	-5.224559
99	6	0	0.006915	-1.381341	-5.301577
100	1	0	-0.600784	-0.487199	-3.434691
101	1	0	2.989671	-2.847442	-3.307128
102	1	0	2.751810	-3.340888	-5.721706
103	1	0	-0.835010	-0.977314	-5.854990
104	1	0	0.840426	-2.406988	-6.999177
105	6	0	2.168539	-2.682097	-0.732364

106	6	0	3.291186	-5.008141	0.360204
107	6	0	3.379335	-2.627148	-0.036314
108	6	0	1.537290	-3.922554	-0.893244
109	6	0	2.092851	-5.075061	-0.347454
110	6	0	3.935809	-3.783650	0.507256
111	1	0	3.908703	-1.686480	0.076639
112	1	0	0.608758	-3.986828	-1.452390
113	1	0	1.589155	-6.027564	-0.478908
114	1	0	4.878547	-3.722882	1.043263
115	1	0	3.723637	-5.908281	0.786458
116	1	0	-5.011331	1.077431	0.217990
117	6	0	-4.750031	1.549887	-0.725826
118	6	0	-4.037417	2.785847	-3.106939
119	6	0	-5.476494	2.645671	-1.183528
120	6	0	-3.656881	1.046212	-1.449411
121	6	0	-3.306981	1.693979	-2.644380
122	6	0	-5.122939	3.269872	-2.377741
123	1	0	-6.316983	3.015254	-0.602649
124	1	0	-2.448275	1.340354	-3.208398
125	1	0	-5.684772	4.127285	-2.735457
126	1	0	-3.753854	3.263844	-4.040688

Zero-point correction=
(Hartree/Particle)

1.048313

Thermal correction to Energy=

1.108686

Thermal correction to Enthalpy=

1.109631

Thermal correction to Gibbs Free Energy=

0.952294

Sum of electronic and zero-point Energies=

-3401.408651

Sum of electronic and thermal Energies=

-3401.348278

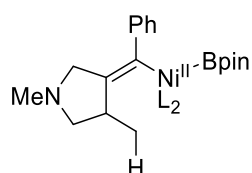
Sum of electronic and thermal Enthalpies=

-3401.347334

Sum of electronic and thermal Free Energies=

-3401.504670

VIIb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	3.677061	3.837906	-2.934832
2	6	0	3.813583	3.230110	-2.032167
3	6	0	2.591032	2.376717	-1.674745
4	6	0	3.213063	1.210891	-0.906938
5	6	0	4.721783	1.326349	-1.102737
6	7	0	4.870346	2.245714	-2.226263
7	1	0	4.058985	3.914366	-1.193336
8	1	0	5.212395	0.369899	-1.308706
9	1	0	5.191841	1.743479	-0.184297
10	6	0	6.187943	2.829614	-2.320642
11	1	0	6.935730	2.042629	-2.459907
12	1	0	6.236460	3.505494	-3.180813
13	6	0	2.560827	0.272927	-0.194181
14	28	0	0.532141	0.185250	-0.512507
15	5	0	-1.143720	0.077270	-1.626516
16	8	0	-1.116762	-0.694507	-2.779994
17	6	0	-2.417474	-0.647057	-3.409367
18	6	0	-3.022275	0.669016	-2.825615
19	8	0	-2.321538	0.803378	-1.574086
20	1	0	1.910751	2.945180	-1.034292
21	6	0	1.836184	1.920957	-2.926085
22	1	0	1.028797	1.220644	-2.669939
23	1	0	2.520723	1.402914	-3.607190
24	1	0	1.390703	2.773901	-3.454428
25	6	0	-3.181308	-1.888705	-2.961784
26	1	0	-2.587610	-2.776316	-3.201136
27	1	0	-4.149254	-1.964454	-3.468420

28	1	0	-3.350622	-1.873715	-1.881615
29	6	0	-2.232291	-0.659826	-4.918867
30	1	0	-1.795419	-1.616200	-5.221141
31	1	0	-1.564828	0.139149	-5.248330
32	1	0	-3.196578	-0.548129	-5.426996
33	6	0	-4.514196	0.625084	-2.528764
34	1	0	-5.092831	0.453092	-3.443028
35	1	0	-4.822021	1.582043	-2.096253
36	1	0	-4.746813	-0.160669	-1.805255
37	6	0	-2.686187	1.901027	-3.665196
38	1	0	-1.610675	1.948769	-3.871213
39	1	0	-2.972685	2.798620	-3.108208
40	1	0	-3.223586	1.896775	-4.618642
41	1	0	6.458570	3.403964	-1.413107
42	1	0	-4.988842	3.756641	1.276735
43	6	0	-4.352461	2.877844	1.278323
44	6	0	-2.738661	0.646170	1.279876
45	6	0	-4.908235	1.618154	1.481488
46	6	0	-2.981731	3.014540	1.079689
47	6	0	-2.149905	1.893748	1.061217
48	6	0	-4.104134	0.478478	1.503373
49	1	0	-5.978324	1.528414	1.636012
50	1	0	-2.557353	3.999744	0.914377
51	6	0	-4.596667	-0.924533	1.834202
52	8	0	-1.908849	-0.452054	1.266344
53	6	0	-4.277673	-1.201446	3.321618
54	1	0	-4.817082	-0.491738	3.957826
55	1	0	-3.205395	-1.098133	3.516960
56	1	0	-4.580396	-2.219196	3.589103
57	6	0	-6.101350	-1.074458	1.611635
58	1	0	-6.374628	-0.886356	0.568044
59	1	0	-6.653554	-0.378687	2.249013
60	1	0	-6.432766	-2.079352	1.886105
61	6	0	-3.788843	-1.908197	0.994447
62	6	0	-2.102882	-3.721450	-0.317592

63	6	0	-4.290528	-3.108933	0.492427
64	6	0	-2.431441	-1.636830	0.800829
65	6	0	-1.557734	-2.526129	0.158296
66	6	0	-3.454280	-4.009853	-0.158499
67	1	0	-5.340830	-3.350070	0.615696
68	1	0	-3.856753	-4.938362	-0.549844
69	1	0	-1.476434	-4.420563	-0.857736
70	15	0	-0.352201	1.993432	0.676059
71	15	0	0.213163	-2.034329	-0.078277
72	6	0	0.866042	-3.259685	-1.265776
73	6	0	1.936709	-4.970351	-3.207776
74	6	0	1.339901	-2.748883	-2.479569
75	6	0	0.925146	-4.642259	-1.041630
76	6	0	1.460545	-5.491363	-2.005707
77	6	0	1.871929	-3.600249	-3.445521
78	1	0	1.294651	-1.678022	-2.661370
79	1	0	0.552245	-5.061177	-0.111230
80	1	0	1.505713	-6.559409	-1.817316
81	1	0	2.241033	-3.189643	-4.379996
82	1	0	2.355956	-5.634457	-3.957390
83	6	0	0.933597	-2.416751	1.579857
84	6	0	1.948516	-2.820114	4.165608
85	6	0	0.629983	-1.523101	2.617348
86	6	0	1.792258	-3.484735	1.845875
87	6	0	2.285789	-3.688495	3.133437
88	6	0	1.129508	-1.725129	3.899164
89	1	0	0.017423	-0.649903	2.423742
90	1	0	2.121606	-4.141990	1.050383
91	1	0	2.961789	-4.518469	3.317098
92	1	0	0.886859	-1.012347	4.682573
93	1	0	2.343228	-2.979451	5.164679
94	6	0	-0.227463	3.697849	0.011241
95	6	0	-0.042733	6.207902	-1.201967
96	6	0	-0.586242	3.863548	-1.331908
97	6	0	0.219857	4.797785	0.744229

98	6	0	0.314204	6.049181	0.133962
99	6	0	-0.499541	5.112250	-1.935167
100	1	0	-0.923329	2.999960	-1.899087
101	1	0	0.501586	4.680370	1.786577
102	1	0	0.668389	6.900589	0.706978
103	1	0	-0.776653	5.228221	-2.978985
104	1	0	0.038149	7.182651	-1.673013
105	6	0	0.391474	2.117325	2.353029
106	6	0	1.636153	2.250001	4.857236
107	6	0	-0.366729	2.035262	3.524741
108	6	0	1.781781	2.261479	2.445868
109	6	0	2.396590	2.340124	3.691703
110	6	0	0.255773	2.093539	4.771417
111	1	0	-1.445650	1.924303	3.470000
112	1	0	2.381743	2.279739	1.538471
113	1	0	3.474958	2.454995	3.751498
114	1	0	-0.343064	2.023954	5.674542
115	1	0	2.119805	2.300644	5.827996
116	1	0	3.440695	0.094883	2.391044
117	6	0	3.823431	-0.706356	1.764516
118	6	0	4.773038	-2.792035	0.193670
119	6	0	3.430440	-0.764309	0.418148
120	6	0	4.682594	-1.656679	2.307528
121	6	0	5.164571	-2.706777	1.527431
122	6	0	3.922973	-1.832238	-0.350812
123	1	0	4.967910	-1.583869	3.354103
124	1	0	5.831474	-3.449799	1.955335
125	1	0	3.643805	-1.890535	-1.399827
126	1	0	5.136423	-3.602999	-0.432715

Zero-point correction=				1.053290	
(Hartree/Particle)					
Thermal correction to Energy=				1.114391	
Thermal correction to Enthalpy=				1.115335	
Thermal correction to Gibbs Free Energy=				0.957351	

Sum of electronic and zero-point Energies= -3401.456000
Sum of electronic and thermal Energies= -3401.394899
Sum of electronic and thermal Enthalpies= -3401.393955
Sum of electronic and thermal Free Energies= -3401.551939

TS_{int-vib}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.988934	3.309088	-3.644436
2	6	0	3.231415	3.219823	-2.578668
3	6	0	2.261380	2.295620	-1.804553
4	6	0	3.180231	1.406402	-1.000494
5	6	0	4.548748	2.039638	-1.054517
6	7	0	4.552422	2.610493	-2.404108
7	1	0	3.208763	4.238148	-2.142410
8	1	0	5.367758	1.325562	-0.923676
9	1	0	4.661677	2.837533	-0.286365
10	6	0	5.636265	3.535533	-2.640086
11	1	0	6.596807	3.027477	-2.508477
12	1	0	5.586441	3.913713	-3.666560
13	6	0	2.769372	0.197181	-0.589779
14	28	0	0.864513	-0.061855	-1.176023
15	5	0	-1.099792	-0.213655	-2.118905
16	8	0	-1.365677	-1.077297	-3.151507
17	6	0	-2.805446	-1.187927	-3.292041
18	6	0	-3.316009	0.094236	-2.552461
19	8	0	-2.242039	0.366826	-1.621652
20	1	0	1.648068	2.919483	-1.141206
21	6	0	1.343546	1.410322	-2.641256
22	1	0	0.039002	0.639977	-2.314504
23	1	0	1.926005	0.763895	-3.307333
24	1	0	0.669680	2.017757	-3.260336
25	6	0	-3.236499	-2.475487	-2.602261

26	1	0	-2.652616	-3.308925	-3.004620
27	1	0	-4.299603	-2.675465	-2.771250
28	1	0	-3.059026	-2.421627	-1.526630
29	6	0	-3.139792	-1.243961	-4.774725
30	1	0	-2.750323	-2.173191	-5.200160
31	1	0	-2.697540	-0.406081	-5.317586
32	1	0	-4.224969	-1.228078	-4.922537
33	6	0	-4.609621	-0.081293	-1.773661
34	1	0	-5.432738	-0.331677	-2.452231
35	1	0	-4.852804	0.853896	-1.258760
36	1	0	-4.518910	-0.867345	-1.019522
37	6	0	-3.415341	1.315437	-3.465989
38	1	0	-2.474673	1.477776	-4.004775
39	1	0	-3.617429	2.198095	-2.851394
40	1	0	-4.222393	1.207763	-4.196744
41	1	0	5.606741	4.403639	-1.952483
42	1	0	-5.351468	3.360553	1.371537
43	6	0	-4.616967	2.561529	1.365633
44	6	0	-2.759783	0.528493	1.339020
45	6	0	-5.000134	1.264552	1.694753
46	6	0	-3.290595	2.838521	1.042930
47	6	0	-2.334744	1.821500	1.022223
48	6	0	-4.071329	0.223171	1.698870
49	1	0	-6.034204	1.067472	1.956593
50	1	0	-2.995368	3.853146	0.792125
51	6	0	-4.373591	-1.197190	2.155405
52	8	0	-1.803688	-0.461539	1.294178
53	6	0	-3.939717	-1.321703	3.634489
54	1	0	-4.518255	-0.628210	4.254015
55	1	0	-2.876790	-1.086844	3.750401
56	1	0	-4.108934	-2.342977	3.991938
57	6	0	-5.861004	-1.533049	2.043517
58	1	0	-6.213903	-1.461264	1.009232
59	1	0	-6.454028	-0.855309	2.662910
60	1	0	-6.056545	-2.542748	2.413753

61	6	0	-3.503898	-2.149476	1.341796
62	6	0	-1.682939	-3.899221	0.128928
63	6	0	-3.882078	-3.448954	1.005474
64	6	0	-2.205773	-1.741161	1.014834
65	6	0	-1.262106	-2.600210	0.431798
66	6	0	-2.980879	-4.317483	0.400067
67	1	0	-4.885259	-3.795526	1.229083
68	1	0	-3.287711	-5.324986	0.139526
69	1	0	-1.002971	-4.587549	-0.356759
70	15	0	-0.573852	2.053707	0.529687
71	15	0	0.446080	-1.982579	0.051474
72	6	0	1.164351	-3.375399	-0.898343
73	6	0	2.280593	-5.388480	-2.498751
74	6	0	1.480686	-3.127575	-2.238906
75	6	0	1.388300	-4.658047	-0.378530
76	6	0	1.950523	-5.654444	-1.170601
77	6	0	2.035149	-4.127861	-3.034797
78	1	0	1.306226	-2.139966	-2.659518
79	1	0	1.110785	-4.885947	0.646513
80	1	0	2.125326	-6.640129	-0.750951
81	1	0	2.280594	-3.915678	-4.070552
82	1	0	2.721417	-6.165979	-3.115047
83	6	0	1.251117	-1.961185	1.713588
84	6	0	2.415436	-1.695937	4.254090
85	6	0	0.899010	-0.901589	2.557960
86	6	0	2.226796	-2.864519	2.143756
87	6	0	2.793089	-2.736107	3.410334
88	6	0	1.474986	-0.767442	3.816886
89	1	0	0.180138	-0.164283	2.229326
90	1	0	2.596354	-3.640086	1.485096
91	1	0	3.558153	-3.441144	3.721521
92	1	0	1.191587	0.076549	4.440106
93	1	0	2.870321	-1.595745	5.235066
94	6	0	-0.679815	3.701562	-0.283871
95	6	0	-0.825121	6.087617	-1.744834

96	6	0	-1.149739	3.702576	-1.604262
97	6	0	-0.279455	4.908073	0.294758
98	6	0	-0.349365	6.094409	-0.436772
99	6	0	-1.230237	4.886793	-2.328050
100	1	0	-1.451631	2.760887	-2.057510
101	1	0	0.092656	4.924605	1.315453
102	1	0	-0.031193	7.026477	0.020808
103	1	0	-1.598911	4.872019	-3.349692
104	1	0	-0.875949	7.012952	-2.310334
105	6	0	0.220459	2.474163	2.137668
106	6	0	1.619031	3.073180	4.491436
107	6	0	-0.467373	2.667034	3.338918
108	6	0	1.619642	2.569066	2.130772
109	6	0	2.312493	2.878056	3.297319
110	6	0	0.230936	2.959972	4.511173
111	1	0	-1.551119	2.591665	3.362064
112	1	0	2.165564	2.373828	1.208353
113	1	0	3.395910	2.953947	3.275996
114	1	0	-0.313397	3.106678	5.439411
115	1	0	2.159479	3.306066	5.403883
116	1	0	3.909731	0.666336	1.812532
117	6	0	4.269535	-0.258408	1.367009
118	6	0	5.147680	-2.642566	0.249133
119	6	0	3.741427	-0.655923	0.128079
120	6	0	5.215534	-1.031041	2.032076
121	6	0	5.661086	-2.229712	1.477544
122	6	0	4.197288	-1.868519	-0.412781
123	1	0	5.599574	-0.700470	2.993759
124	1	0	6.399639	-2.834088	1.996309
125	1	0	3.809923	-2.193750	-1.374389
126	1	0	5.490337	-3.571518	-0.199663

Zero-point correction=
(Hartree/Particle)

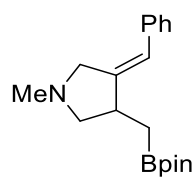
1.049429

Thermal correction to Energy=

1.109604

Thermal correction to Enthalpy=	1.110548
Thermal correction to Gibbs Free Energy=	0.956248
Sum of electronic and zero-point Energies=	-3401.415742
Sum of electronic and thermal Energies=	-3401.355567
Sum of electronic and thermal Enthalpies=	-3401.354623
Sum of electronic and thermal Free Energies=	-3401.508923

VIIIb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.897019	1.582535	0.794271
2	6	0	-0.867899	2.057623	-0.637153
3	7	0	0.558392	2.267427	-0.849038
4	6	0	1.024499	2.941300	0.356776
5	6	0	0.301754	2.207640	1.505199
6	1	0	-1.439444	3.002022	-0.762840
7	1	0	-1.269854	1.323137	-1.343831
8	1	0	0.741017	4.011202	0.345722
9	1	0	2.115113	2.873216	0.428722
10	1	0	-0.039321	2.934671	2.251694
11	6	0	-1.688013	0.641992	1.317462
12	5	0	1.663157	0.051276	1.187370
13	8	0	0.991657	-1.132946	1.010743
14	6	0	1.471321	-1.703813	-0.225081
15	6	0	2.901670	-1.077392	-0.344004
16	8	0	2.757185	0.170211	0.369168
17	6	0	1.200363	1.160751	2.203466
18	1	0	0.642778	0.697476	3.025339
19	1	0	2.059959	1.677390	2.645421

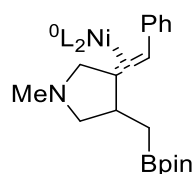
20	6	0	0.876933	2.967051	-2.072764
21	1	0	0.516001	2.392527	-2.932050
22	1	0	1.962226	3.073955	-2.162182
23	6	0	-2.765270	-0.074868	0.613261
24	6	0	-4.755071	-1.529452	-0.735828
25	6	0	-3.613607	0.554815	-0.305844
26	6	0	-2.947063	-1.443529	0.860136
27	6	0	-3.927049	-2.165875	0.188100
28	6	0	-4.597177	-0.166961	-0.977093
29	1	0	-3.516000	1.623554	-0.475047
30	1	0	-2.292835	-1.939175	1.573338
31	1	0	-4.046807	-3.226895	0.385659
32	1	0	-5.248277	0.339176	-1.683549
33	1	0	-5.523987	-2.090344	-1.257869
34	6	0	0.522534	-1.224784	-1.322942
35	1	0	0.576102	-0.134632	-1.415202
36	1	0	-0.500804	-1.500056	-1.046705
37	1	0	0.763156	-1.682539	-2.287874
38	6	0	1.440548	-3.219465	-0.115117
39	1	0	1.989829	-3.569529	0.761541
40	1	0	1.874108	-3.678219	-1.010362
41	1	0	0.402692	-3.554637	-0.027857
42	6	0	3.346045	-0.775847	-1.766392
43	1	0	2.676550	-0.053530	-2.238474
44	1	0	3.365276	-1.691092	-2.367762
45	1	0	4.354918	-0.353083	-1.753522
46	6	0	3.966868	-1.887952	0.391037
47	1	0	4.889043	-1.301955	0.435819
48	1	0	4.178008	-2.831264	-0.121901
49	1	0	3.650049	-2.108545	1.415297
50	1	0	-1.483405	0.303188	2.332594
51	1	0	0.422443	3.974893	-2.111919

Zero-point correction=
(Hartree/Particle)

0.450067

Thermal correction to Energy=	0.472160
Thermal correction to Enthalpy=	0.473104
Thermal correction to Gibbs Free Energy=	0.399418
Sum of electronic and zero-point Energies=	-970.154518
Sum of electronic and thermal Energies=	-970.132425
Sum of electronic and thermal Enthalpies=	-970.131481
Sum of electronic and thermal Free Energies=	-970.205168

VIIIb-Ni



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.814281	-4.666537	4.304596
2	6	0	-1.919534	-3.711714	3.799858
3	6	0	-2.196817	-1.302347	2.517965
4	6	0	-2.416377	-2.611851	4.496160
5	6	0	-1.549517	-3.595791	2.463420
6	6	0	-1.665068	-2.371262	1.796405
7	6	0	-2.574245	-1.382686	3.859351
8	1	0	-2.687053	-2.720877	5.541247
9	1	0	-1.150682	-4.459529	1.941798
10	6	0	-3.175439	-0.131649	4.493206
11	8	0	-2.350013	-0.113560	1.843493
12	6	0	-4.649651	-0.022586	4.041395
13	1	0	-5.215780	-0.890799	4.394757
14	1	0	-4.723563	0.021205	2.950381
15	1	0	-5.100514	0.886076	4.453650
16	6	0	-3.124360	-0.177655	6.019601
17	1	0	-2.096316	-0.260282	6.386396
18	1	0	-3.700259	-1.027855	6.395773

19	1	0	-3.576372	0.723276	6.443562
20	6	0	-2.416426	1.064474	3.926232
21	6	0	-1.135525	3.209790	2.637748
22	6	0	-2.092397	2.223768	4.629186
23	6	0	-2.067344	1.016878	2.576339
24	6	0	-1.428104	2.056382	1.903070
25	6	0	-1.461174	3.289150	3.989285
26	1	0	-2.333704	2.303695	5.684097
27	1	0	-1.219058	4.186234	4.549760
28	1	0	-0.635517	4.042037	2.151676
29	15	0	-1.054147	-2.058255	0.078134
30	15	0	-1.004361	1.789379	0.124964
31	6	0	0.124864	3.218368	-0.124030
32	6	0	2.031038	5.242821	-0.470437
33	6	0	1.451159	3.031078	0.292249
34	6	0	-0.233085	4.427799	-0.721195
35	6	0	0.719261	5.434394	-0.894920
36	6	0	2.397306	4.036345	0.127813
37	1	0	1.757403	2.078600	0.725408
38	1	0	-1.251002	4.582715	-1.068257
39	1	0	0.431877	6.368504	-1.368411
40	1	0	3.419498	3.861259	0.451087
41	1	0	2.768921	6.026407	-0.612310
42	6	0	-2.577304	2.266276	-0.694537
43	6	0	-4.935162	2.903158	-2.055622
44	6	0	-3.389831	3.315946	-0.246795
45	6	0	-2.970302	1.526195	-1.812559
46	6	0	-4.141472	1.848742	-2.495413
47	6	0	-4.561389	3.634151	-0.926651
48	1	0	-3.104406	3.882423	0.636983
49	1	0	-2.358904	0.695196	-2.154951
50	1	0	-4.422762	1.268098	-3.368639
51	1	0	-5.185225	4.450977	-0.576256
52	1	0	-5.848787	3.156103	-2.585381
53	6	0	-0.330629	-3.709085	-0.283355

54	6	0	0.943452	-6.174323	-0.673431
55	6	0	-0.983628	-4.742485	-0.960379
56	6	0	0.962266	-3.929057	0.202972
57	6	0	1.594905	-5.154462	0.018956
58	6	0	-0.343458	-5.964977	-1.162222
59	1	0	-1.994081	-4.598324	-1.330752
60	1	0	1.475957	-3.127091	0.729896
61	1	0	2.599450	-5.307144	0.402038
62	1	0	-0.857649	-6.757963	-1.696548
63	1	0	1.436944	-7.128338	-0.830611
64	6	0	-2.599097	-2.034096	-0.919893
65	6	0	-4.817849	-1.721256	-2.604217
66	6	0	-3.855567	-1.738178	-0.386779
67	6	0	-2.471650	-2.187068	-2.306446
68	6	0	-3.571207	-2.035348	-3.144014
69	6	0	-4.956488	-1.579236	-1.226796
70	1	0	-3.984814	-1.625968	0.684916
71	1	0	-1.500795	-2.439052	-2.727193
72	1	0	-3.453541	-2.161029	-4.216367
73	1	0	-5.925501	-1.340433	-0.799254
74	1	0	-5.677243	-1.592753	-3.255375
75	6	0	6.716197	0.327922	1.154526
76	8	0	6.077682	-0.039442	-0.087342
77	5	0	4.862915	0.600917	-0.129948
78	8	0	4.556575	1.217258	1.066840
79	6	0	5.498288	0.728905	2.045322
80	6	0	5.780718	1.824720	3.059679
81	1	0	4.872975	2.038607	3.631120
82	1	0	6.102390	2.746162	2.569746
83	1	0	6.560914	1.507010	3.759889
84	6	0	4.843760	-0.473821	2.723872
85	1	0	4.651040	-1.271713	1.998057
86	1	0	3.886587	-0.160283	3.150112
87	1	0	5.471057	-0.873819	3.526132
88	6	0	7.639047	1.506059	0.850002

89	1	0	7.066246	2.371403	0.501874
90	1	0	8.333093	1.213096	0.057709
91	1	0	8.217729	1.799648	1.731010
92	6	0	7.520499	-0.856785	1.665147
93	1	0	6.905314	-1.756601	1.729861
94	1	0	7.936965	-0.640995	2.654951
95	1	0	8.349585	-1.058204	0.980920
96	6	0	3.846240	0.568815	-1.315630
97	1	0	4.315750	0.400930	-2.290929
98	1	0	3.337636	1.537975	-1.350927
99	6	0	2.822650	-0.567267	-1.063328
100	1	0	2.537298	-0.551299	0.000295
101	6	0	1.566887	-0.520571	-1.967179
102	6	0	1.679078	-1.709796	-2.916434
103	1	0	1.442436	-1.454480	-3.955168
104	1	0	1.021043	-2.552097	-2.614405
105	7	0	3.084783	-2.105633	-2.824000
106	6	0	3.442814	-1.925477	-1.423662
107	1	0	4.532899	-1.939080	-1.299982
108	1	0	3.018794	-2.732871	-0.801289
109	6	0	3.325866	-3.447142	-3.305909
110	1	0	3.047760	-3.517997	-4.362506
111	1	0	2.745750	-4.205181	-2.743611
112	1	0	4.389762	-3.689238	-3.215672
113	6	0	0.993114	0.734467	-2.262258
114	28	0	-0.007297	-0.139055	-0.738967
115	1	0	1.482095	1.615688	-1.854006
116	1	0	-1.172109	3.904485	-4.827733
117	6	0	-1.042194	2.844939	-4.625436
118	6	0	-0.690946	0.144325	-4.082791
119	6	0	-1.795614	1.902885	-5.324441
120	6	0	-0.122844	2.437470	-3.666561
121	6	0	0.069221	1.077870	-3.357854
122	6	0	-1.606644	0.550275	-5.049183
123	1	0	-2.515865	2.218724	-6.072986

124	1	0	0.459687	3.180975	-3.127128
125	1	0	-2.181814	-0.199079	-5.586710
126	1	0	-0.589059	-0.911493	-3.864345

Zero-point correction=	1.055717
(Hartree/Particle)	
Thermal correction to Energy=	1.116107
Thermal correction to Enthalpy=	1.117052
Thermal correction to Gibbs Free Energy=	0.959414
Sum of electronic and zero-point Energies=	-3401.513008
Sum of electronic and thermal Energies=	-3401.452618
Sum of electronic and thermal Enthalpies=	-3401.451674
Sum of electronic and thermal Free Energies=	-3401.609312

TSivb-viii

Imaginary frequency: -669.7744

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	28	0	-0.233855	0.086243	0.183126
2	1	0	-3.399957	0.476160	2.980779
3	6	0	-3.041733	0.352859	1.947906
4	1	0	-2.110816	0.930672	1.878447
5	6	0	-2.763801	-1.135956	1.677284
6	6	0	-3.893964	-2.061895	2.143576
7	7	0	-3.775579	-3.219836	1.267505
8	6	0	-3.539173	-2.664005	-0.060110
9	6	0	-2.609128	-1.495813	0.200441
10	1	0	-1.837223	-1.434549	2.195189
11	1	0	-4.871566	-1.559604	2.016332
12	1	0	-3.796450	-2.360828	3.193628
13	1	0	-4.492922	-2.313730	-0.511717
14	1	0	-3.114388	-3.423808	-0.729277
15	1	0	-4.748136	-4.958772	0.649224
16	6	0	-1.700532	-0.919185	-0.612920

17	6	0	-4.912251	-4.107917	1.319452
18	1	0	-5.036349	-4.494161	2.336237
19	1	0	-5.854641	-3.609182	1.019896
20	1	0	-1.453862	0.680024	-0.486315
21	5	0	-4.077465	0.965933	0.932929
22	8	0	-5.159942	0.289958	0.418562
23	6	0	-5.660389	1.063897	-0.691077
24	6	0	-5.189309	2.508377	-0.326608
25	8	0	-4.002586	2.254431	0.453136
26	6	0	-7.167512	0.885641	-0.779364
27	1	0	-7.395875	-0.155751	-1.023659
28	1	0	-7.584410	1.522093	-1.567437
29	1	0	-7.655751	1.129718	0.166318
30	6	0	-4.984511	0.520782	-1.948274
31	1	0	-5.238920	-0.538384	-2.048452
32	1	0	-3.894028	0.600465	-1.875890
33	1	0	-5.323680	1.043629	-2.847662
34	6	0	-6.170941	3.243618	0.582780
35	1	0	-6.448650	2.624027	1.441162
36	1	0	-7.080522	3.525795	0.043984
37	1	0	-5.693362	4.153459	0.958307
38	6	0	-4.817094	3.371452	-1.522062
39	1	0	-3.974577	2.941228	-2.068062
40	1	0	-4.531572	4.372425	-1.185447
41	1	0	-5.669275	3.471668	-2.202984
42	1	0	3.400110	-4.711171	-2.488470
43	6	0	3.277221	-3.696058	-2.125640
44	6	0	2.986105	-1.133552	-1.200404
45	6	0	3.827006	-2.635623	-2.842934
46	6	0	2.552746	-3.464548	-0.959489
47	6	0	2.368230	-2.161997	-0.486810
48	6	0	3.698177	-1.325375	-2.383648
49	1	0	4.363756	-2.837513	-3.764075
50	1	0	2.098301	-4.297559	-0.433870
51	6	0	4.307292	-0.091879	-3.045328

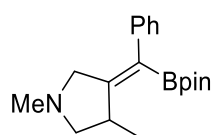
52	8	0	2.834708	0.137128	-0.698329
53	6	0	5.604422	0.270772	-2.286634
54	1	0	6.328195	-0.546951	-2.367750
55	1	0	5.400137	0.449701	-1.225935
56	1	0	6.046160	1.177965	-2.712317
57	6	0	4.638911	-0.332109	-4.517138
58	1	0	3.746343	-0.594192	-5.094470
59	1	0	5.370495	-1.138437	-4.618767
60	1	0	5.089674	0.561918	-4.956917
61	6	0	3.319165	1.056411	-2.857449
62	6	0	1.609578	3.198809	-2.199796
63	6	0	3.071211	2.078512	-3.774621
64	6	0	2.661199	1.134361	-1.632503
65	6	0	1.817064	2.182535	-1.266133
66	6	0	2.224173	3.136706	-3.449197
67	1	0	3.545159	2.058828	-4.750599
68	1	0	2.046979	3.923243	-4.175386
69	1	0	0.957021	4.030756	-1.952307
70	15	0	1.188799	-1.689075	0.853070
71	15	0	0.999034	2.038294	0.372918
72	6	0	0.158221	3.661347	0.548347
73	6	0	-1.210082	6.078601	0.859575
74	6	0	-1.236129	3.692876	0.498671
75	6	0	0.867385	4.852286	0.752445
76	6	0	0.185360	6.055327	0.899459
77	6	0	-1.918404	4.897689	0.661788
78	1	0	-1.793433	2.776242	0.334447
79	1	0	1.953340	4.834292	0.804849
80	1	0	0.740018	6.975517	1.056500
81	1	0	-3.004329	4.894705	0.647709
82	1	0	-1.738540	7.018314	0.990249
83	6	0	2.415400	2.274872	1.528029
84	6	0	4.427460	2.696245	3.429549
85	6	0	3.704795	2.633579	1.125840
86	6	0	2.148253	2.118518	2.891755

87	6	0	3.144711	2.335522	3.837322
88	6	0	4.706380	2.839815	2.073484
89	1	0	3.931172	2.763065	0.070674
90	1	0	1.152435	1.820843	3.214280
91	1	0	2.923855	2.204778	4.892382
92	1	0	5.704313	3.119253	1.748862
93	1	0	5.207552	2.857794	4.167368
94	6	0	0.442681	-3.323169	1.246433
95	6	0	-0.779628	-5.803830	1.697141
96	6	0	-0.432158	-3.869394	0.296873
97	6	0	0.709757	-4.042783	2.414989
98	6	0	0.096564	-5.273937	2.639805
99	6	0	-1.034340	-5.103237	0.520847
100	1	0	-0.628672	-3.334276	-0.628360
101	1	0	1.402157	-3.650452	3.152291
102	1	0	0.311947	-5.820470	3.552959
103	1	0	-1.712160	-5.512273	-0.222681
104	1	0	-1.258377	-6.761856	1.875545
105	6	0	2.245544	-1.349255	2.312366
106	6	0	3.733501	-0.822492	4.622914
107	6	0	3.636497	-1.258202	2.248842
108	6	0	1.602967	-1.140334	3.540168
109	6	0	2.343052	-0.899696	4.692455
110	6	0	4.375324	-0.985322	3.399181
111	1	0	4.147695	-1.407061	1.301901
112	1	0	0.516222	-1.188516	3.595730
113	1	0	1.835053	-0.760406	5.642117
114	1	0	5.456524	-0.907702	3.336697
115	1	0	4.312391	-0.620359	5.519182
116	1	0	-3.500619	-2.029523	-2.440691
117	6	0	-2.501954	-1.890387	-2.838348
118	6	0	0.017367	-1.473594	-3.939145
119	6	0	-2.238538	-2.272167	-4.151742
120	6	0	-1.508589	-1.306143	-2.033199
121	6	0	-0.254261	-1.085676	-2.632497

122	6	0	-0.975882	-2.078199	-4.707394
123	1	0	-3.029446	-2.721258	-4.746099
124	1	0	0.521524	-0.594213	-2.050356
125	1	0	-0.773736	-2.381208	-5.730331
126	1	0	1.006602	-1.296501	-4.353983

Zero-point correction=				1.050021	
(Hartree/Particle)					
Thermal correction to Energy=				1.110020	
Thermal correction to Enthalpy=				1.110964	
Thermal correction to Gibbs Free Energy=				0.955185	
Sum of electronic and zero-point Energies=				-3401.479464	
Sum of electronic and thermal Energies=				-3401.419465	
Sum of electronic and thermal Enthalpies=				-3401.418521	
Sum of electronic and thermal Free Energies=				-3401.574299	

IXb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.487116	-0.748287	0.110950
2	6	0	2.996091	-0.593617	0.097527
3	7	0	3.486817	-1.922369	-0.246302
4	6	0	2.576928	-2.831665	0.440140
5	6	0	1.197094	-2.244473	0.118224
6	1	0	3.347905	-0.296542	1.107052
7	1	0	3.347329	0.168930	-0.606609
8	1	0	2.755691	-2.828865	1.533843
9	1	0	2.705779	-3.856355	0.074490
10	1	0	0.452165	-2.498804	0.875120
11	6	0	0.585500	0.252708	0.068112

12	5	0	-0.950119	-0.019031	0.088660
13	8	0	-1.534929	-1.219502	0.424273
14	6	0	-2.938089	-1.117137	0.097740
15	6	0	-3.175539	0.424335	0.155049
16	8	0	-1.881529	0.945234	-0.215073
17	6	0	0.714602	-2.717810	-1.258776
18	1	0	1.493913	-2.539958	-2.005811
19	1	0	-0.190487	-2.184664	-1.558079
20	1	0	0.491495	-3.789929	-1.237151
21	6	0	4.877327	-2.122363	0.094964
22	1	0	5.501655	-1.413161	-0.457066
23	1	0	5.183522	-3.135886	-0.180860
24	6	0	1.032348	1.675293	-0.004109
25	6	0	1.874243	4.353865	-0.171095
26	6	0	1.908624	2.214440	0.945137
27	6	0	0.568323	2.511633	-1.027476
28	6	0	0.989991	3.834499	-1.115123
29	6	0	2.328702	3.539585	0.862709
30	1	0	2.249311	1.590177	1.766546
31	1	0	-0.130669	2.113638	-1.756808
32	1	0	0.625524	4.463600	-1.921827
33	1	0	3.008262	3.936880	1.610864
34	1	0	2.201264	5.386994	-0.237644
35	6	0	-3.742735	-1.924990	1.102642
36	1	0	-3.499898	-1.639932	2.128093
37	1	0	-3.521879	-2.989124	0.980087
38	1	0	-4.815565	-1.776688	0.939170
39	6	0	-3.110975	-1.691667	-1.307137
40	1	0	-2.547447	-1.105861	-2.041150
41	1	0	-4.163186	-1.709089	-1.606351
42	1	0	-2.728554	-2.716250	-1.319101
43	6	0	-3.467020	0.924629	1.568619
44	1	0	-2.727475	0.540969	2.278527
45	1	0	-4.464058	0.622173	1.902671
46	1	0	-3.412177	2.016402	1.574185

47	6	0	-4.219609	0.946721	-0.818221
48	1	0	-4.316167	2.030123	-0.704738
49	1	0	-5.194944	0.492443	-0.612928
50	1	0	-3.942964	0.733712	-1.852764
51	1	0	5.068668	-1.983253	1.176190

Zero-point correction= 0.449780
(Hartree/Particle)

Thermal correction to Energy= 0.472357

Thermal correction to Enthalpy= 0.473301

Thermal correction to Gibbs Free Energy= 0.399040

Sum of electronic and zero-point Energies= -970.157817

Sum of electronic and thermal Energies= -970.135239

Sum of electronic and thermal Enthalpies= -970.134295

Sum of electronic and thermal Free Energies= -970.208556

TS_{Vb-IXb}

Imaginary frequencies = -815.3482 cm⁻¹

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	1	0	-7.119045	1.940932	-2.291494
2	6	0	-6.372338	1.305365	-1.826631
3	6	0	-4.479502	-0.301871	-0.659944
4	6	0	-6.592867	-0.067122	-1.735069
5	6	0	-5.199448	1.869014	-1.332546
6	6	0	-4.218049	1.067642	-0.739701
7	6	0	-5.646590	-0.898721	-1.138786
8	1	0	-7.511281	-0.486536	-2.132273
9	1	0	-5.036313	2.937460	-1.427119
10	6	0	-5.805333	-2.401483	-0.921643
11	8	0	-3.511396	-1.089852	-0.076791
12	6	0	-6.217665	-2.634509	0.549525
13	1	0	-7.184067	-2.158536	0.746070

14	1	0	-5.476216	-2.215050	1.236392
15	1	0	-6.305575	-3.707687	0.748493
16	6	0	-6.866067	-3.008197	-1.838704
17	1	0	-6.615028	-2.866105	-2.894672
18	1	0	-7.842290	-2.554429	-1.646602
19	1	0	-6.971031	-4.079216	-1.644059
20	6	0	-4.431829	-3.029587	-1.137690
21	6	0	-1.814430	-4.047524	-1.323977
22	6	0	-4.190387	-4.270907	-1.725872
23	6	0	-3.328120	-2.322648	-0.663445
24	6	0	-2.015733	-2.787777	-0.754096
25	6	0	-2.895312	-4.779297	-1.809781
26	1	0	-5.016744	-4.853993	-2.119098
27	1	0	-2.728505	-5.752354	-2.260191
28	1	0	-0.807703	-4.446614	-1.402963
29	15	0	-2.551956	1.670435	-0.217792
30	15	0	-0.701775	-1.647857	-0.164339
31	6	0	0.844463	-2.529354	-0.611403
32	6	0	3.369661	-3.457554	-1.405689
33	6	0	1.169938	-2.640258	-1.970631
34	6	0	1.798801	-2.894569	0.340661
35	6	0	3.058778	-3.344377	-0.054771
36	6	0	2.416010	-3.115890	-2.365057
37	1	0	0.445339	-2.337039	-2.724988
38	1	0	1.566055	-2.820790	1.398773
39	1	0	3.799574	-3.598601	0.697394
40	1	0	2.650859	-3.200153	-3.422242
41	1	0	4.354695	-3.796142	-1.711667
42	6	0	-0.796656	-1.883547	1.653901
43	6	0	-0.819202	-2.152782	4.436176
44	6	0	-1.171365	-3.096528	2.241444
45	6	0	-0.439207	-0.808039	2.470822
46	6	0	-0.448123	-0.941958	3.858367
47	6	0	-1.182427	-3.229344	3.626649
48	1	0	-1.452518	-3.937413	1.612210

49	1	0	-0.157477	0.138455	2.012895
50	1	0	-0.176593	-0.094519	4.481314
51	1	0	-1.474587	-4.173552	4.076362
52	1	0	-0.831139	-2.259540	5.516661
53	6	0	-2.677864	3.455535	-0.636886
54	6	0	-2.848589	6.143403	-1.392464
55	6	0	-3.446539	4.353640	0.112568
56	6	0	-1.992024	3.918331	-1.762412
57	6	0	-2.082029	5.255760	-2.143232
58	6	0	-3.529151	5.691643	-0.262210
59	1	0	-3.979699	4.002939	0.993239
60	1	0	-1.371665	3.225769	-2.326565
61	1	0	-1.543778	5.605110	-3.019118
62	1	0	-4.123458	6.382103	0.328492
63	1	0	-2.911027	7.187813	-1.682602
64	6	0	-2.657835	1.718248	1.618996
65	6	0	-2.577256	1.757820	4.417967
66	6	0	-3.623126	1.037832	2.361713
67	6	0	-1.644723	2.417313	2.292456
68	6	0	-1.609272	2.442728	3.682045
69	6	0	-3.579051	1.055381	3.755988
70	1	0	-4.417554	0.494562	1.858247
71	1	0	-0.880252	2.938549	1.718910
72	1	0	-0.822638	2.992075	4.191533
73	1	0	-4.334514	0.519726	4.322701
74	1	0	-2.547219	1.771308	5.503368
75	6	0	3.789829	1.102626	-1.664858
76	6	0	2.452211	1.771061	-1.369252
77	6	0	2.085091	2.425363	-2.713653
78	7	0	3.338167	2.495374	-3.455977
79	6	0	4.008151	1.236456	-3.153978
80	1	0	2.573171	2.527225	-0.588971
81	1	0	1.348893	1.783503	-3.241876
82	1	0	1.638293	3.419468	-2.603087
83	1	0	5.063178	1.256668	-3.446232

84	1	0	3.523812	0.391177	-3.692288
85	6	0	3.155240	2.717823	-4.871902
86	1	0	2.552306	1.918930	-5.346364
87	1	0	4.127530	2.757798	-5.372980
88	1	0	2.646295	3.673006	-5.034007
89	6	0	4.609960	0.517504	-0.767432
90	6	0	1.416653	0.722418	-0.937497
91	1	0	1.745182	0.270411	0.008749
92	1	0	1.426564	-0.068387	-1.703896
93	28	0	-0.559169	0.660373	-0.671650
94	1	0	0.267533	1.876748	-0.842788
95	5	0	4.323665	0.600077	0.763813
96	8	0	4.930272	-0.223749	1.685376
97	8	0	3.496759	1.523895	1.365042
98	6	0	4.293500	0.012832	2.957964
99	6	0	3.734283	1.459809	2.784144
100	6	0	3.183668	-1.025399	3.100514
101	1	0	2.684040	-0.954652	4.071971
102	1	0	3.617987	-2.024754	3.000443
103	1	0	2.431032	-0.897823	2.315063
104	6	0	5.322346	-0.148190	4.065348
105	1	0	4.887222	0.118667	5.034660
106	1	0	6.198975	0.478286	3.887453
107	1	0	5.649899	-1.190616	4.111728
108	6	0	2.427907	1.734936	3.512766
109	1	0	2.550347	1.595289	4.592813
110	1	0	2.119077	2.768786	3.330819
111	6	0	4.766474	2.537038	3.112524
112	1	0	4.956346	2.596120	4.188550
113	1	0	4.388586	3.503730	2.769205
114	1	0	5.713307	2.338429	2.599769
115	1	0	1.634247	1.073729	3.157314
116	6	0	5.832349	-0.213852	-1.198369
117	6	0	8.156522	-1.586325	-2.009124
118	6	0	7.044664	-0.050036	-0.513865

119	6	0	5.809130	-1.097201	-2.286036
120	6	0	6.956742	-1.773971	-2.690672
121	6	0	8.194329	-0.721291	-0.916855
122	1	0	7.081841	0.613788	0.345421
123	1	0	4.868420	-1.270338	-2.801414
124	1	0	6.911310	-2.453698	-3.536947
125	1	0	9.123778	-0.570310	-0.375669
126	1	0	9.052797	-2.113675	-2.321343

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Zero-point correction=                1.048464
(Hartree/Particle)

Thermal correction to Energy=          1.109245

Thermal correction to Enthalpy=        1.110189

Thermal correction to Gibbs Free Energy= 0.950529

Sum of electronic and zero-point Energies= -3401.457855
Sum of electronic and thermal Energies=    -3401.397074
Sum of electronic and thermal Enthalpies=   -3401.396129
Sum of electronic and thermal Free Energies= -3401.555790

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TS_{vib-vib}

Imaginary frequency: -110.9665

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.994981	1.990131	-4.084139
2	6	0	3.504143	2.194728	-3.136618
3	6	0	2.546379	2.153416	-1.923335
4	6	0	3.443290	1.571617	-0.830515
5	6	0	4.804958	1.331337	-1.439491
6	7	0	4.502325	1.168231	-2.855750
7	1	0	3.986059	3.190564	-3.213566
8	1	0	5.306229	0.442378	-1.035843
9	1	0	5.477257	2.202160	-1.276213

10	6	0	5.670050	1.255744	-3.703881
11	1	0	6.388427	0.473723	-3.435175
12	1	0	5.380585	1.111347	-4.749191
13	6	0	3.047188	1.282593	0.416080
14	28	0	-0.220600	0.527542	-1.126618
15	5	0	-0.082889	2.393462	-0.754179
16	8	0	0.127907	2.679672	0.599236
17	6	0	0.270404	4.098502	0.785834
18	6	0	-0.362722	4.678283	-0.528369
19	8	0	-0.268002	3.583227	-1.454749
20	1	0	2.283755	3.186964	-1.664927
21	6	0	1.242112	1.396809	-2.207562
22	1	0	1.994706	1.429826	0.654761
23	1	0	1.517648	0.418363	-2.630311
24	1	0	0.732880	1.939813	-3.015693
25	6	0	1.757879	4.409213	0.956682
26	1	0	2.138139	3.842416	1.812120
27	1	0	1.919910	5.475271	1.146497
28	1	0	2.342132	4.115159	0.082681
29	6	0	-0.454890	4.498950	2.065112
30	1	0	0.015347	3.998069	2.916776
31	1	0	-1.505451	4.206652	2.043051
32	1	0	-0.390501	5.581730	2.221254
33	6	0	0.383917	5.869433	-1.114771
34	1	0	0.377741	6.714573	-0.417563
35	1	0	-0.106447	6.185434	-2.040269
36	1	0	1.420600	5.614509	-1.347497
37	6	0	-1.842414	5.028534	-0.375835
38	1	0	-2.412005	4.179839	0.017032
39	1	0	-2.251998	5.271807	-1.360393
40	1	0	-1.983662	5.889013	0.286066
41	1	0	6.178657	2.234647	-3.614964
42	1	0	3.262335	-3.630042	2.885296
43	6	0	2.337211	-3.149362	2.584266
44	6	0	0.006461	-1.925162	1.828212

45	6	0	1.447004	-2.697453	3.556123
46	6	0	2.067135	-2.963705	1.231613
47	6	0	0.885176	-2.336892	0.825442
48	6	0	0.258948	-2.064323	3.192920
49	1	0	1.688107	-2.838419	4.604992
50	1	0	2.786087	-3.294360	0.489461
51	6	0	-0.805420	-1.560907	4.165370
52	8	0	-1.175315	-1.360703	1.412534
53	6	0	-1.905607	-2.640875	4.275468
54	1	0	-1.484106	-3.567989	4.677879
55	1	0	-2.340127	-2.855052	3.293017
56	1	0	-2.704973	-2.296989	4.940292
57	6	0	-0.224591	-1.286051	5.551878
58	1	0	0.568208	-0.531569	5.510102
59	1	0	0.184217	-2.202755	5.985597
60	1	0	-1.005912	-0.936693	6.232491
61	6	0	-1.438113	-0.313672	3.551200
62	6	0	-2.788235	1.772327	2.219180
63	6	0	-1.906664	0.796425	4.255268
64	6	0	-1.644432	-0.316318	2.174595
65	6	0	-2.322417	0.685464	1.481220
66	6	0	-2.569612	1.829527	3.594742
67	1	0	-1.760362	0.860968	5.328477
68	1	0	-2.920473	2.688146	4.158532
69	1	0	-3.306739	2.583949	1.717445
70	15	0	0.481858	-1.901882	-0.924405
71	15	0	-2.370160	0.462416	-0.336999
72	6	0	-3.528989	1.748633	-0.948489
73	6	0	-5.304260	3.613835	-2.036229
74	6	0	-3.183627	2.462392	-2.097895
75	6	0	-4.784527	1.956926	-0.361913
76	6	0	-5.659820	2.897617	-0.891746
77	6	0	-4.074630	3.386274	-2.645116
78	1	0	-2.205825	2.310725	-2.546751
79	1	0	-5.077117	1.372315	0.507417

80	1	0	-6.625628	3.062411	-0.424084
81	1	0	-3.797595	3.937027	-3.538869
82	1	0	-5.992918	4.341578	-2.454563
83	6	0	-3.489639	-0.996881	-0.514868
84	6	0	-5.291687	-3.084757	-0.991345
85	6	0	-4.198371	-1.572761	0.541376
86	6	0	-3.680528	-1.488529	-1.810202
87	6	0	-4.583200	-2.518207	-2.049421
88	6	0	-5.091419	-2.616583	0.303287
89	1	0	-4.065009	-1.203857	1.554959
90	1	0	-3.118029	-1.059485	-2.637809
91	1	0	-4.718392	-2.892798	-3.059377
92	1	0	-5.636313	-3.057621	1.132945
93	1	0	-5.991021	-3.894755	-1.176348
94	6	0	1.969421	-2.585139	-1.772429
95	6	0	4.321415	-3.538339	-2.962378
96	6	0	3.042456	-1.724120	-2.017032
97	6	0	2.092018	-3.937417	-2.120764
98	6	0	3.261013	-4.409109	-2.709592
99	6	0	4.208960	-2.195908	-2.616534
100	1	0	2.979590	-0.677515	-1.741624
101	1	0	1.273801	-4.625278	-1.928151
102	1	0	3.344021	-5.459490	-2.972276
103	1	0	5.013904	-1.495441	-2.817684
104	1	0	5.229030	-3.909380	-3.429150
105	6	0	-0.770885	-3.163492	-1.407852
106	6	0	-2.578981	-5.100152	-2.315690
107	6	0	-1.482572	-3.945403	-0.497489
108	6	0	-1.000445	-3.337531	-2.779411
109	6	0	-1.888698	-4.307175	-3.231074
110	6	0	-2.385307	-4.906269	-0.951723
111	1	0	-1.327444	-3.820656	0.570209
112	1	0	-0.454423	-2.730928	-3.499660
113	1	0	-2.041071	-4.444433	-4.297567
114	1	0	-2.935195	-5.506296	-0.232860

115	1	0	-3.275722	-5.855897	-2.666027
116	6	0	3.876139	0.801911	1.534230
117	6	0	5.354219	-0.091954	3.761188
118	6	0	3.255257	0.110139	2.585125
119	6	0	5.252783	1.056294	1.638505
120	6	0	5.983662	0.608427	2.734372
121	6	0	3.984337	-0.334475	3.682388
122	1	0	2.185179	-0.084051	2.529942
123	1	0	5.751246	1.642861	0.874208
124	1	0	7.046944	0.821755	2.793596
125	1	0	3.478182	-0.871026	4.480049
126	1	0	5.923921	-0.433592	4.620082

Zero-point correction=				1.054115	
(Hartree/Particle)					
Thermal correction to Energy=				1.113762	
Thermal correction to Enthalpy=				1.114706	
Thermal correction to Gibbs Free Energy=				0.961179	
Sum of electronic and zero-point Energies=				-3401.463575	
Sum of electronic and thermal Energies=				-3401.403928	
Sum of electronic and thermal Enthalpies=				-3401.402984	
Sum of electronic and thermal Free Energies=				-3401.556511	

Xb

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	2.752691	-5.399802	-2.299760
2	6	0	2.726331	-4.404787	-1.867461
3	6	0	2.667439	-1.891603	-0.772648
4	6	0	3.842810	-3.576952	-1.973592
5	6	0	1.574060	-3.962920	-1.222787
6	6	0	1.521280	-2.679286	-0.671500
7	6	0	3.834931	-2.298991	-1.417201

8	1	0	4.724477	-3.936044	-2.494487
9	1	0	0.703059	-4.608189	-1.166089
10	6	0	5.007874	-1.323442	-1.416993
11	8	0	2.609219	-0.638726	-0.203127
12	6	0	5.690135	-1.386312	-0.031649
13	1	0	6.090951	-2.390348	0.142524
14	1	0	4.979483	-1.151321	0.766742
15	1	0	6.512845	-0.665029	0.013929
16	6	0	6.036829	-1.657874	-2.495569
17	1	0	5.596310	-1.623973	-3.497150
18	1	0	6.454484	-2.654813	-2.329497
19	1	0	6.872824	-0.953953	-2.456047
20	6	0	4.420287	0.073965	-1.595640
21	6	0	3.221230	2.617335	-1.681929
22	6	0	4.999810	1.108792	-2.328413
23	6	0	3.228158	0.354235	-0.928299
24	6	0	2.601319	1.599126	-0.951969
25	6	0	4.408171	2.370021	-2.367605
26	1	0	5.922910	0.936499	-2.872246
27	1	0	4.876203	3.166006	-2.937650
28	1	0	2.765812	3.602221	-1.724123
29	15	0	0.008440	-1.901638	0.034670
30	15	0	1.010038	1.760337	-0.037058
31	6	0	0.501825	3.450018	-0.542287
32	6	0	-0.472621	5.926667	-1.405527
33	6	0	-0.157986	3.563148	-1.773608
34	6	0	0.668536	4.586324	0.250211
35	6	0	0.173676	5.818945	-0.177612
36	6	0	-0.629804	4.796605	-2.209048
37	1	0	-0.329864	2.672445	-2.375457
38	1	0	1.170014	4.509979	1.210974
39	1	0	0.293091	6.694651	0.453092
40	1	0	-1.133228	4.875578	-3.167926
41	1	0	-0.857044	6.886473	-1.736454
42	6	0	1.604315	1.963227	1.687614

43	6	0	2.386139	2.221900	4.359110
44	6	0	2.864526	2.480536	2.006793
45	6	0	0.742598	1.573422	2.717104
46	6	0	1.131735	1.704090	4.048170
47	6	0	3.252038	2.610143	3.337556
48	1	0	3.542989	2.781477	1.212317
49	1	0	-0.230145	1.154211	2.468951
50	1	0	0.457988	1.387305	4.838319
51	1	0	4.231944	3.011886	3.577401
52	1	0	2.693339	2.318737	5.396069
53	6	0	-1.206312	-3.260821	-0.156366
54	6	0	-3.071239	-5.296721	-0.593244
55	6	0	-1.358170	-4.289691	0.778099
56	6	0	-1.996043	-3.261557	-1.310545
57	6	0	-2.919753	-4.278472	-1.532143
58	6	0	-2.291601	-5.300787	0.561546
59	1	0	-0.747815	-4.299214	1.677006
60	1	0	-1.898055	-2.448390	-2.025850
61	1	0	-3.536959	-4.261551	-2.424583
62	1	0	-2.408627	-6.092390	1.295445
63	1	0	-3.802920	-6.082081	-0.757210
64	6	0	0.325558	-1.901639	1.847564
65	6	0	0.653245	-1.734066	4.624520
66	6	0	1.570586	-2.149702	2.427001
67	6	0	-0.755018	-1.563068	2.674552
68	6	0	-0.596588	-1.492206	4.053750
69	6	0	1.733313	-2.057341	3.809411
70	1	0	2.420061	-2.420871	1.806838
71	1	0	-1.722490	-1.350573	2.223732
72	1	0	-1.445202	-1.237562	4.681879
73	1	0	2.709009	-2.243419	4.247913
74	1	0	0.783573	-1.667407	5.700545
75	28	0	-0.749981	0.280197	-0.204983
76	6	0	-2.588196	2.776511	0.614664
77	1	0	-2.158583	2.870620	1.624334

78	1	0	-2.058399	3.508188	-0.004684
79	6	0	-2.282439	1.391271	0.134466
80	6	0	-2.692837	0.211584	-0.149672
81	7	0	-3.982787	3.196465	0.681348
82	6	0	-4.513082	3.655389	-0.596035
83	1	0	-3.915648	4.517817	-0.921758
84	1	0	-5.532492	4.020235	-0.406548
85	6	0	-4.546317	2.638396	-1.709747
86	1	0	-5.069827	1.704234	-1.505846
87	6	0	-3.980886	2.831051	-2.898751
88	1	0	-4.031454	2.087270	-3.689198
89	1	0	-3.444341	3.750865	-3.123378
90	6	0	-4.845685	2.259098	1.376406
91	1	0	-4.409438	2.035977	2.356712
92	1	0	-4.994910	1.302029	0.853010
93	1	0	-5.824740	2.723569	1.537298
94	1	0	-3.877210	-0.238128	-2.500709
95	6	0	-4.297086	-0.852258	-1.708150
96	6	0	-5.329757	-2.438754	0.326231
97	6	0	-3.775287	-0.720290	-0.409885
98	6	0	-5.324713	-1.749952	-1.978523
99	6	0	-5.846033	-2.550691	-0.963544
100	6	0	-4.310031	-1.533793	0.601448
101	1	0	-5.717097	-1.828420	-2.988723
102	1	0	-6.642905	-3.257070	-1.175317
103	1	0	-3.920883	-1.445097	1.612046
104	1	0	-5.723368	-3.061013	1.124898

Zero-point correction=				0.854984	
(Hartree/Particle)					
Thermal correction to Energy=				0.906493	
Thermal correction to Enthalpy=				0.907437	
Thermal correction to Gibbs Free Energy=				0.768435	
Sum of electronic and zero-point Energies=				-2989.932665	
Sum of electronic and thermal Energies=				-2989.881156	

Sum of electronic and thermal Enthalpies= -2989.880212
Sum of electronic and thermal Free Energies= -2990.019215

Xlb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	28	0	-0.149177	0.043667	-0.716581
2	5	0	-2.182822	-0.061773	-0.432970
3	8	0	-3.169772	-0.032933	-1.411235
4	6	0	-4.462342	-0.261782	-0.808147
5	6	0	-4.199282	0.026823	0.707965
6	8	0	-2.775199	-0.141202	0.824508
7	6	0	-4.526381	1.460957	1.120513
8	1	0	-5.608227	1.628306	1.159564
9	1	0	-4.086316	2.185711	0.432468
10	1	0	-4.107713	1.641564	2.116039
11	6	0	-4.877602	-0.943372	1.668083
12	1	0	-5.966621	-0.911358	1.552147
13	1	0	-4.637970	-0.660617	2.697932
14	1	0	-4.534394	-1.968042	1.507494
15	6	0	-5.478538	0.663000	-1.464811
16	1	0	-6.462014	0.550964	-0.994760
17	1	0	-5.575158	0.400930	-2.523177
18	1	0	-5.172547	1.708904	-1.396237
19	6	0	-4.846762	-1.712831	-1.075687
20	1	0	-5.848467	-1.934819	-0.692650
21	1	0	-4.132223	-2.400966	-0.617096
22	1	0	-4.839389	-1.889443	-2.155008
23	6	0	1.841607	0.218516	-0.886586
24	6	0	2.599389	0.082749	0.225214
25	1	0	2.088080	-0.183879	1.156100
26	6	0	2.478972	0.572607	-2.223394
27	1	0	3.437636	0.045108	-2.343177

28	1	0	2.712377	1.649573	-2.227682
29	7	0	1.716684	0.319680	-3.447929
30	6	0	1.471405	-1.088485	-3.688817
31	1	0	0.691212	-1.492625	-3.021269
32	1	0	2.387813	-1.664550	-3.521626
33	1	0	1.142406	-1.239628	-4.721842
34	6	0	0.496534	1.091671	-3.558317
35	1	0	-0.350905	0.608932	-3.019787
36	1	0	0.651884	2.061776	-3.065788
37	6	0	0.063555	1.349220	-4.980381
38	1	0	-0.945444	1.746881	-5.092058
39	6	0	0.818637	1.142339	-6.055099
40	1	0	0.456597	1.360828	-7.054814
41	1	0	1.826614	0.751168	-5.950612
42	1	0	1.261035	-4.796189	3.681911
43	6	0	0.913141	-3.840815	3.303899
44	6	0	0.068508	-1.390995	2.340487
45	6	0	0.675296	-2.786633	4.184867
46	6	0	0.690343	-3.670035	1.943803
47	6	0	0.257397	-2.440152	1.431832
48	6	0	0.232112	-1.551269	3.721514
49	1	0	0.830600	-2.939414	5.247618
50	1	0	0.870064	-4.493192	1.257520
51	6	0	-0.214426	-0.401452	4.614238
52	8	0	-0.284249	-0.173351	1.834338
53	6	0	-1.759974	-0.454827	4.687672
54	1	0	-2.080820	-1.395890	5.147394
55	1	0	-2.197046	-0.388461	3.685036
56	1	0	-2.134056	0.380974	5.288902
57	6	0	0.359076	-0.501240	6.026723
58	1	0	1.453264	-0.466608	6.023372
59	1	0	0.038105	-1.431246	6.503612
60	1	0	-0.015916	0.314960	6.649999
61	6	0	0.155930	0.904653	3.924319
62	6	0	0.481273	3.309190	2.522796

63	6	0	0.527101	2.070534	4.587629
64	6	0	-0.004223	0.964369	2.535058
65	6	0	0.113561	2.159034	1.812723
66	6	0	0.700974	3.266253	3.893436
67	1	0	0.678818	2.054821	5.661642
68	1	0	0.997893	4.164152	4.424764
69	1	0	0.622824	4.241469	1.983265
70	15	0	-0.027447	-2.209321	-0.371705
71	15	0	-0.182646	2.203082	-0.001723
72	6	0	1.114296	3.392861	-0.565616
73	6	0	3.153422	5.017135	-1.606907
74	6	0	2.409227	3.341100	-0.033040
75	6	0	0.852820	4.283576	-1.612192
76	6	0	1.866993	5.085847	-2.132550
77	6	0	3.418554	4.148482	-0.549563
78	1	0	2.635574	2.659558	0.780338
79	1	0	-0.146693	4.357927	-2.031516
80	1	0	1.645595	5.765846	-2.949290
81	1	0	4.416792	4.086234	-0.126029
82	1	0	3.943649	5.640239	-2.014073
83	6	0	-1.697718	3.221322	-0.234174
84	6	0	-3.956408	4.756674	-0.851376
85	6	0	-2.178689	4.166935	0.676307
86	6	0	-2.365179	3.046269	-1.452087
87	6	0	-3.479047	3.821691	-1.767118
88	6	0	-3.308766	4.922235	0.371755
89	1	0	-1.689926	4.303357	1.635553
90	1	0	-2.024094	2.280156	-2.144878
91	1	0	-3.982400	3.679075	-2.718568
92	1	0	-3.684777	5.641869	1.092376
93	1	0	-4.834042	5.350412	-1.087390
94	6	0	1.353230	-3.227452	-1.072986
95	6	0	3.539951	-4.536332	-2.257411
96	6	0	2.653953	-3.033019	-0.589550
97	6	0	1.163290	-4.111893	-2.139013

98	6	0	2.249395	-4.759315	-2.726892
99	6	0	3.737187	-3.676845	-1.178233
100	1	0	2.828687	-2.370638	0.249565
101	1	0	0.168115	-4.303146	-2.526340
102	1	0	2.079449	-5.440185	-3.555431
103	1	0	4.735278	-3.499763	-0.788371
104	1	0	4.384745	-5.035235	-2.722263
105	6	0	-1.473241	-3.270559	-0.771164
106	6	0	-3.530993	-4.957192	-1.643615
107	6	0	-2.050699	-4.190131	0.107433
108	6	0	-1.968432	-3.172542	-2.078464
109	6	0	-2.969626	-4.031483	-2.521059
110	6	0	-3.085107	-5.019496	-0.325649
111	1	0	-1.696718	-4.263430	1.131059
112	1	0	-1.564290	-2.419625	-2.752914
113	1	0	-3.330809	-3.957386	-3.542257
114	1	0	-3.532194	-5.725097	0.367926
115	1	0	-4.323995	-5.616888	-1.981903
116	1	0	6.998181	1.439420	-0.730272
117	6	0	6.330494	0.849212	-0.108832
118	6	0	4.604629	-0.615369	1.485967
119	6	0	6.846187	0.079810	0.930614
120	6	0	4.960058	0.877972	-0.360344
121	6	0	4.064173	0.130659	0.422270
122	6	0	5.971279	-0.650835	1.734132
123	1	0	7.914855	0.057848	1.120517
124	1	0	4.583742	1.510897	-1.155446
125	1	0	6.355250	-1.245168	2.558484
126	1	0	3.924362	-1.178536	2.124036

Zero-point correction=				1.052822	
(Hartree/Particle)					
Thermal correction to Energy=				1.113869	
Thermal correction to Enthalpy=				1.114813	
Thermal correction to Gibbs Free Energy=				0.958839	

Sum of electronic and zero-point Energies=	-3401.428780
Sum of electronic and thermal Energies=	-3401.367733
Sum of electronic and thermal Enthalpies=	-3401.366789
Sum of electronic and thermal Free Energies=	-3401.522764

TS_{Xb-XIb}

Imaginary frequency: -920.9477

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	28	0	-0.308854	0.469502	1.406383
2	5	0	0.959088	1.889529	0.778290
3	8	0	1.606679	2.810066	1.587975
4	6	0	2.622558	3.461927	0.795070
5	6	0	2.075716	3.277411	-0.652411
6	8	0	1.342001	2.040176	-0.541012
7	6	0	1.063254	4.346916	-1.061804
8	1	0	1.542005	5.315923	-1.235000
9	1	0	0.288274	4.469313	-0.296619
10	1	0	0.576101	4.022423	-1.986664
11	6	0	3.147782	3.134187	-1.719483
12	1	0	3.784638	4.026054	-1.743037
13	1	0	2.676746	3.013684	-2.699336
14	1	0	3.771237	2.255692	-1.530988
15	6	0	2.750241	4.907212	1.247608
16	1	0	3.439572	5.454532	0.595045
17	1	0	3.143984	4.941142	2.267603
18	1	0	1.781516	5.412516	1.236732
19	6	0	3.927679	2.704056	1.023602
20	1	0	4.767808	3.185323	0.512381
21	1	0	3.840793	1.673861	0.664489
22	1	0	4.139210	2.677045	2.096746
23	6	0	-2.135136	0.237756	2.186576
24	6	0	-2.005903	1.479070	1.872741

25	1	0	-0.681553	1.945957	1.247445
26	6	0	-3.192599	-0.646224	2.792902
27	1	0	-3.960519	-0.032467	3.285789
28	1	0	-2.743677	-1.287922	3.559259
29	7	0	-3.876144	-1.512989	1.837199
30	6	0	-4.574577	-0.739863	0.822351
31	1	0	-3.899414	-0.093845	0.230537
32	1	0	-5.327419	-0.104338	1.301804
33	1	0	-5.096664	-1.420347	0.144077
34	6	0	-2.984050	-2.503326	1.250406
35	1	0	-2.327230	-2.068275	0.473940
36	1	0	-2.301489	-2.856013	2.034795
37	6	0	-3.707208	-3.698443	0.688025
38	1	0	-3.095030	-4.344813	0.061429
39	6	0	-4.982467	-4.004698	0.914871
40	1	0	-5.434214	-4.896621	0.491222
41	1	0	-5.603795	-3.371231	1.541666
42	1	0	1.126027	1.930988	-5.650094
43	6	0	1.245674	1.336574	-4.749823
44	6	0	1.562842	-0.148258	-2.457759
45	6	0	2.504037	0.849836	-4.404094
46	6	0	0.137620	1.041643	-3.957701
47	6	0	0.280846	0.285472	-2.795385
48	6	0	2.683523	0.085138	-3.250494
49	1	0	3.352548	1.070866	-5.043200
50	1	0	-0.846949	1.403539	-4.240480
51	6	0	3.987216	-0.590023	-2.847462
52	8	0	1.673725	-0.872044	-1.291785
53	6	0	3.927108	-2.055658	-3.337689
54	1	0	3.838370	-2.083111	-4.429016
55	1	0	3.063770	-2.573874	-2.906795
56	1	0	4.834491	-2.592294	-3.040906
57	6	0	5.206159	0.090975	-3.470601
58	1	0	5.293635	1.134872	-3.151052
59	1	0	5.140031	0.064156	-4.561510

60	1	0	6.123884	-0.437885	-3.200354
61	6	0	4.053259	-0.618146	-1.323142
62	6	0	4.040596	-0.969780	1.457214
63	6	0	5.239717	-0.551927	-0.593973
64	6	0	2.864691	-0.829554	-0.616132
65	6	0	2.822311	-1.030687	0.771299
66	6	0	5.234285	-0.725633	0.785807
67	1	0	6.180110	-0.374397	-1.104536
68	1	0	6.163136	-0.669784	1.343810
69	1	0	4.060763	-1.083282	2.534047
70	15	0	-1.093137	-0.216072	-1.677317
71	15	0	1.191387	-1.181074	1.648021
72	6	0	1.706584	-1.220693	3.408859
73	6	0	2.454871	-1.151343	6.105819
74	6	0	1.315686	-0.155922	4.225665
75	6	0	2.479394	-2.253244	3.959376
76	6	0	2.850489	-2.219079	5.298904
77	6	0	1.689513	-0.121332	5.569263
78	1	0	0.715829	0.648762	3.805914
79	1	0	2.788773	-3.088294	3.334944
80	1	0	3.447345	-3.024840	5.714894
81	1	0	1.379291	0.711638	6.192064
82	1	0	2.744030	-1.126831	7.152019
83	6	0	0.599077	-2.900481	1.329030
84	6	0	-0.582655	-5.394809	0.796843
85	6	0	0.385232	-3.326013	0.011301
86	6	0	0.190485	-3.736315	2.375669
87	6	0	-0.385162	-4.977739	2.109703
88	6	0	-0.204269	-4.559095	-0.252136
89	1	0	0.663540	-2.689713	-0.819878
90	1	0	0.303326	-3.419412	3.407086
91	1	0	-0.690936	-5.611747	2.936382
92	1	0	-0.378773	-4.852934	-1.284035
93	1	0	-1.043759	-6.356683	0.593588
94	6	0	-2.389117	1.005608	-2.143765

95	6	0	-4.323025	2.988240	-2.574744
96	6	0	-2.333359	2.223676	-1.453592
97	6	0	-3.417606	0.799837	-3.068518
98	6	0	-4.378364	1.788070	-3.280446
99	6	0	-3.292735	3.209207	-1.662379
100	1	0	-1.530619	2.394226	-0.741079
101	1	0	-3.473778	-0.133697	-3.621151
102	1	0	-5.174399	1.616803	-3.999052
103	1	0	-3.241485	4.136115	-1.096337
104	1	0	-5.082284	3.747848	-2.734097
105	6	0	-1.634183	-1.766761	-2.525878
106	6	0	-2.450534	-4.259051	-3.548716
107	6	0	-0.796445	-2.502618	-3.373179
108	6	0	-2.885850	-2.306087	-2.199124
109	6	0	-3.294853	-3.534144	-2.710013
110	6	0	-1.201191	-3.738721	-3.876866
111	1	0	0.177612	-2.110481	-3.653961
112	1	0	-3.554259	-1.756534	-1.540529
113	1	0	-4.269858	-3.925970	-2.435287
114	1	0	-0.537005	-4.292146	-4.534470
115	1	0	-2.765273	-5.219848	-3.944281
116	1	0	-0.835620	3.931504	1.789297
117	6	0	-2.659762	2.790007	1.843354
118	6	0	-3.960516	5.274883	1.736386
119	6	0	-1.922965	3.979988	1.782642
120	6	0	-4.059150	2.864086	1.857199
121	6	0	-4.701981	4.095911	1.804178
122	6	0	-2.568054	5.211910	1.730280
123	1	0	-4.635949	1.945458	1.886909
124	1	0	-5.787066	4.135155	1.805520
125	1	0	-1.980648	6.124328	1.686941
126	1	0	-4.464628	6.235155	1.689020

Zero-point correction=
(Hartree/Particle)

1.046986

Thermal correction to Energy=	1.108580
Thermal correction to Enthalpy=	1.109524
Thermal correction to Gibbs Free Energy=	0.951009
Sum of electronic and zero-point Energies=	-3401.393071
Sum of electronic and thermal Energies=	-3401.331476
Sum of electronic and thermal Enthalpies=	-3401.330532
Sum of electronic and thermal Free Energies=	-3401.489048