

SUPPORTING INFORMATION

1,2-Bis-perfluoroalkylations of alkenes and alkynes with perfluorocarboxylic anhydrides *via* the formation of perfluoroalkylcopper intermediates

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1. General Experimental

General: All reactions involving air- and/or moisture-sensitive compounds were conducted in a dry vessel under a positive pressure of nitrogen gas by using a balloon filled with it. Analytical thin-layer chromatography (TLC) was performed on glass plates coated with 0.25 mm 230–400 mesh silica gel (Merck, Silica gel 60 F₂₅₄) containing a fluorescent indicator. Visualization was accomplished by means of ultraviolet irradiation at 254 nm and/or by spraying an ethanolic solution of 12-molybdo(VI)phosphoric acid as a developing agent. Flash column chromatography was performed using Silica gel N-60 (spherical, neutral, 40–50 μ m, Kanto Chemical Co., Inc. (Kanto)).

Instrumentation:

NMR analysis

¹H, ¹³C, and ¹⁹F NMR spectra were recorded at room temperature on a JEOL JNM-ECS-400 NMR spectrometer at 400, 100, and 376 MHz, respectively. The proton chemical shift values are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and referenced to the proton resonance of CHCl₃ (δ 7.26). The carbon chemical shift values are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and referenced to the carbon resonance of CDCl₃ (δ 77.16). The fluorine chemical shift values are reported in parts per million (ppm, δ scale) with CFCl₃ (δ 0.00) as an external standard. Chemical shifts are reported in ppm and *J* values in hertz (Hz). The data are presented in the following order: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet and/or multiple resonances, and br = broad), signal area integration in natural numbers.

IR analysis

Infrared spectra were measured on a Thermo Nicolet iS5. Only diagnostic absorptions are listed.

HRMS analysis

ESI-MS spectra were measured on a Bruker micrOTOF-QII-RSL. The samples were diluted with MeOH for the measurement. EI-MS were taken on a JMS-T100GCV.

Materials: Chemical reagents were purchased from Wako Pure Chemical Industries, Ltd., Tokyo Chemical Industry Co., Ltd., Sigma-Aldrich Inc., and other commercial suppliers.

Preparation of known alkenes and alkynes (1):

The known alkenes (**1a**,¹ **1c**,² **1e**,³ **1f**,⁴ **1g**,⁵) and alkynes (**4c**,⁶ **4g**⁷) were prepared according to the literatures.

¹ H. Clavier, S. P. Nolan and M. Mauduit, *Organometallics*, 2008, **27**, 2287.

² K. Mori, *Tetrahedron*, 2009, **65**, 2798.

³ J. D. Neukom, N. S. Perch, J. P. Wolfe, *J. Am. Chem. Soc.* 2010, **132**, 6276.

⁴ P. R. Walker, C. D. Campbell, A. Suleman, G. Carr and E. A. Anderson, *Angew. Chem., Int. Ed.*, 2013, **52**, 9139.

⁵ J. Mo, S. H. Kim, P. H. Lee, *Org. Lett.* 2010, **12**, 424.

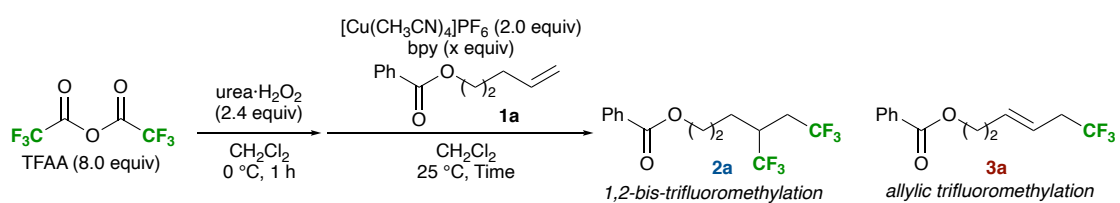
⁶ W.-K. Chan, C.-M. Ho, M.-K. Wong and C.-M. Che, *J. Am. Chem. Soc.* 2006, **128**, 14796.

⁷ Y. R. Malpani, B. K. Biswas, H. S. Han, Y.-S. Jung and S. B. Han, *Org. Lett.* 2018, **20**, 1693.

2. Additional Results

2-1. Optimization of the amount of bpy

The amount of bpy used in the 1,2-bis-trifluoromethylation of alkene **1a** was optimised (Table S1). The conversion of **1a** was very rapid without bpy present, and the desired product **2a** was obtained despite the low yield and problematic amount of allylic trifluoromethylation product **3a** that was also formed (entry 1). To sufficiently suppress the formation of by-product **3a**, the use of 4.0 equiv. of bpy with respect to **1a** (2.0 equiv. of Cu salt) is essential (entries 2 vs. 3), in which the (bpy)₂Cu(I) complex was presumably formed as a reactive Cu intermediate. Although the 4.0 equiv. of bpy slightly decreased the rate of conversion, the use of this amount remarkably improved the selectivity and yield of **2a**.

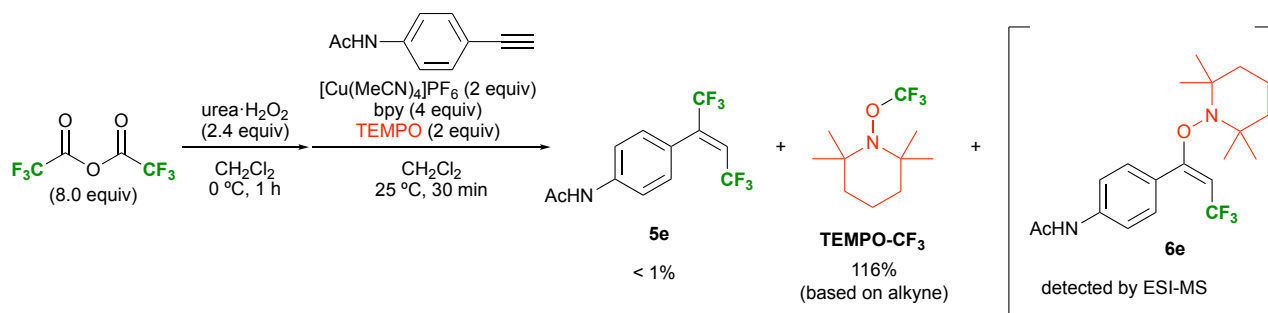


Entry	Amount of bpy (equiv)	Time (min)	Conversion of 1a (%)	NMR Yield		
				2a	3a (E/Z)	2a:3a
1	0	5	>99%	32	28 (78/22)	53:47
2	2.0	5	>99%	48	25 (78/22)	66:34
3	4.0	5	78%	42	4 (91/19)	91:9
4	4.0	30	>99%	75	4 (91/19)	94:6

Table S1. Optimisation of the amount of 2,2'-bipyridine (bpy).

2-2. TEMPO trapping test

The 1,2-bis-trifluoromethylation reaction was performed in the presence of TEMPO to trap the radical intermediate of this reaction (Scheme S1). As a result, the 1,2-bis-trifluoromethylation reaction was suppressed and a TEMPO-CF₃ adduct was obtained. In addition, the ESI-MS analysis of the crude mixture (HRMS-ESI (*m/z*) [M+Na]⁺ calcd. for C₂₀H₂₇F₃N₂NaO₂, 407.1917; found, 407.1916) confirmed the formation of TEMPO-bearing oxy-trifluoromethylation product **6e**, suggesting the generation of a vinyl radical intermediate.



Scheme S1. TEMPO trapping test to detect the radical intermediate of the 1,2-bis-trifluoromethylation.

2-3. Detection of (bpy)Cu(CF₃)₃ by ¹⁹F NMR analysis

¹⁹F NMR analysis (using acetone-*d*₆) revealed the presence of a (bpy)Cu(CF₃)₃ complex in the crude mixture obtained after the workup of the 1,2-bis-trifluoromethylation reaction of **4e**.⁸

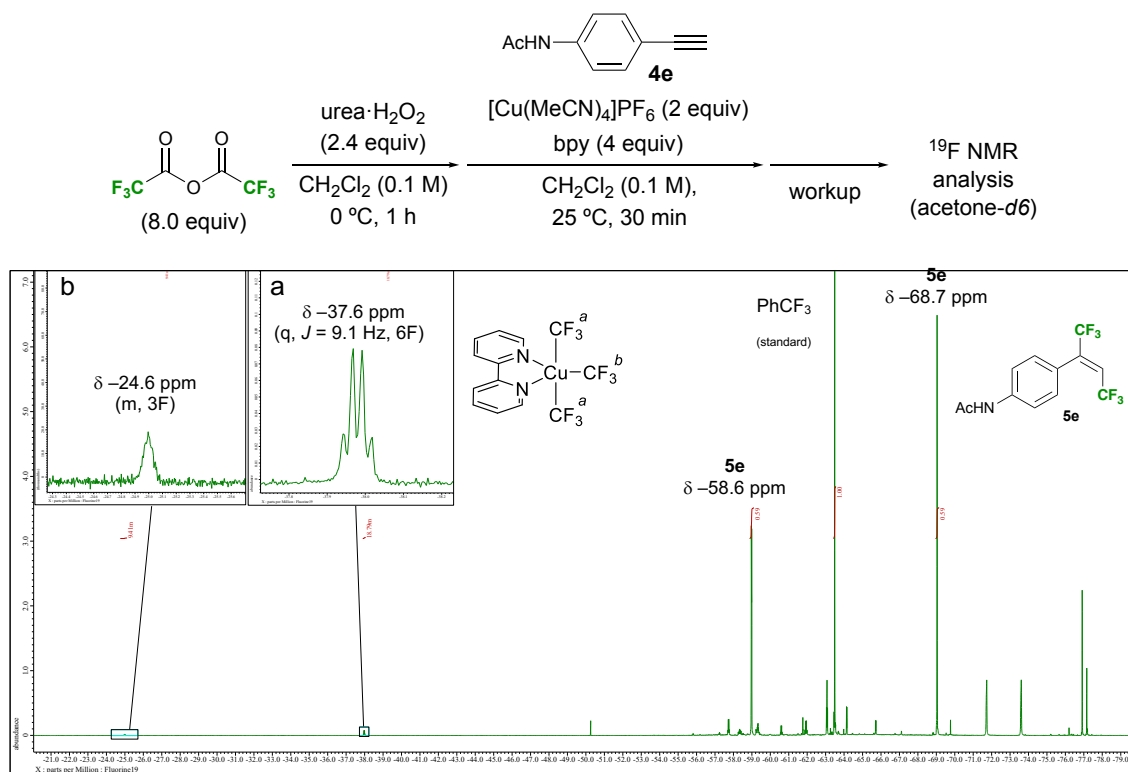


Figure S1. ¹⁹F NMR analysis of the crude mixture obtained from the 1,2-bis-trifluoromethylation reaction of **4e**.

2-4. Stability comparison of copper intermediates

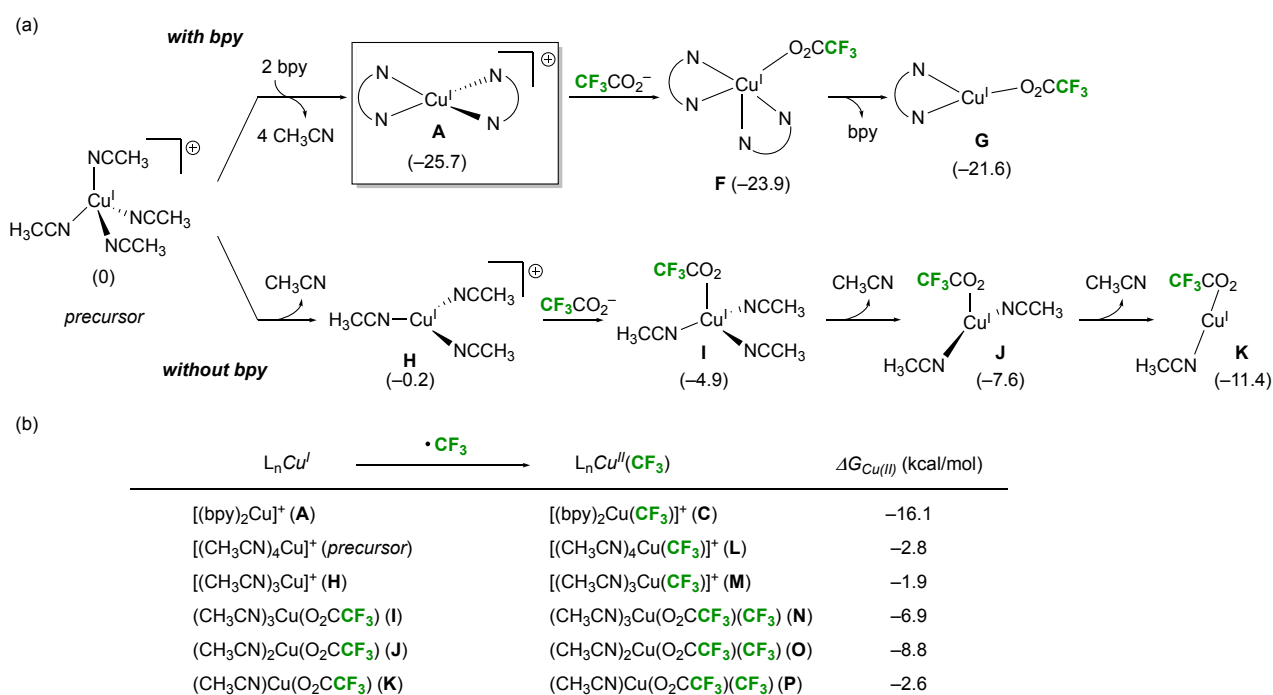
The thermal stabilities of several Cu(I) intermediates in the presence and absence of the bpy ligand (2.0 equiv. with respect to Cu) were compared to that of the precursor ([Cu(CH₃CN)₄]⁺) by means of DFT calculations (Scheme S2a). According to the literature⁹ and experimental results in Table S1, in the presence of bpy, cationic intermediate **A** bearing two bpy ligands is formed. Under the optimal conditions determined for the 1,2-bis-trifluoromethylation process of the present study, a relatively high concentration of trifluoroacetic acid was found to exist in the reaction mixture. Therefore, neutral trifluoroacetate intermediate **F** and intermediate **G** bearing one bpy unit were also proposed to have formed; however, the calculated free energy relative to that of [Cu(CH₃CN)₄]⁺ indicated that

⁸ The ¹⁹F NMR shifts and coupling patterns in acetone-*d*₆ were in good agreement with those reported in the literature: A. M. Romine, N. Nebra, A. I. Kononov, E. Martin, J. Benet-Buchholz and V. V. Grushin, *Angew. Chem., Int. Ed.*, 2015, **54**, 2745.

⁹ (a) X. Lin, C. Hou, H. Li and Z. Weng, *Chem. Eur. J.*, 2016, **22**, 2075; (b) X. Lin, Z. Li, X. Han and Z. Weng, *RSC Adv.*, 2016, **6**, 75465.

intermediate **A** is the most stable (-25.7 kcal/mol for **A** vs. -23.9 and -21.6 kcal/mol for **F** and **G**, respectively). Thus, **A** was concluded to be the reactive Cu(I) intermediate formed during 1,2-bis-trifluoromethylation. In the absence of bpy, the formation of a neutral species *via* the substitution of the precursor acetonitrile ligand with trifluoroacetate is favoured; this is in contrast to what was observed for the bpy complex. Furthermore, intermediates **J** and **K**, which are formed when one or two acetonitrile ligands, respectively, dissociate from **I**, are more stable than intermediate **I**.

We then examined the effect of the ligand on the free energy change for the formation of Cu(II)–CF₃ intermediates from Cu(I) intermediates and CF₃ radicals (Scheme S2b). As a result, the formation of [(bpy)₂Cu(II)(CF₃)]⁺ (**C**) from [(bpy)₂Cu]⁺ (**A**) and CF₃ radicals ($\Delta G_{Cu(II)} = -16.1$ kcal/mol) decreased the free energy to a greater extent than the acetonitrile–Cu(II)–CF₃ complexes did ($\Delta G_{Cu(II)} \geq -8.8$ kcal/mol).

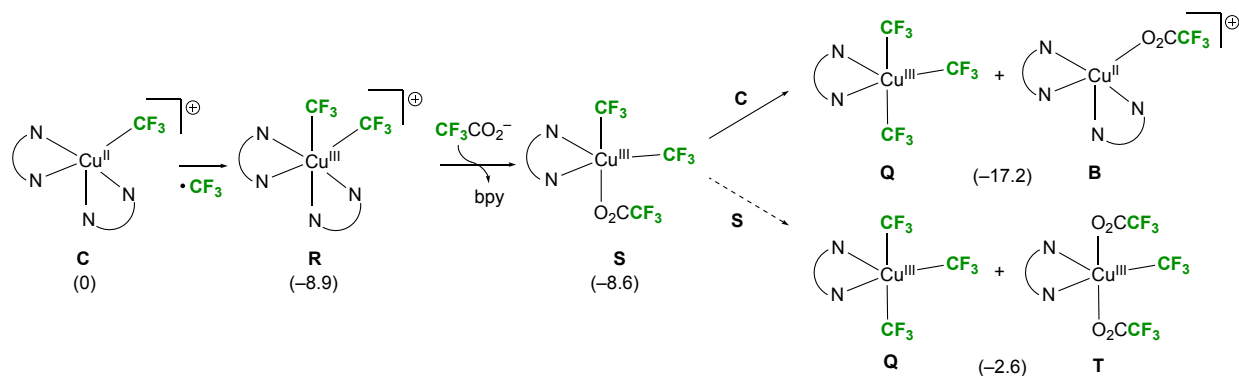


Scheme S2. Ligand effect on the 1,2-bis-trifluoromethylation of alkenes: (a) Identification of stable Cu(I) intermediates (the free energies of each intermediate relative to that of [Cu(CH₃CN)₄]⁺ are shown in parentheses). (b) A comparison of the free energy change upon the formation of Cu(II)–CF₃ intermediates.

2-5. Possible pathways to (bpy)Cu(CF₃)₃ (**Q**)

Here, we discuss possible pathways for the formation of (bpy)Cu(CF₃)₃ (**Q**), which was observed in the crude mixture by NMR analysis. First, Cu(II)–CF₃ intermediate **C** reacts with the CF₃ radical, affording Cu(III) intermediate **R**. Then, the ligand exchange of intermediate **R** replaces the bpy ligand with trifluoroacetate and generates intermediate **S**. Finally, **Q** can be formed from **S** by ligand exchange

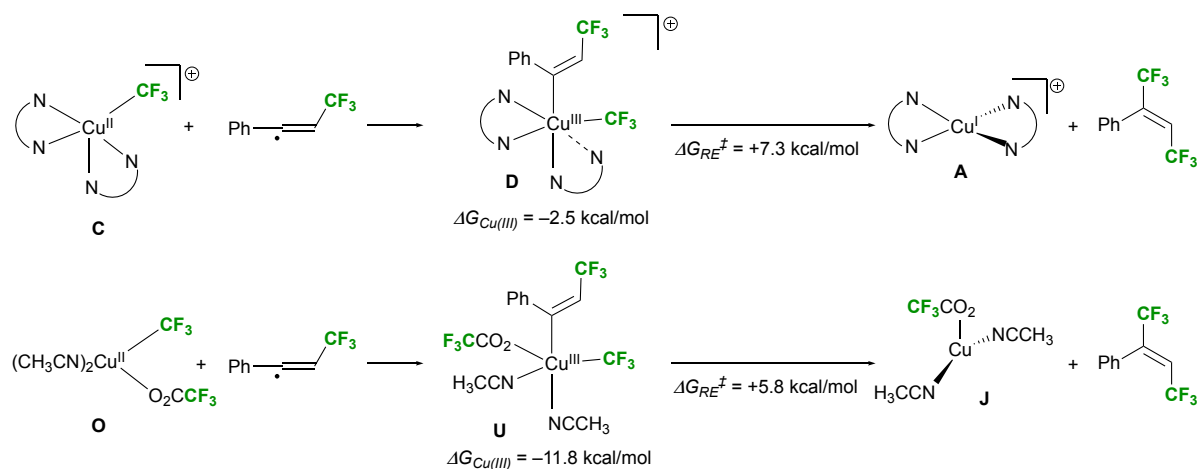
with **C** or the disproportionation of **S**. The free energy changes of these steps suggest that ligand exchange between **S** and **C** is more likely than the disproportionation of **S**.



Scheme S3. Possible pathways for the formation of (bpy)Cu(CF₃)₃ (Q). The free energy of each intermediate relative to that of C are shown in parentheses.

2-6. Ligand effect on the coupling reaction with Cu(II)–CF₃ intermediates

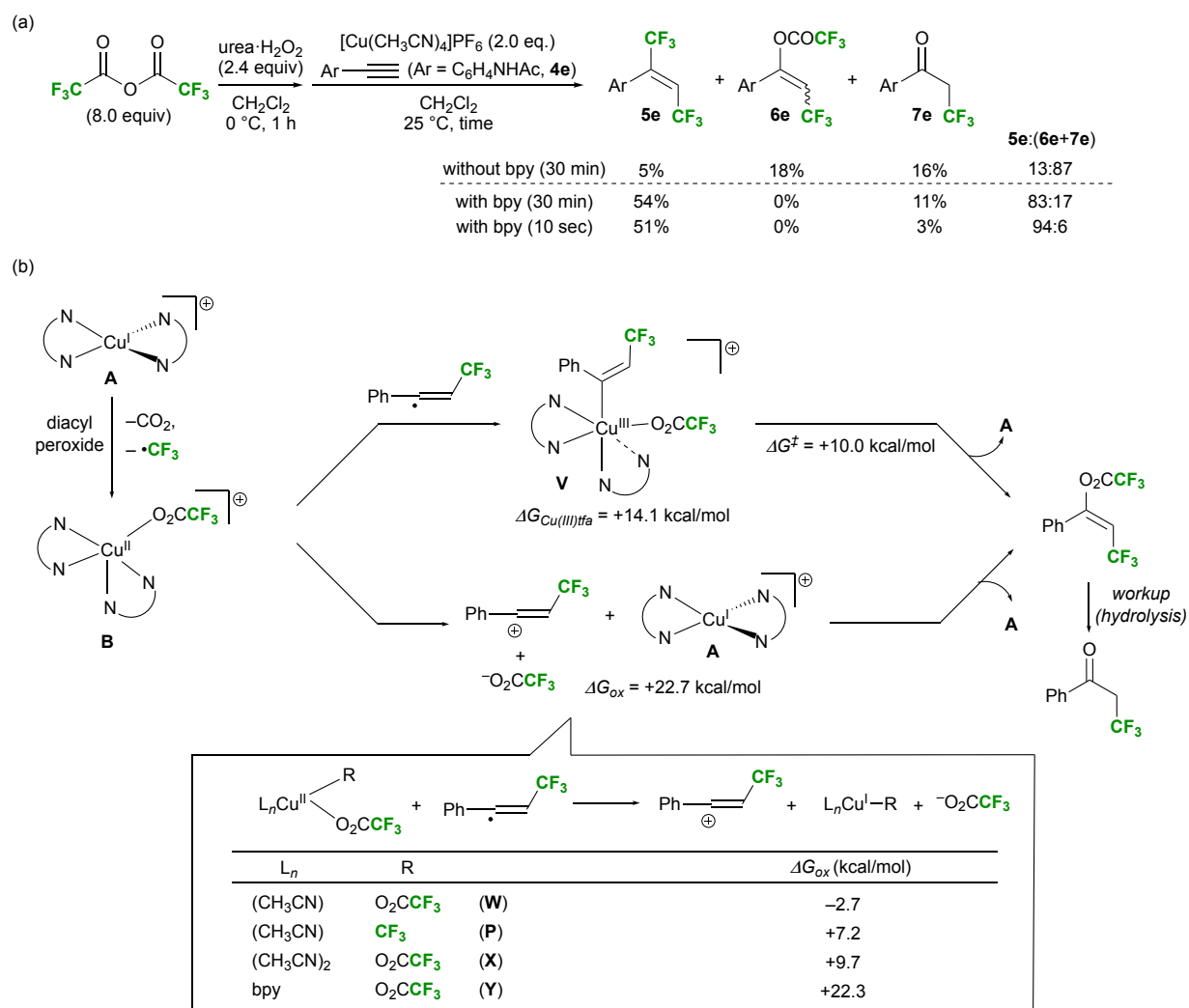
The effect of the ligand on the coupling step was investigated by comparing the free energy changes between the reactions of the vinyl radical with [(bpy)₂CuCF₃]⁺ (**C**) and the corresponding acetonitrile complex (CH₃CN)₂Cu(O₂CCF₃)(CF₃) (**O**). The results indicate that bpy does not stabilise the Cu(III) intermediate because the decrease in the free energy of the formation of **D** is much smaller than that of the free energy of the formation of acetonitrile–Cu(III) intermediate **U** ($\Delta G_{\text{Cu(III)}} = -2.5$ kcal/mol for the formation of **D** from **C** and -11.8 kcal/mol for the formation of **U** from **O**). This could be due to steric repulsion between the ligands on **D**. In addition, the activation energies for the reductive eliminations of **D** and **U** indicated that bpy did not accelerate either process ($\Delta G_{\text{RE}}^\ddagger = +7.3$ kcal/mol for the reductive elimination of **D** and $+5.8$ kcal/mol for that of **U**). Thus, we concluded that the crucial role of bpy is to stabilise Cu(II)–CF₃ intermediate **C**, as discussed in the manuscript.



Scheme S4. Ligand effect on the coupling step.

2-7. Discussion of ligand effect on the product selectivity

When the reaction of **4e** was carried out in the absence of a ligand, we found that significant amounts of oxy-trifluoromethylation products, vinyl trifluoroacetate **6e** and ketone **7e**, were obtained instead of the desired bis-trifluoromethylated product (**5e**) (Scheme S5a). Ketone **7e** was considered to be formed by the hydrolysis of **6e** during the workup; it was also observed in low yield in the crude mixture of the reaction in the presence of bpy. Interestingly, the ratio of **7e** to **5e** was found to increase with increasing reaction time under optimal conditions using bpy.



Scheme S5. Proposed pathways of the oxy-trifluoromethylation side-reaction.

The proposed mechanism for the formation of **6e** and **7e** is depicted in Scheme S5b. Cationic Cu(II) trifluoroacetate intermediate **B**, which is formed during the CF₃-radical formation reaction that occurs between diacyl peroxide and **A**, was postulated to give the oxy-trifluoromethylation products. We proposed two pathways involving **B**; the first involves a C–O coupling reaction between **B** and the vinyl radical (top arrow). DFT calculations suggested that Cu(III) intermediate **V**, bearing vinyl and

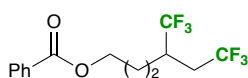
trifluoroacetate groups, could be formed ($\Delta G_{Cu(III)TFA} = +14.1$ kcal/mol), and subsequent reductive elimination would afford the oxy-trifluoromethylation products ($\Delta G^\ddagger = +10.0$ kcal/mol). The concentration of intermediate **V** should increase at a later stage of the reaction. Furthermore, the stability of **V** is lower than that of $(bpy)_2Cu(CF_3)(vinyl)$ (**D**) ($\Delta G_{Cu(III)TFA} = +14.1$ kcal/mol for the formation of **V** vs. $\Delta G_{Cu(III)} = -2.5$ kcal/mol for the formation of **D**), which suggests that the oxy-trifluoromethylation is much slower than the desired 1,2-bis-trifluoromethylation. This is in good agreement with the experimental results. The second proposed route is a vinyl cation-forming pathway that proceeds *via* the single-electron transfer (SET) between **B** and the vinyl radical (lower arrow). This pathway may also occur, but it is likely much slower than the other pathway due to the large increase in the free energy of the latter ($\Delta G_{ox} = +22.7$ kcal/mol). On the other hand, without bpy, the SET event can proceed smoothly; this is according to its small change in free energy. Specifically, the change in free energy for the SET of the vinyl radical with $(CH_3CN)Cu(O_2CCF_3)_2$ is $\Delta G = -2.7$ kcal/mol. In the absence of bpy, not only does the C–O coupling increase the yield of the oxy-trifluoromethylation products (the change in the free energy change of the formation of $(CH_3CN)Cu^{III}(O_2CCF_3)_2(vinyl)$, $\Delta G = -13.2$ kcal/mol; the activation energy of reductive elimination of $(CH_3CN)Cu^{III}(O_2CCF_3)_2(vinyl)$, $\Delta G^\ddagger = +8.4$ kcal/mol), but the SET process does as well. Therefore, bpy was considered to play a role in inhibiting the undesired oxidation of the vinyl radical and in improving the product selectivity. This is also supported by the improvement in the selectivity of the 1,2-bis-trifluoromethylation of alkenes brought about by bpy (Table 1). Furthermore, the allylic trifluoromethylation side reaction, which is known to proceed *via* a carbocation generated by oxidation of the alkyl radical intermediate with a Cu(II) species (Scheme 1a), could be suppressed by bpy.

3. Experimental Procedures

General procedure

Trifluoroacetic anhydride (220 μ L, 1.6 mmol) was slowly added to a suspension of urea·H₂O₂ (45 mg, 0.48 mmol) in CH₂Cl₂ (2.0 mL) at 0 °C. After stirring for 1 h, the alkene or alkyne (0.20 mmol), 2,2'-bipyridine (125 mg, 0.80 mmol), and [Cu(CH₃CN)₄]PF₆ (149 mg, 0.40 mmol) were added at 0 °C. The mixture was immediately warmed to 25 °C and stirred for 30 min. After the addition of 5 mL of CH₂Cl₂, the reaction was quenched with an aqueous NaHCO₃ solution at 0 °C and then stirred at room temperature for 20 min. The aqueous layer was extracted three times with 5 mL of CH₂Cl₂. The combined organic phases were checked with XploSens PS[®] to confirm the absence of peroxide, and the water phase was treated with saturated Na₂S₂O₃ to decompose H₂O₂. The combined organic phases were dried over Na₂SO₄ and the solvent was evaporated. Then, α,α,α -trifluorotoluene (20 mg) was added as an internal standard, followed by a deuterated solvent (CDCl₃ or acetone-*d*₆). ¹H and ¹⁹F NMR analyses were conducted to estimate the NMR yield.^{10,11} After the evaporation of the deuterated solvent, flash column chromatography of the crude mixture on silica gel afforded the target compound.

6,6,6-Trifluoro-4-(trifluoromethyl)hexyl benzoate (2a)



The reaction was carried out according to general procedure. The target compound was obtained as a colorless oil (38 mg, 58% yield) after silica gel column chromatography (CH₂Cl₂/hexane = 50/50).

¹H NMR (400 MHz, CDCl₃)

1.73–2.03 (m, 4H), 2.17–2.32 (m, 1H), 2.44–2.65 (m, 2H), 4.30–4.55 (m, 2H), 7.45 (t, *J* = 7.4 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 8.03 (d, *J* = 7.4 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃)

25.1, 25.7, 32.7 (q, *J* = 30 Hz), 38.4 (q, *J* = 27 Hz), 64.2, 126.0 (q, *J* = 274 Hz), 127.2 (q, *J* = 277 Hz), 128.6 (2C), 129.7 (2C), 130.2, 133.2, 166.6

¹⁹F NMR (376 MHz, CDCl₃)

–71.0 (d, *J* = 8.6 Hz, 3F), –64.3 (t, *J* = 10.1 Hz, 3F)

IR (neat, cm⁻¹)

2965, 1721, 1453, 1276, 1253, 1213, 1149, 1116, 1017, 1028, 712

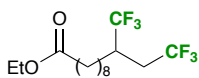
HRMS-ESI (m/z)

[M+Na]⁺ calcd. for C₁₄H₁₄F₆O₂, 351.0790; found, 351.0792

¹⁰ The stereochemistry of 1,2-bis-perfluoroalkylated alkenes **5a**, **5d–5f** was assigned by comparison with literature data. The stereochemistry of the other alkenes (**5b**, **5c**, **5g–5k**) was determined by the characteristic coupling pattern of their ¹⁹F NMR spectra; only *Z*-isomers show F–F coupling. See, S. Guo, D. I. AbuSalim, S. P. Cook, *Angew. Chem., Int. Ed.*, 2019, **58**, 11704.

¹¹ The *E/Z* ratio of 1,2-bis-perfluoroalkylated alkenes **5a–k** was determined by ¹⁹F NMR analysis of the crude product.

Ethyl 12,12,12-trifluoro-10-(trifluoromethyl)dodecanoate (2b)



The reaction was carried out on according to general procedure. The target compound was obtained as a colorless oil (44mg, 62% yield) after silica gel column chromatography (CH₂Cl₂/hexane = 50/50).

¹H NMR (400 MHz, CDCl₃)

1.25 (t, *J* = 7.2 Hz, 3H), 1.25–1.34 (m, 6H), 1.36–1.45 (m, 2H), 1.48–1.76 (m, 6H), 2.12–2.24 (m, 1H), 2.28 (t, *J* = 7.6 Hz, 2H), 2.35–2.53 (m, 2H), 4.12 (q, *J* = 7.2 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃)

14.4, 25.1, 26.2, 28.4, 29.2 (2C), 29.3, 29.5, 32.8 (q, *J* = 30 Hz), 34.5, 38.0 (q, *J* = 27 Hz), 60.3, 126.1 (q, *J* = 274 Hz), 127.4 (q, *J* = 277 Hz), 174.0

¹⁹F NMR (376 MHz, CDCl₃)

–71.1 (d, *J* = 8.6 Hz, 3F), –64.5 (t, *J* = 10.2 Hz, 3F)

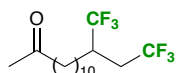
IR (neat, cm⁻¹)

2932, 2860, 1738, 1467, 1374, 1252, 1176, 1143, 1115, 1037, 801

HRMS-ESI (m/z)

[M+Na]⁺ calcd. for C₁₅H₂₄F₆O₂, 373.1573; found, 373.1578

15,15,15-Trifluoro-13-(trifluoromethyl)pentadecan-2-one (2c)



The reaction was carried out on according to general procedure. The target compound was obtained as a colorless oil (37 mg, 55% yield) after silica gel column chromatography (CH₂Cl₂/hexane = 40/60).

¹H NMR (400 MHz, CDCl₃)

1.24–1.30 (m, 12H), 1.36–1.45 (m, 2H), 1.50–1.60 (m, 3H), 1.65–1.76 (m, 1H), 2.13 (s, 3H), 2.15–2.29 (m, 1H), 2.37–2.52 (m, 2H), 2.41 (t, *J* = 7.6 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃)

24.0, 26.3, 28.4, 29.3, 29.4, 29.5 (3C), 29.6, 30.0, 32.8 (q, *J* = 30 Hz), 37.9 (q, *J* = 27 Hz), 44.0, 126.0 (q, *J* = 274 Hz), 127.3 (q, *J* = 277 Hz), 209.6

¹⁹F NMR (376 MHz, CDCl₃)

–117.5 (m, 1F), –71.1 (d, *J* = 8.6 Hz, 3F), –64.5 (t, *J* = 10.2 Hz, 3F)

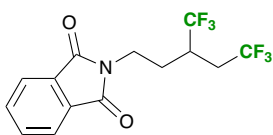
IR (neat, cm⁻¹)

2929, 2858, 1717, 1409, 1362, 1251, 1142, 1118

HRMS-ESI (m/z)

[M+Na]⁺ calcd. for C₁₆H₂₆F₆O, 371.1780; found, 371.1780.

2-(5,5,5-Trifluoro-3-(trifluoromethyl)pentyl)isoindoline-1,3-dione (2d)



The reaction was carried out on according to general procedure. The target compound was obtained as a white solid (37 mg, 54% yield) after silica gel column chromatography (CH₂Cl₂/hexane = 60/40). The compound was identified by comparison of its spectra with the literature data.¹¹

¹H NMR (400 MHz, CDCl₃)

1.92–2.03 (m, 1H), 2.08–2.20 (m, 1H), 2.24–2.39 (m, 1H), 2.47–2.66 (m, 2H), 3.82 (t, *J* = 7.2 Hz, 2H), 7.74 (dd, *J* = 5.6, 3.2 Hz, 2H), 7.86 (dd, *J* = 5.6, 3.2 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃)

27.6, 32.9 (q, *J* = 30 Hz), 35.3, 36.3 (q, *J* = 28 Hz), 123.6 (2C), 125.8 (q, *J* = 274 Hz), 126.9 (q, *J* = 277 Hz), 132.0 (2C), 134.3 (2C), 168.2 (2C)

¹⁹F NMR (376 MHz, CDCl₃)

–71.4 (d, *J* = 8.6 Hz, 3F), –64.3 (t, *J* = 10.2 Hz, 3F)

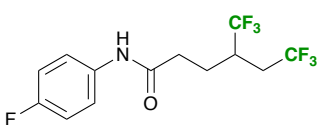
IR (neat, cm⁻¹)

2962, 2924, 2854, 1773, 1718, 1399, 1386, 1253, 1175, 1145, 1093, 1020, 870, 798

HRMS-ESI (m/z)

[M+Na]⁺ calcd. for C₁₄H₁₁F₆NO₂, 362.0586; found, 362.0578.

6,6,6-Trifluoro-*N*-(4-fluorophenyl)-4-(trifluoromethyl)hexanamide (2e)



The reaction was carried out on according to general procedure. The target compound was obtained as a coreless oil (30 mg, 46% yield) after silica gel column chromatography (CH₂Cl₂).

¹H NMR (400 MHz, CDCl₃)

2.04–2.33 (m, 3H), 2.44–2.69 (m, 4H), 7.02 (t, *J* = 8.7 Hz, 2H), 7.16 (br, 1H), 7.40–7.48 (m, 2H)

¹³C NMR (100 MHz, CDCl₃)

24.0, 33.0 (q, *J* = 30 Hz), 33.6, 37.3 (q, *J* = 27 Hz), 115.9 (d, *J* = 22 Hz, 2C), 122.0 (d, *J* = 8 Hz, 2C), 125.9 (q, *J* = 274 Hz), 127.1 (q, *J* = 278 Hz), 133.6 (d, *J* = 2 Hz), 159.5 (d, *J* = 243 Hz), 169.3

¹⁹F NMR (376 MHz, CDCl₃)

–117.5 (m, 1F), –70.7 (d, *J* = 8.6 Hz, 3F), –62.3 (t, *J* = 11.3 Hz, 3F)

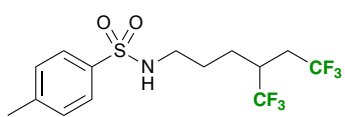
IR (neat, cm⁻¹)

3291, 1662, 1617, 1558, 1539, 1509, 1409, 1250, 1214, 1144, 1109, 834

HRMS-ESI (m/z)

[M+Na]⁺ calcd. for C₁₃H₁₁F₇NO, 354.0699; found, 354.0695

4-Methyl-*N*-(6,6,6-trifluoro-4-(trifluoromethyl)hexyl)benzenesulfonamide (2f)



The reaction was carried out on according to general procedure. The target compound was obtained as a colorless oil (49 mg, 66% yield) after silica gel column chromatography (CH₂Cl₂).

¹H NMR (400 MHz, CDCl₃)

1.52–1.78 (m, 4H), 2.00–2.28 (m, 1H), 2.31–2.51 (m, 2H), 2.43 (s, 3H), 2.92–3.01 (m, 2H), 4.37 (t, *J* = 6.0 Hz, 1H), 7.32 (d, *J* = 8.3 Hz, 2H), 7.74 (d, *J* = 8.3 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃)

21.6, 25.5, 26.6, 32.6 (q, *J* = 30 Hz), 37.7 (q, *J* = 28 Hz), 43.0, 125.9 (q, *J* = 274 Hz), 127.0 (q, *J* = 277 Hz), 127.2 (2C), 130.0 (2C), 136.9, 143.8

¹⁹F NMR (376 MHz, CDCl₃)

–71.0 (d, *J* = 8.6 Hz, 3F), –64.4 (t, *J* = 10.2 Hz, 3F)

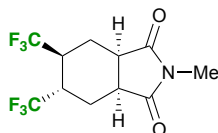
IR (neat, cm^{–1})

3287, 2929, 1326, 1300, 1288, 1202, 1151, 1117, 1094, 816, 670, 662

HRMS-ESI (*m/z*)

[*M*+Na]⁺ calcd. for C₁₄H₁₇F₆NO₂S, 400.0776; found, 400.0771.

2-Methyl-5,6-bis(trifluoromethyl)hexahydro-1*H*-isoindole-1,3(2*H*)-dione (2g)



The reaction was carried out on according to general procedure. The target compound was obtained as a white solid (24 mg, 39% yield) after silica gel column chromatography (CH₂Cl₂/hexane = 50/50).¹²

¹H NMR (400 MHz, CDCl₃)

1.54 (q, *J* = 13.9 Hz, 1H), 1.68–1.78 (m, 1H), 2.41 (dt, *J* = 13.9, 5.4 Hz, 1H), 2.49 (ddd, *J* = 15.3, 6.9, 2.5 Hz, 1H), 2.53–2.66 (m, 1H), 2.70–2.81 (m, 1H), 2.83–2.92 (m, 1H), 3.00 (s, 3H), 2.98–3.08 (m, 1H)

¹³C NMR (100 MHz, CDCl₃)

19.3, 21.1, 25.1, 35.7, 35.7 (q, *J* = 30 Hz), 36.8 (q, *J* = 28 Hz), 37.3, 125.3 (d, *J* = 41 Hz), 128.1 (d, *J* = 40 Hz), 177.9, 178.2

¹⁹F NMR (376 MHz, CDCl₃)

–73.2 (m, 3F), –70.0 (m, 3F)

IR (neat, cm^{–1})

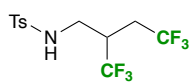
1703, 1700, 1286, 1256, 1218, 1183, 1163, 1130, 1102, 980, 970, 608

HRMS-ESI (*m/z*)

¹² The stereochemistry was confirmed by NOESY experiments.

[M+Na]⁺ calcd. for C₁₁H₁₁F₆NO₂, 326.0587; found, 326.0581

4-Methyl-N-(4,4,4-trifluoro-2-(trifluoromethyl)butyl)benzenesulfonamide (2h)



The reaction was carried out on according to general procedure. The target compound was obtained as a white solid (47 mg, 68% yield) after silica gel column chromatography (CH₂Cl₂).

¹H NMR (400 MHz, CDCl₃)

2.33–2.52 (m, 2H), 2.44 (s, 3H), 2.55–2.70 (m, 1H), 3.20–3.32 (m, 2H), 4.71 (br, 1H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃)

21.7, 30.1 (q, *J* = 31 Hz), 38.6 (q, *J* = 27 Hz), 40.9, 125.7 (q, *J* = 274 Hz), 126.3 (q, *J* = 277 Hz), 127.2 (2C), 130.2 (2C), 136.4, 144.4

¹⁹F NMR (376 MHz, CDCl₃)

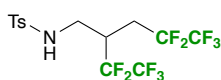
–69.9 (d, *J* = 8.6 Hz, 3F), –64.5 (t, *J* = 10.2 Hz, 3F)

IR (neat, cm⁻¹)

3282, 1599, 1496, 1436, 1390, 1332, 1307, 1291, 1274, 1251, 1155, 1119, 1092, 815, 667

HRMS-ESI (m/z) [M+Na]⁺ calcd. for C₁₂H₁₃F₆NO₂S, 372.0463; found, 372.0464

4-Methyl-N-(4,4,5,5,5-pentafluoro-2-(perfluoroethyl)pentyl)benzenesulfonamide (2i)



The reaction was carried out on according to general procedure. The target compound was obtained as a white solid (45 mg, 50% yield) after silica gel column chromatography (CH₂Cl₂).

¹H NMR (400 MHz, CDCl₃)

2.28–2.60 (m, 2H), 2.44 (s, 3H), 2.70–2.85 (m, 1H), 3.22–3.38 (m, 2H), 4.69 (t, *J* = 7.2 Hz, 1H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃)¹³

21.7, 25.9 (t, *J* = 21 Hz), 34.8 (t, *J* = 21 Hz), 41.3, 127.2 (2C), 130.2 (2C), 136.3, 144.4

¹⁹F NMR (376 MHz, CDCl₃)

–118.0 (m, 2F), –116.5 (m, 2F), –85.5 (s, 3F), –82.3 (s, 3F)

IR (neat, cm⁻¹)

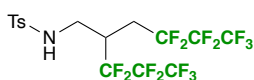
3304, 1339, 1307, 1195, 1162, 1093, 1069, 1043, 814, 668, 663

HRMS-ESI (m/z)

[M+Na]⁺ calcd. for C₁₄H₁₃F₁₀NO₂S, 472.0400; found, 472.0400.

¹³ The carbons of perfluoroalkyl group could not be assigned because of low intensity of signals and their complex coupling.

4-Methyl-*N*-(4,4,5,5,6,6,6-heptafluoro-2-(perfluoropropyl)hexyl)benzenesulfonamide (2j)



The reaction was carried out according to general procedure. The target compound was obtained as a white solid (47 mg, 43% yield) after silica gel column chromatography (CH₂Cl₂).

¹H NMR (400 MHz, CDCl₃)

2.35–2.65 (m, 2H), 2.44 (s, 3H), 2.82–2.97 (m, 1H), 3.22–3.38 (m, 2H), 4.78 (t, *J* = 7.2 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃)¹³

21.7, 25.8 (t, *J* = 21 Hz), 35.1 (t, *J* = 21 Hz), 41.3, 127.2 (2C), 130.1 (2C), 136.2, 144.4

¹⁹F NMR (376 MHz, CDCl₃)

–127.5 (m, 2F), –125.0 (m, 2F), –114.9 (m, 2F), –113.2 (m, 2F), –80.4 (s, 3F), –80.3 (s, 3F)

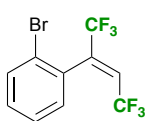
IR (neat, cm^{–1})

3296, 1436, 1330, 1123, 1176, 1158, 1107, 1081, 922, 814, 746, 714

HRMS-ESI (*m/z*)

[*M*+Na]⁺ calcd. for C₁₆H₁₃F₁₄NO₂S, 572.0336; found, 572.0336.

(*E*)-1-bromo-2-(1,1,1,4,4,4-hexafluorobuten-2-yl)benzene (5a)



The reaction was carried out according to general procedure. The target compound was obtained as a colorless oil (28 mg, 42% yield) after silica gel column chromatography (pentane).

¹H NMR (400 MHz, CDCl₃)

6.58 (qq, *J* = 7.0, 1.4 Hz, 1H), 7.22 (dd, *J* = 7.5, 1.9 Hz, 1H), 7.31 (td, *J* = 7.7, 1.9 Hz, 1H), 7.38 (dt, *J* = 7.5, 1.3 Hz, 1H), 7.66 (dd, *J* = 7.7, 1.3 Hz, 1H)

¹³C NMR (100 MHz, CDCl₃)

121.3 (q, *J* = 271 Hz), 121.6 (q, *J* = 275), 123.3, 124.6 (qq, *J* = 35, 6 Hz), 127.3, 130.3, 130.6, 131.3, 133.2, 139.4 (qq, *J* = 32, 6 Hz)

¹⁹F NMR (376 MHz, CDCl₃)

–67.8 (d, *J* = 1.4 Hz, 3F), –60.6 (m, 3F)

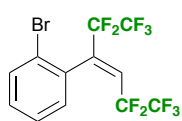
IR (neat, cm^{–1})

1269, 1187, 1145, 756, 738, 663, 646, 613

HRMS-EI (*m/z*)

[*M*] calcd. for C₁₀H₅BrF₆, 317.9479; found, 317.9476

(E)-1-bromo-2-(1,1,1,2,2,5,5,6,6,6-decafluorohexen-3-yl)benzene (5b)



The reaction was carried out on according to general procedure. The target compound was obtained as a colorless oil (38 mg, 45% yield) after silica gel column chromatography (pentane).

^1H NMR (400 MHz, CDCl_3)

6.49 (t, $J = 12.8$ Hz, 1H), 7.15 (m, 1H), 7.30 (td, $J = 7.7, 1.9$ Hz, 1H), 7.35 (td, $J = 7.5, 1.4$ Hz, 1H), 7.67 (dd, $J = 7.7, 1.4$ Hz, 1H)

^{13}C NMR (100 MHz, CDCl_3)¹³

123.8, 125.2 (m), 127.0, 130.5, 130.7, 131.3, 133.0, 141.9 (m)

^{19}F NMR (376 MHz, CDCl_3)

-117.11 (d, $J = 268$ Hz, 1F), -114.88 (dd, $J = 275, 14$ Hz, 1F), -113.17 (dd, $J = 275, 11$ Hz, 1F), -110.60 (d, $J = 268$ Hz, 1F), -82.28 (d, $J = 6.2$ Hz, 3F), -84.76 (d, $J = 6.7$ Hz, 3F)

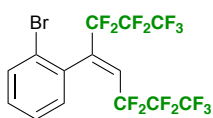
IR (neat, cm^{-1})

1327, 1120, 1168, 1130, 1065, 1048, 1034, 753, 744, 721, 707, 666, 658

HRMS-EI (m/z)

[M] calcd. for $\text{C}_{12}\text{H}_5\text{BrF}_{10}$, 417.9415; found, 417.9403

(E)-1-bromo-2-(1,1,1,2,2,3,3,6,6,7,7,8,8,8-tetradecafluoroocten-4-yl)benzene (5c)



The reaction was carried out on according to general procedure. The target compound was obtained as a colorless oil (62 mg, 60% yield) after silica gel column chromatography (pentane)

^1H NMR (400 MHz, CDCl_3)

6.49 (dd, $J = 14.3, 11.8$ Hz, 1H), 7.17 (m, 1H), 7.30 (td, $J = 7.8, 1.8$ Hz, 1H), 7.38 (dt, $J = 7.5, 1.4$ Hz, 1H), 7.66 (dd, $J = 7.8, 1.4$ Hz, 1H)

^{13}C NMR (100 MHz, CDCl_3)¹³

124.0, 125.8 (m), 127.0, 130.4, 130.9, 131.3, 133.0, 142.0 (m)

^{19}F NMR (376 MHz, CDCl_3)

-127.46 (m, 2F), -124.41 to -125.64 (m, 1F), -123.31 to -124.41 (m, 1F), -114.41 (m, 1F), -111.49 to -113.78 (m, 1F), -108.53 to -111.01 (m, 1F), -106.51 (m, 1F), -80.37 (m, 3F), -79.84 to -80.21 (m, 3F)

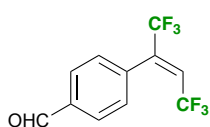
IR (neat, cm^{-1})

1345, 1229, 1184, 1118, 988, 961, 745, 724

HRMS-EI (m/z)

[M] calcd. for $\text{C}_{14}\text{H}_5\text{BrF}_{14}$, 517.9351; found, 517.9336

(E)-4-(1,1,1,4,4,4-hexafluorobuten-2-yl)benzaldehyde (5d)



The reaction was carried out on according to general procedure. The target compound was obtained as a colorless oil (21 mg, 40% yield) after silica gel column chromatography (CH₂Cl₂/hexane = 20/80).

¹H NMR (400 MHz, CDCl₃)

6.57 (qq, *J* = 7.2, 1.5 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 2H), 7.96 (d, *J* = 8.2 Hz, 2H), 10.07 (s, 1H)

¹³C NMR (100 MHz, CDCl₃)

121.3 (q, *J* = 272 Hz), 121.7 (q, *J* = 275 Hz), 123.9 (qq, *J* = 35, 6 Hz), 129.7 (2C), 129.8 (2C), 134.8, 137.3, 140.2 (qq, *J* = 31, 5 Hz), 191.5

¹⁹F NMR (376 MHz, CDCl₃)

-67.9 (s, 3F), -58.1 (d, *J* = 7.2 Hz, 3F)

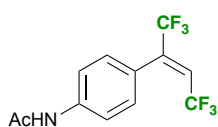
IR (neat, cm⁻¹)

1710, 1267, 1185, 1140, 825, 740, 649, 634, 623

HRMS-EI (*m/z*)

[M] calcd. for C₁₁H₆F₆O, 268.0323; found, 268.0310

(E)-N-(4-(1,1,1,4,4,4-hexafluorobuten-2-yl)phenyl)acetamide (5e)



The reaction was carried out on according to general procedure. The target compound was obtained as a white solid (29 mg, 48% yield) after silica gel column chromatography (AcOEt/hexane = 30/70).

¹H NMR (400 MHz, acetone-*d*₆)

2.10 (s, 3H), 6.84 (qq, *J* = 7.2, 1.5 Hz, 1H), 7.29 (d, *J* = 8.6 Hz, 2H), 7.77 (d, *J* = 8.6 Hz, 2H), 9.37 (bs, 1H)

¹³C NMR (100 MHz, acetone-*d*₆)

24.3, 119.5 (2C), 121.5 (q, *J* = 271 Hz), 123.1 (q, *J* = 274 Hz), 123.9 (qq, *J* = 35, 5.5 Hz), 130.2 (2C), 141.6 (qq, *J* = 31, 5 Hz), 142.1, 169.3

¹⁹F NMR (376 MHz, acetone-*d*₆)

-68.7 (s, 3F), -58.6 (d, *J* = 7.2 Hz, 3F)

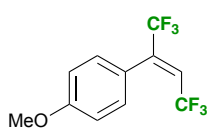
IR (neat, cm⁻¹)

1671, 1606, 1543, 1538, 1515, 1403, 1321, 1269, 1199, 1136

HRMS-ESI (*m/z*)

[M+Na]⁺ calcd. for C₁₂H₉F₆NO, 320.0481; found: 320.0479.

(E)-1-(1,1,1,4,4,4-hexafluorobuten-2-yl)-4-methoxybenzene (5f)



The reaction was carried out on according to general procedure. The target compound was obtained as a colorless oil (9 mg, 15% yield) after silica gel column chromatography (hexane).

^1H NMR (400 MHz, CDCl_3)

3.84 (s, 3H), 6.45 (qq, $J = 7.2, 1.4$ Hz, 1H), 6.94 (d, $J = 8.8$ Hz, 2H), 7.23 (d, $J = 8.8$ Hz, 2H)

^{13}C NMR (100 MHz, CDCl_3)

55.4, 114.0 (2C), 121.0, 121.7 (q, $J = 272$ Hz), 122.1 (q, $J = 276$ Hz), 122.6 (qq, $J = 35, 5$ Hz), 130.3 (2C), 141.2 (qq, $J = 31, 5$ Hz), 160.9

^{19}F NMR (376 MHz, CDCl_3)

-68.2 (s, 3F), -57.9 (d, $J = 7.2$ Hz, 3F)

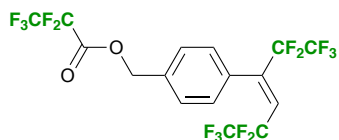
IR (neat, cm^{-1})

2956, 2923, 2853, 1734, 1730, 1654, 1632, 1468, 1287, 1263, 1222, 1183, 1163, 1135, 808, 722

HRMS-EI (m/z)

[M] calcd. for $\text{C}_{11}\text{H}_8\text{F}_6\text{O}$, 270.0479; found, 270.0475

(E)-4-(1,1,1,2,2,5,5,6,6,6-decafluorohexen-3-yl)benzyl 2,2,3,3,3-pentafluoropropoate (5g)



The reaction of (4-ethynylphenyl)methane **4e** was carried out on according to general procedure. The target compound was obtained as a colorless oil (56 mg, 54% yield) after silica gel column chromatography ($\text{CH}_2\text{Cl}_2/\text{hexane} = 5/95$).

^1H NMR (400 MHz, CDCl_3)

5.42 (s, 2H), 6.47 (t, $J = 13.0$ Hz, 1H), 7.28 (d, $J = 8.2$ Hz, 2H), 7.41 (d, $J = 8.2$ Hz, 2H)

^{13}C NMR (100 MHz, CDCl_3)¹³

69.0, 123.9 (m), 127.9 (2C), 129.7 (2C), 129.9, 135.1, 142.3 (m), 158.4 (t, $J = 30$ Hz)

^{19}F NMR (376 MHz, CDCl_3)

-121.5 (s, 2F), -115.0 (s, 2F), -110.9 (dd, $J = 13.0, 2.9$ Hz, 2F), -85.0 (s, 3F), -82.8 (s, 3F), -81.7 (s, 3F)

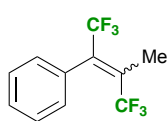
IR (neat, cm^{-1})

1784, 1331, 1302, 1120, 1150, 1129, 1063, 1034, 746, 713, 664

HRMS-EI (m/z)

[M] calcd. for $\text{C}_{16}\text{H}_7\text{F}_{15}\text{O}_2$, 516.0207; found, 516.0173

(1,1,1,4,4,4-hexafluoro-3-methylbuten-2-yl)benzene (**5h**)¹⁴



The reaction was carried out according to general procedure. After the extraction, the organic phase was very carefully evaporated because of high volatility of the product (200 mmHg, 20 °C). The target compound was identified by ¹H and ¹⁹F NMR analyses, and the ¹⁹F NMR yield was estimated (Figure S6, 46% yield, *E*:*Z* = 67:33).

E-isomer

¹H NMR (400 MHz, CDCl₃)

2.18–2.22 (m, 3H), 7.13–7.20 (m, 2H), 7.30–7.42 (m, 3H)

¹⁹F NMR (376 MHz, CDCl₃)

–61.7 (s, 3F), –59.3 (s, 3F)

Z-isomer

¹H NMR (400 MHz, CDCl₃)

1.75 (q, *J* = 2.2 Hz, 3H), 7.16–7.19 (m, 2H), 7.41–7.46 (m, 3H)

¹⁹F NMR (376 MHz, CDCl₃)

–62.1 (q, *J* = 14.5 Hz, 3F), –58.7 (q, *J* = 14.5 Hz, 3F)

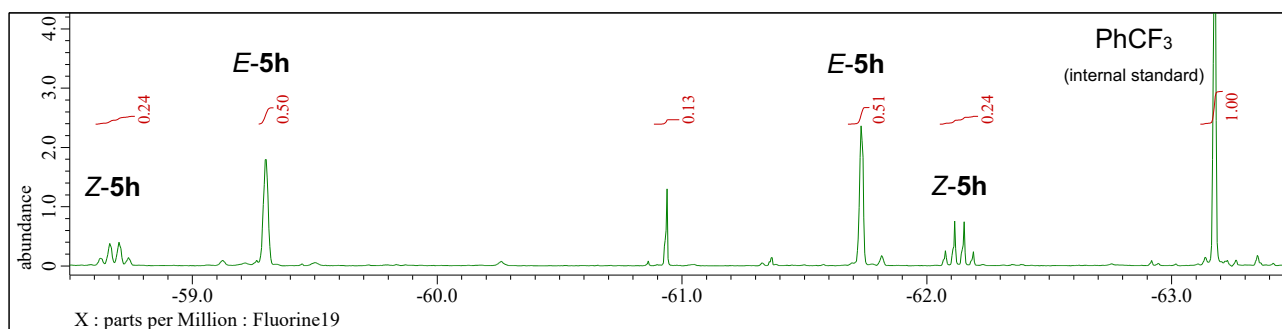
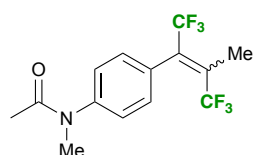


Figure S2. ¹⁹F NMR analysis of the crude product.

N-(4-(1,1,1,4,4,4-hexafluoro-3-methylbuten-2-yl)phenyl)-*N*-methylacetamide (**5i**)¹⁵



The reaction was carried out according to general procedure. The target compound was obtained after silica gel column chromatography (AcOEt/hexane = 60/40).

E-isomer: white solid, 19 mg, 29% yield

¹⁴ The stereochemistry was analogously determined by comparing the chemical shifts and coupling patterns of the ¹⁹F NMR spectra of **5h** and **5i**; a unique F–F coupling was observed only in the case of the *Z*-isomer.

¹⁵ The stereochemistry was determined by NOESY experiments; only the *Z*-isomer showed a correlation between the aromatic proton and methyl proton on the double bond.

¹H NMR (400 MHz, CDCl₃)

1.88 (s, 3H), 2.22 (q, *J* = 2.4 Hz, 3H), 3.29 (s, 3H), 7.19–7.25 (m, 4H)

¹³C NMR (100 MHz, CDCl₃)

14.5, 22.5, 37.2, 122.7 (q, *J* = 277 Hz), 122.9 (q, *J* = 277 Hz), 127.0 (2C), 130.5 (2C), 131.8, 135.3 (m), 135.5 (m), 145.2, 170.6

¹⁹F NMR (376 MHz, CDCl₃)

–61.2 (s, 3F), –58.6 (s, 3F)

IR (neat, cm^{–1})

1348, 1230, 1214, 1189, 1139, 1114, 1013, 941, 897, 832, 751, 723, 698

HRMS-ESI (*m/z*)

[*M*+Na]⁺ calcd. for C₁₄H₁₃F₆NO, 348.0794; found: 348.0791

Z-isomer: colorless oil, 8 mg, 12% yield

¹H NMR (400 MHz, CDCl₃)

1.79 (q, *J* = 2.1 Hz, 3H), 1.92 (bs, 3H), 3.31 (s, 3H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃)

17.3, 22.6, 37.3, 121.3 (q, *J* = 275 Hz), 122.2 (q, *J* = 276 Hz), 127.8 (2C), 130.3 (2C), 132.9, 135.0 (m), 135.3 (m), 145.4, 170.4

¹⁹F NMR (376 MHz, CDCl₃)

–61.6 (q, *J* = 14.2 Hz, 3F), –58.0 (qd, *J* = 14.2, 2.1 Hz, 3F)

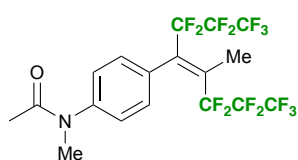
IR (neat, cm^{–1})

1662, 1606, 1511, 1381, 1321, 1292, 1227, 1143, 1104, 1086, 1020, 932, 712, 672

HRMS-ESI (*m/z*)

[*M*+Na]⁺ calcd. for C₁₄H₁₃F₆NO, 348.0794; found: 348.0794

(*E*)-*N*-methyl-*N*-(4-(1,1,1,2,2,3,3,6,6,7,7,8,8,8-tetrafluoro-5-methylocten-4-yl)phenyl)acetamide (5j**)¹⁶**



The reaction was carried out on according to general procedure. The target compound was obtained as a white solid (68 mg, 65% yield) after silica gel column chromatography (AcOEt/hexane = 60/40).

¹H NMR (400 MHz, CDCl₃)

1.83 (s, 3H), 2.19 (s, 3H), 3.26 (s, 3H), 7.11–7.21 (m, 4H)

¹⁶ The stereochemistry was analogously determined by comparing the chemical shifts and coupling patterns of the ¹⁹F NMR spectra of **5j** and the CF₃ analog (**5i**); a unique F–F coupling was observed only in the case of the *Z*-isomer.

^{13}C NMR (100 MHz, CDCl_3)¹³

15.7, 22.3, 37.1, 126.2 (2C), 131.3 (2C), 131.5, 136.5 (t, $J = 24$ Hz), 137.3 (t, $J = 20$ Hz), 145.1, 170.5

^{19}F NMR (376 MHz, CDCl_3)

-122.9 (s, 2F), -122.7 (s, 2F), -105.5 (q, $J = 10.1$ Hz, 2F), -102.9 (q, $J = 10.1$ Hz, 2F), -80.8 (t, $J = 10.1$ Hz, 3F), -80.4 (t, $J = 10.1$ Hz, 3F)

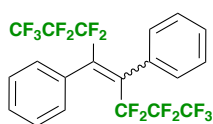
IR (neat, cm^{-1})

1167, 1508, 1343, 1224, 1184, 1151, 1112, 1030, 955, 906, 865, 843, 749, 730, 716, 701, 668, 648

HRMS-ESI (m/z)

$[\text{M}+\text{Na}]^+$ calcd. for $\text{C}_{18}\text{H}_{13}\text{F}_{14}\text{NO}$, 548.0666; found: 548.0671

(1,1,1,2,2,3,3,6,6,7,7,8,8,8-tetradecafluorooct-4-en-4,5-diyl)dibenzene (5k)¹⁷



The reaction was carried out according to general procedure. The target compound was obtained after silica gel column chromatography (hexane).

E-isomer: white solid, 44 mg, 43%

^1H NMR (400 MHz, CDCl_3)

7.31–7.44 (m, 10H)

^{13}C NMR (100 MHz, CDCl_3)¹³

127.6 (4C), 129.2 (2C), 129.9 (4C), 131.1 (2C), 139.4 (t, $J = 26.6$ Hz, 2C)

^{19}F NMR (376 MHz, CDCl_3)

-120.2 (s, 4F), -102.0 (q, $J = 10.1$ Hz, 4F), -80.7 (t, $J = 10.1$ Hz, 6F)

IR (neat, cm^{-1})

1342, 1220, 1188, 1147, 1112, 960, 720, 702

HRMS-EI (m/z)

$[\text{M}]$ calcd. for $\text{C}_{20}\text{H}_{10}\text{F}_{14}$, 516.0559; found, 516.0549

Z-isomer: colorless oil, 17 mg, 16%

^1H NMR (400 MHz, CDCl_3)

6.97–7.02 (m, 4H), 7.06–7.11 (m, 6H)

^{13}C NMR (100 MHz, CDCl_3)¹³

127.7 (4C), 128.4 (2C), 130.5 (4C), 133.5 (2C), 140.8 (q, $J = 13.5$ Hz, 2C)

^{19}F NMR (376 MHz, CDCl_3)

-119.7 (m, 4F), -102.6 (m, 4F), -80.6 (m, 6F)

¹⁷ The stereochemistry was determined by the chemical shifts and unique coupling patterns in the ^{19}F NMR spectra, which depend on the geometrical configuration of the two perfluoroalkyl groups on the double bond.

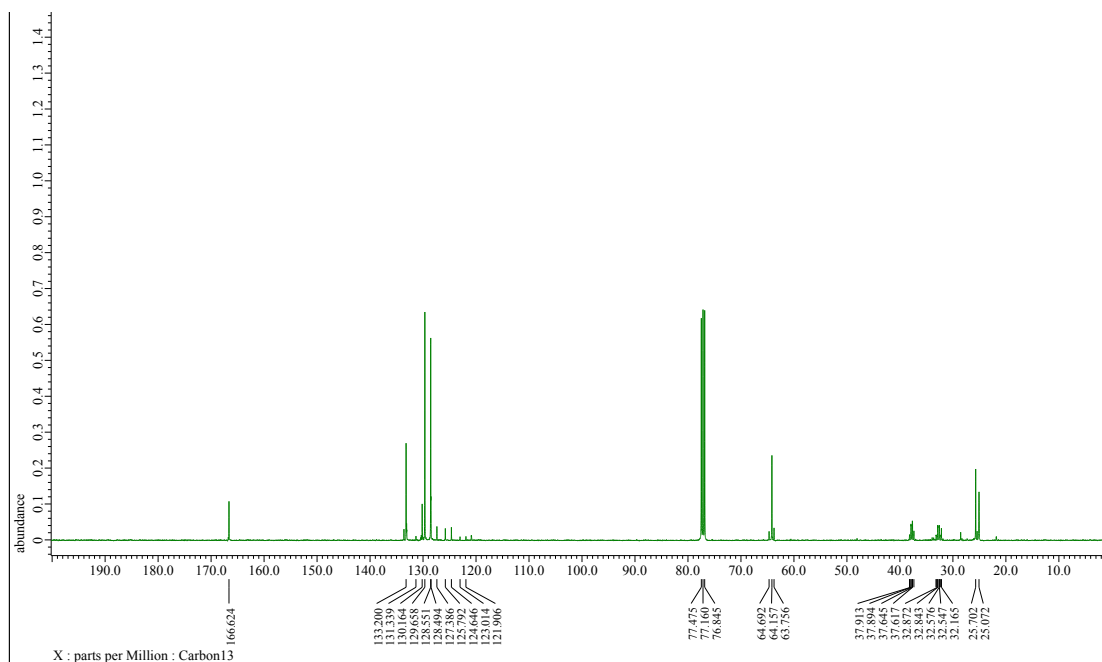
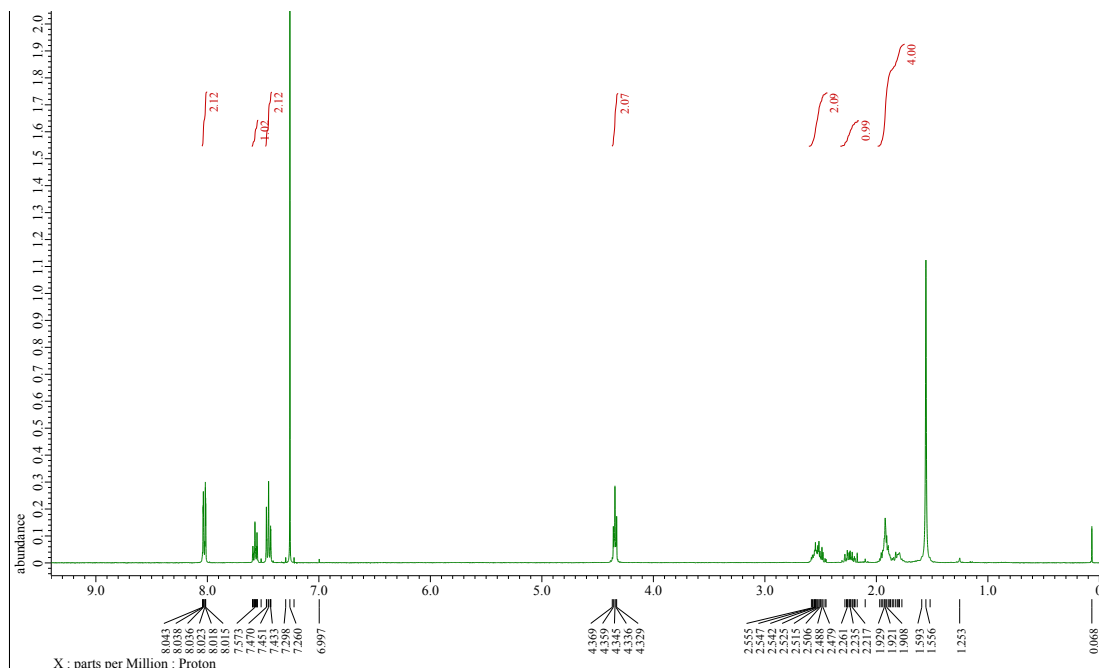
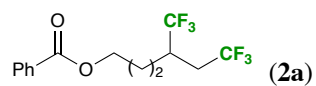
IR (neat, cm^{-1})

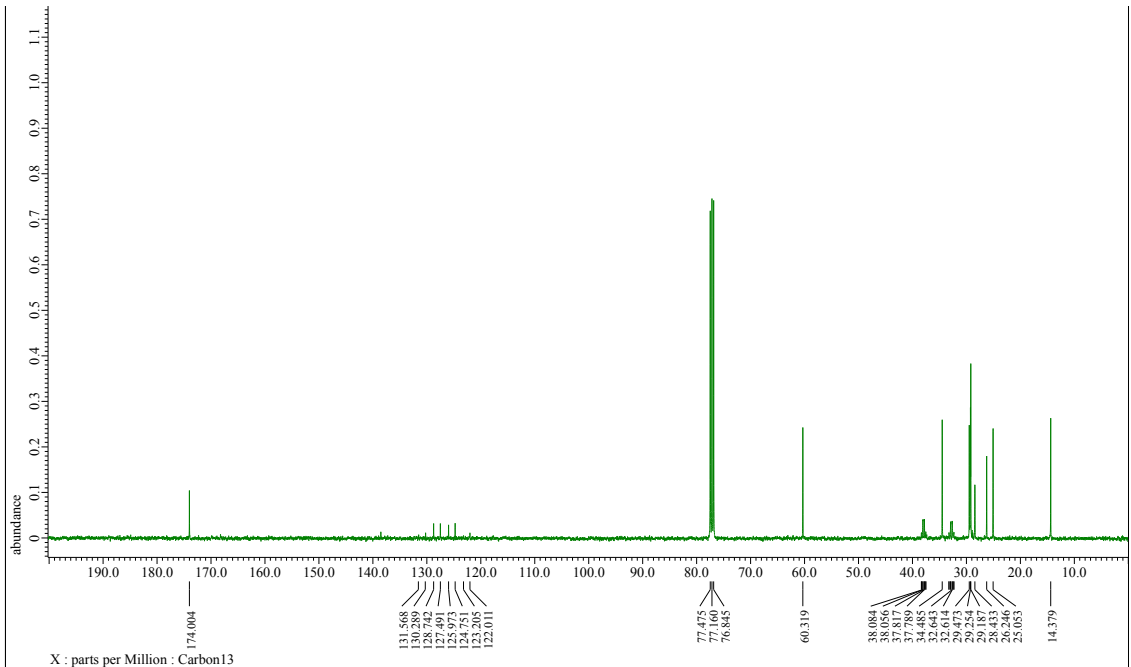
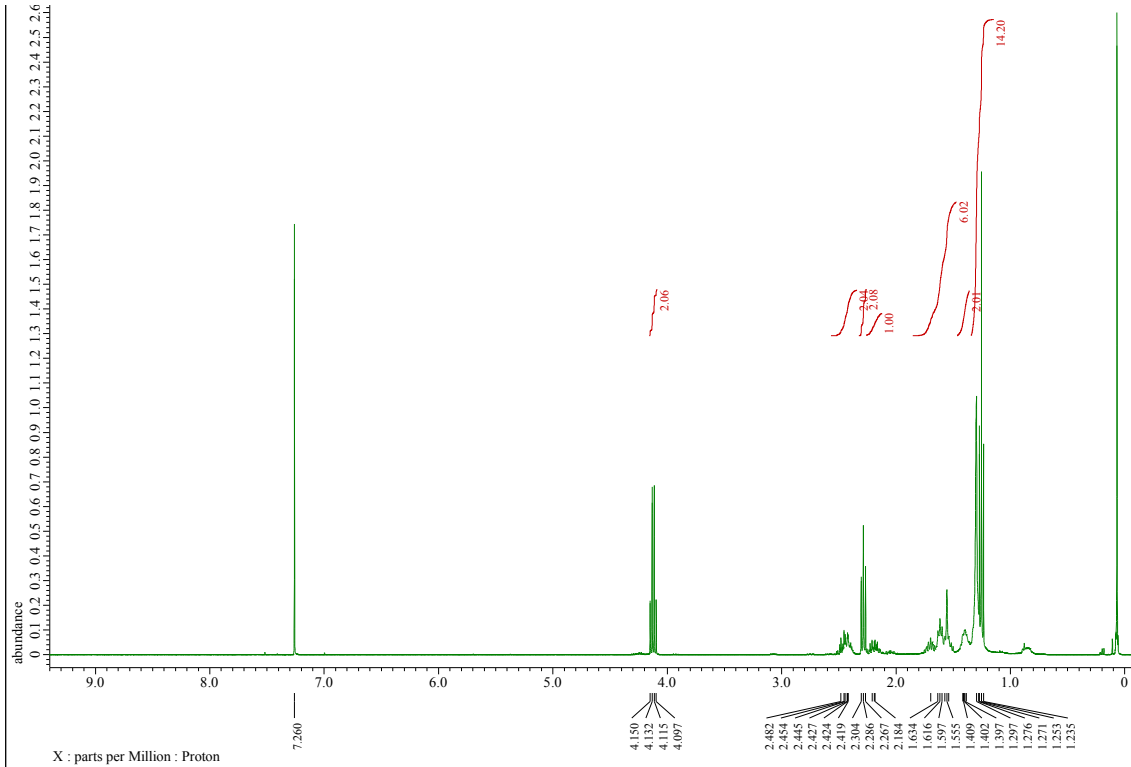
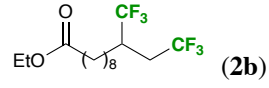
1668, 1608, 1511, 1378, 1260, 1226, 1180, 1138, 1112, 1030, 927, 659

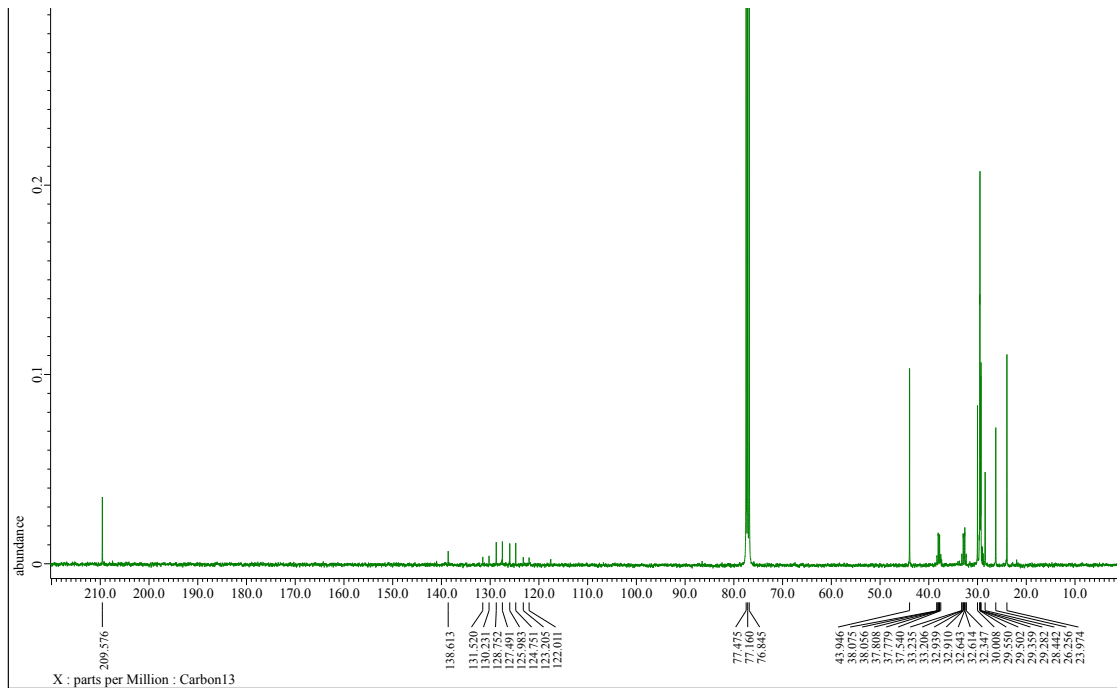
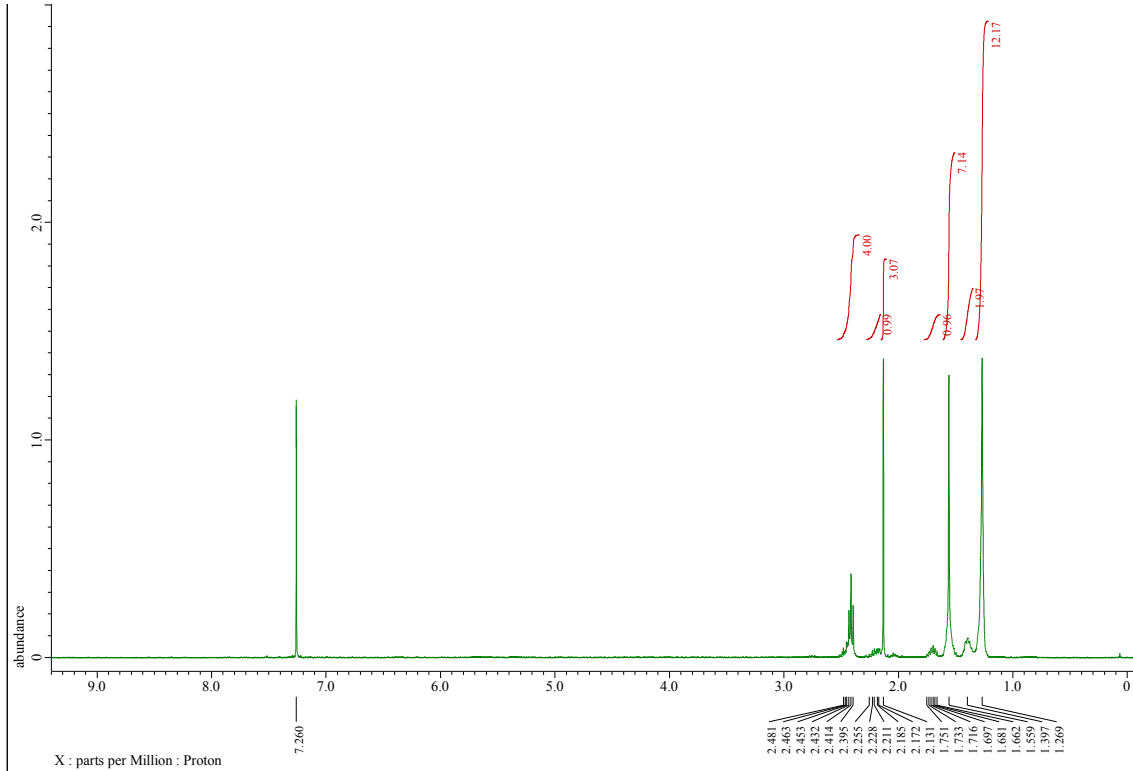
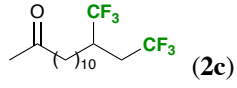
HRMS-EI (m/z)

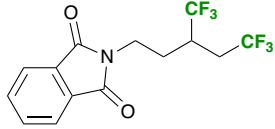
[M] calcd. for $\text{C}_{20}\text{H}_{10}\text{F}_{14}$, 516.0559; found, 516.0548

4. ¹H and ¹³C NMR spectra

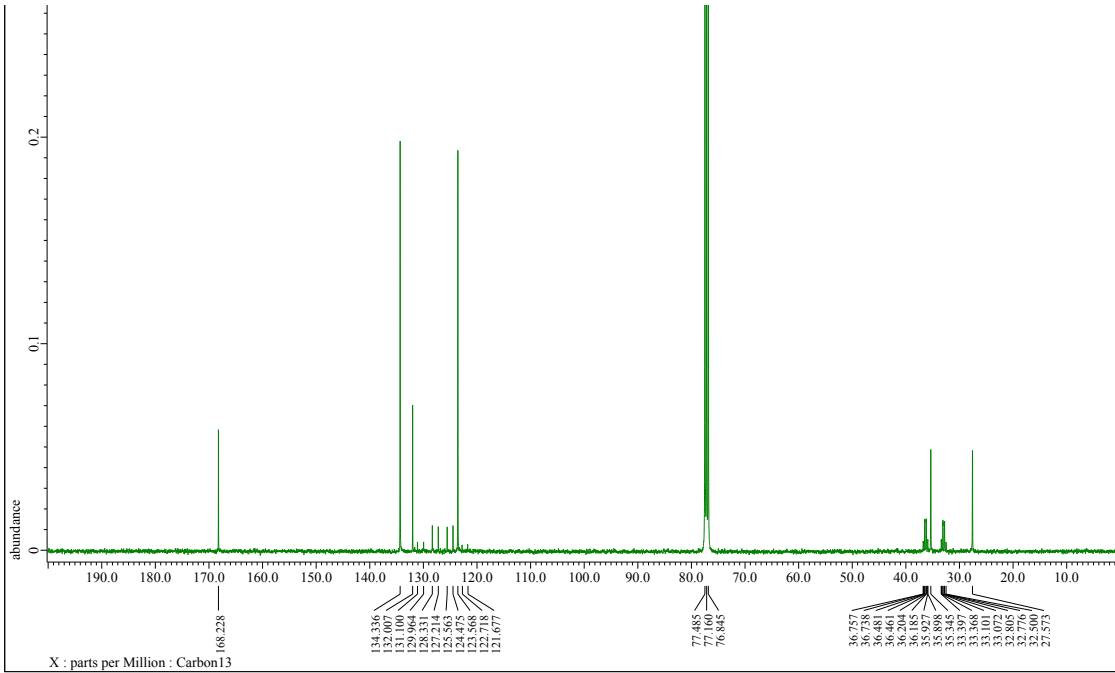
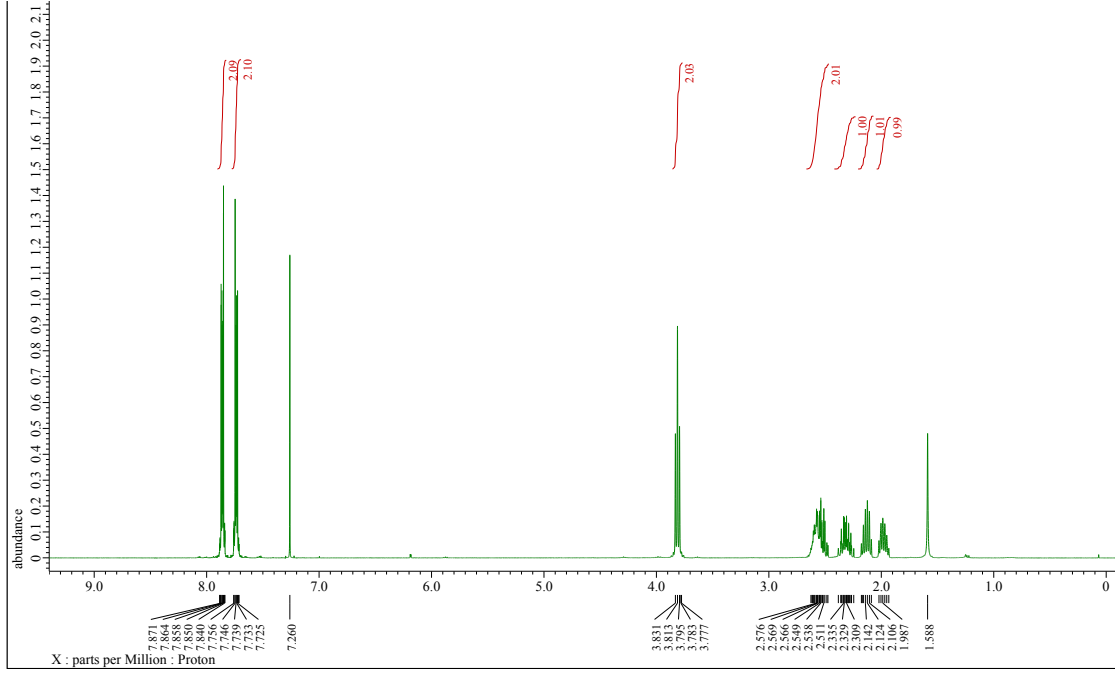


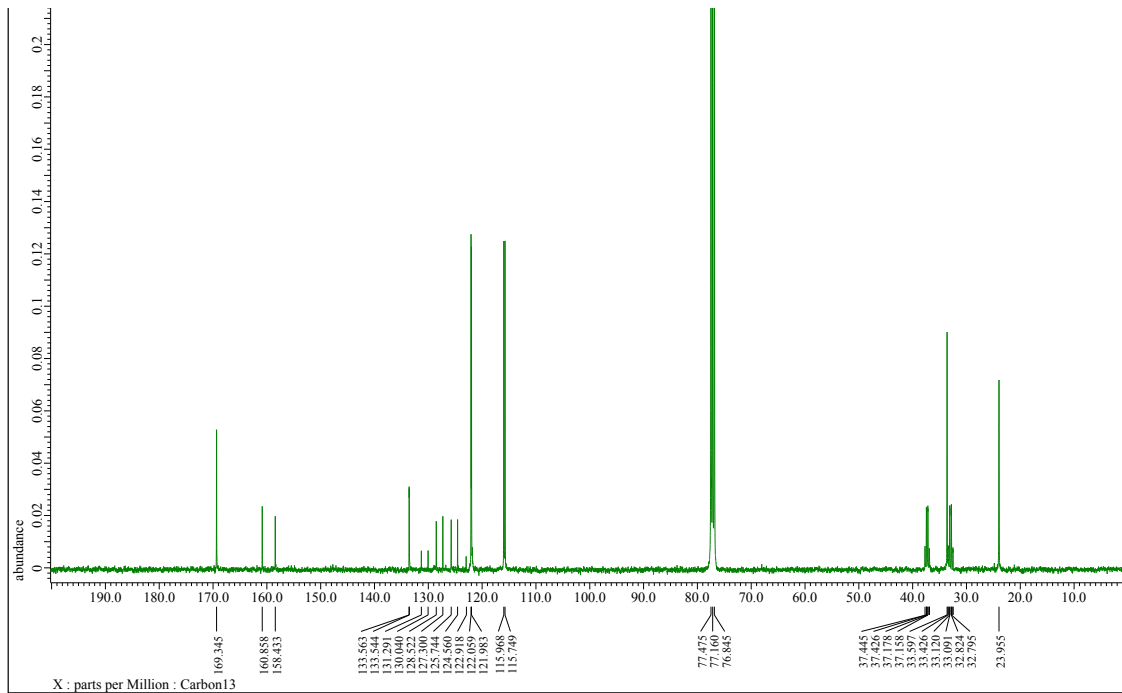
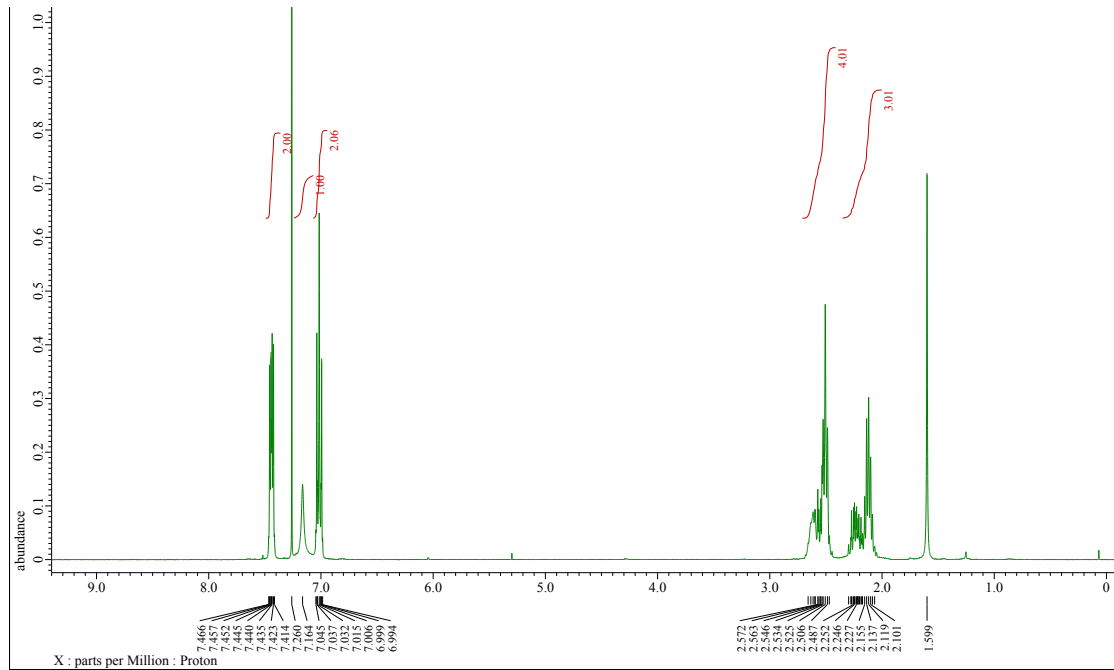
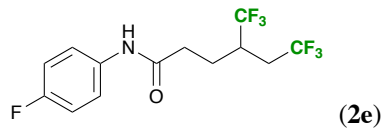


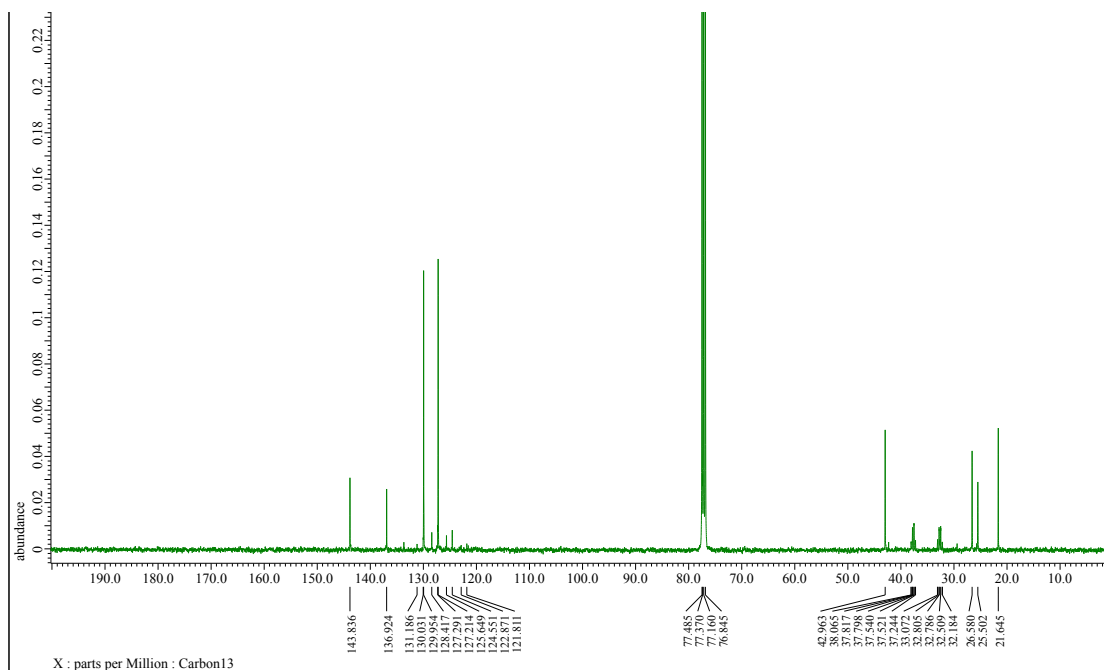
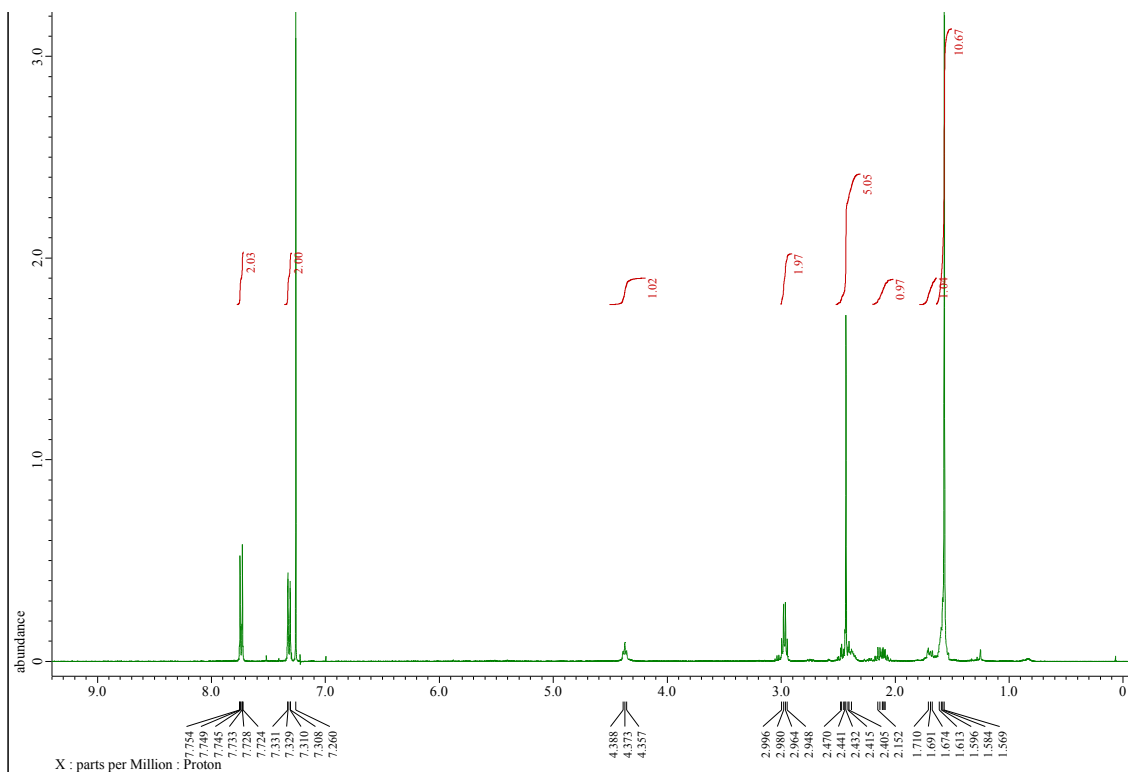
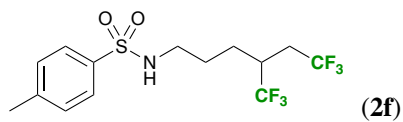


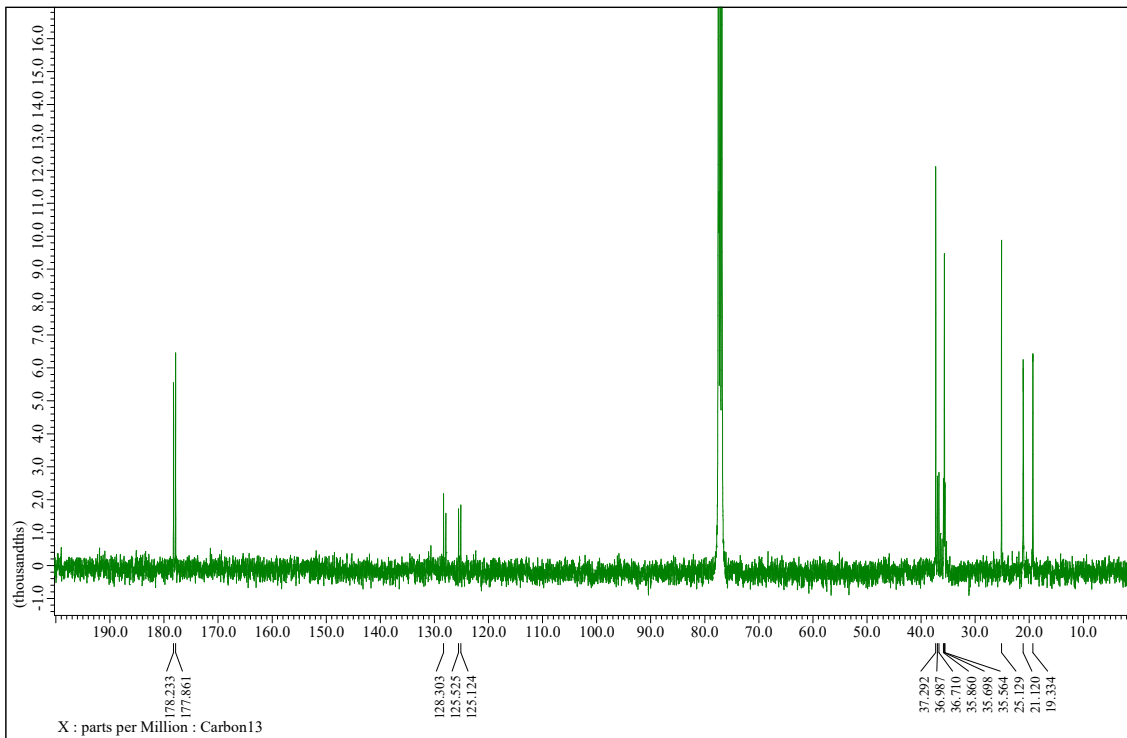
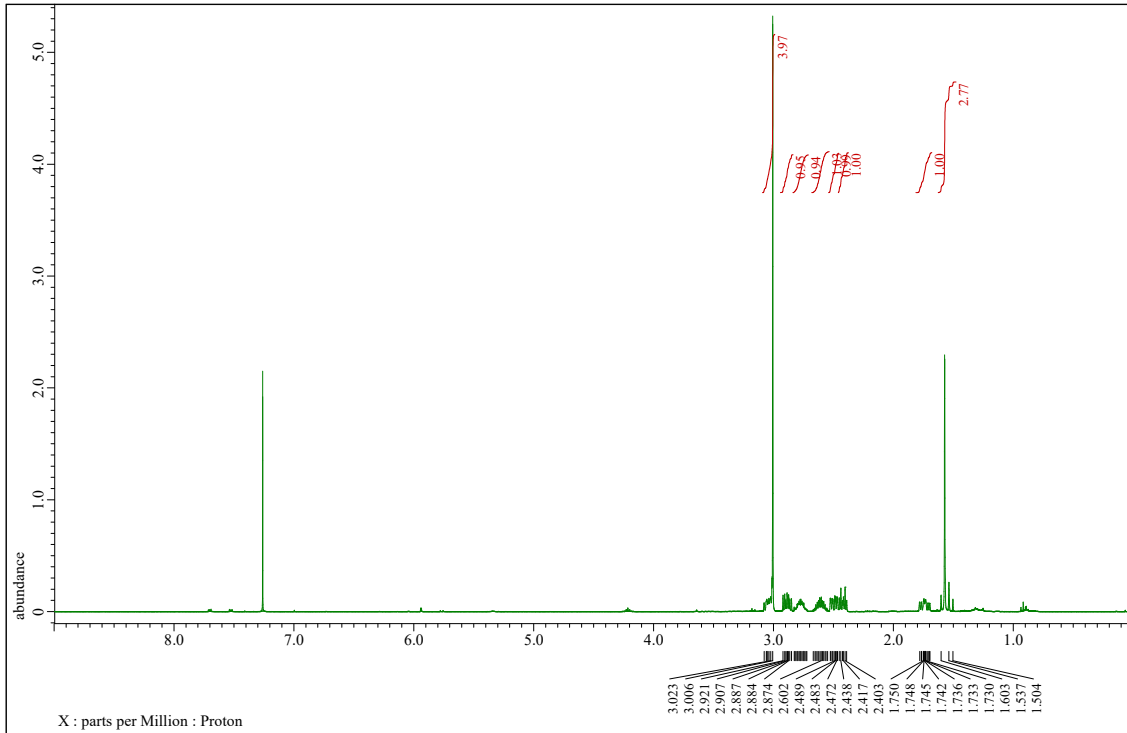
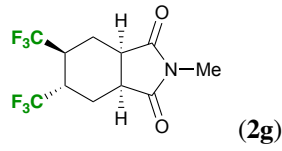


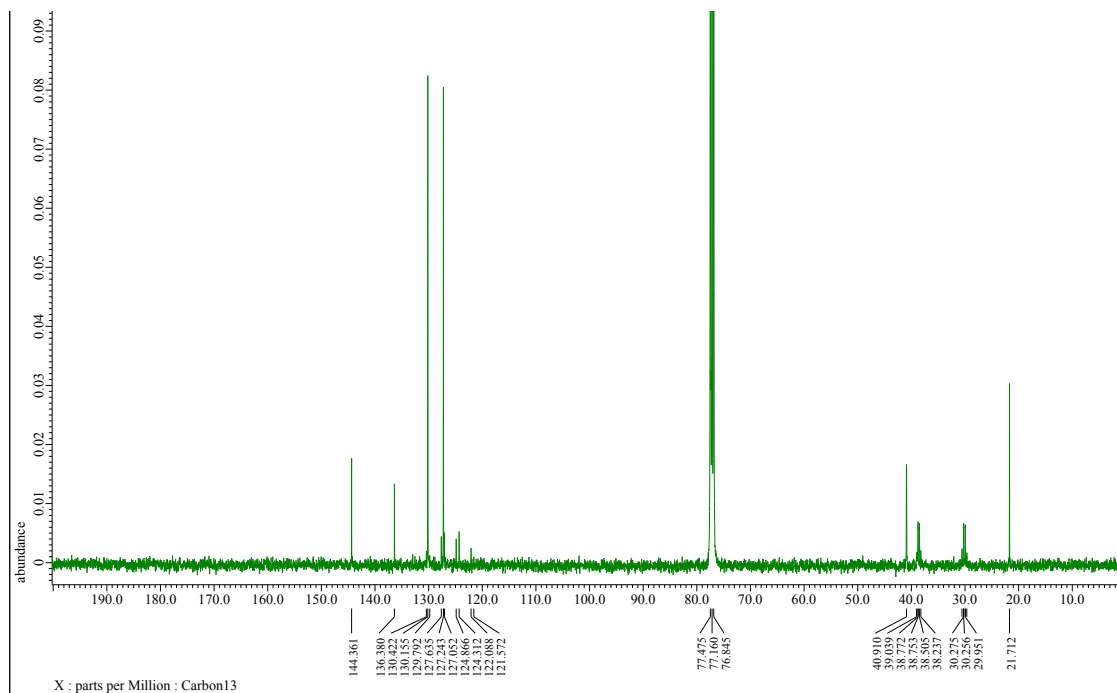
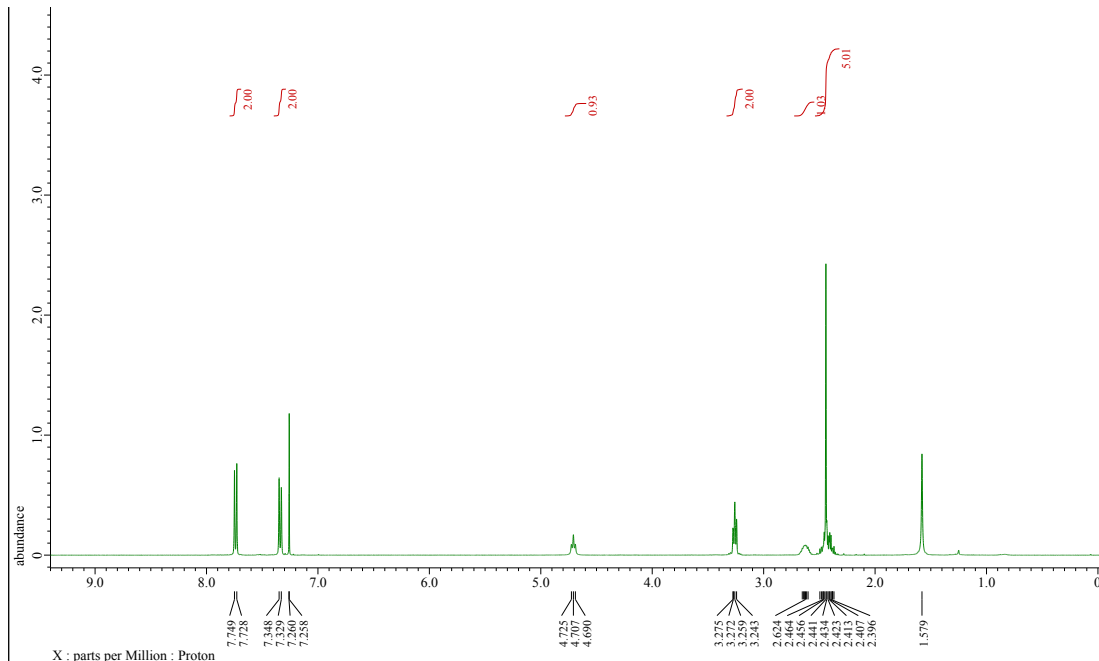
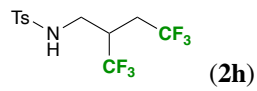
(2d)

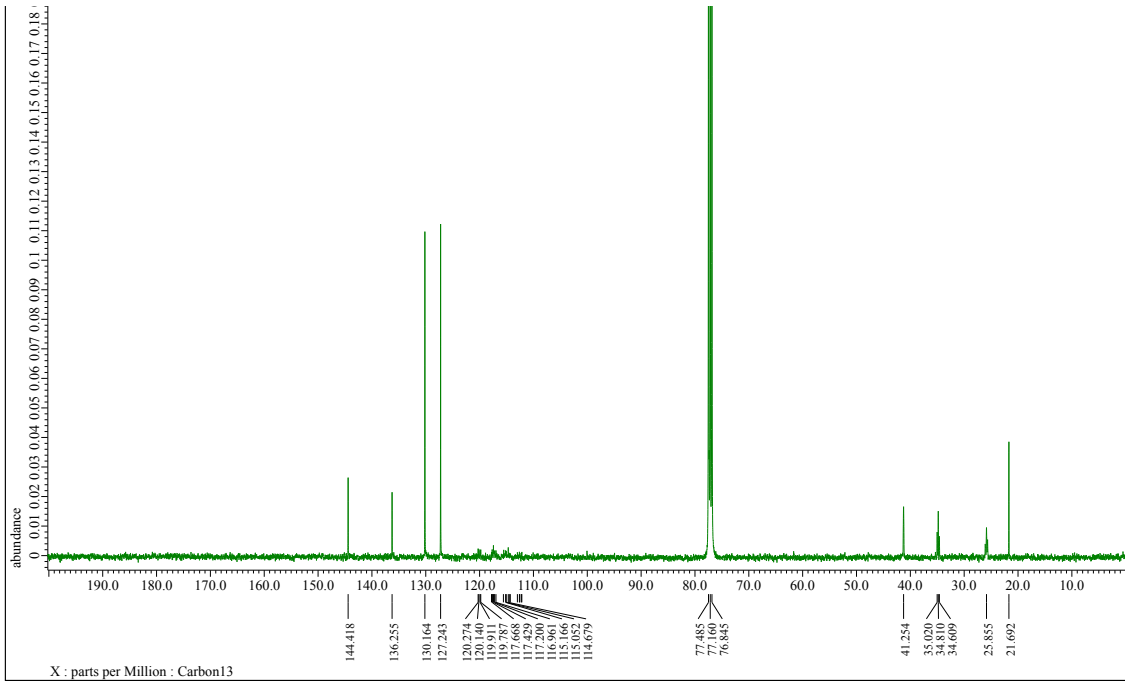
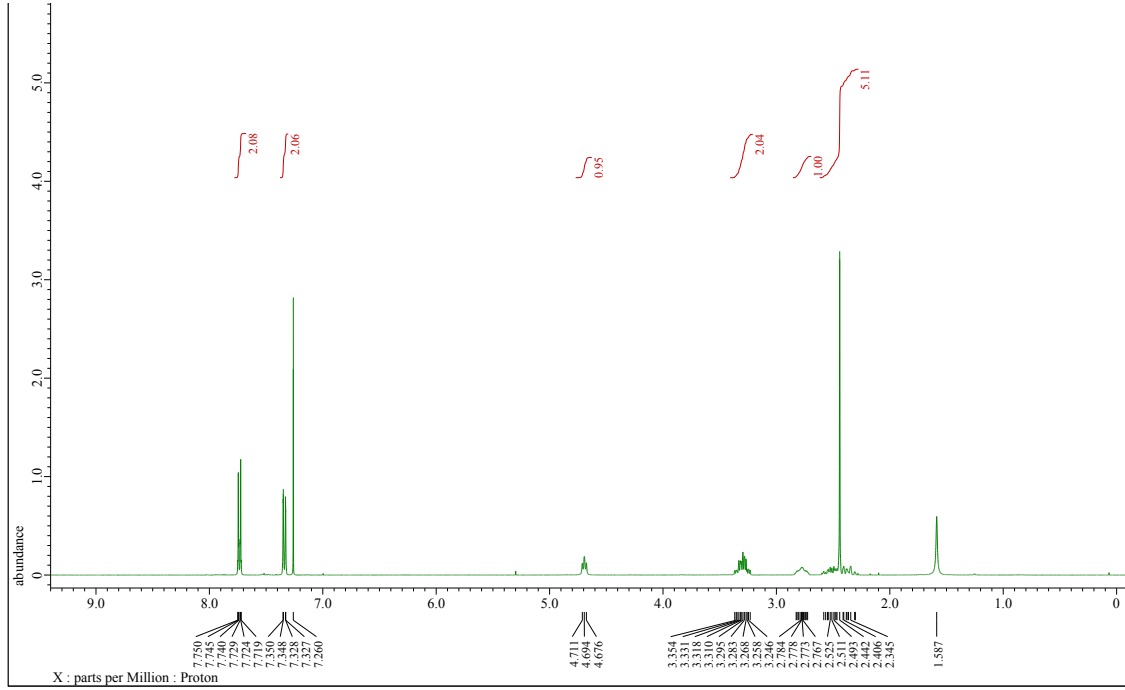
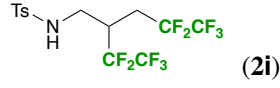


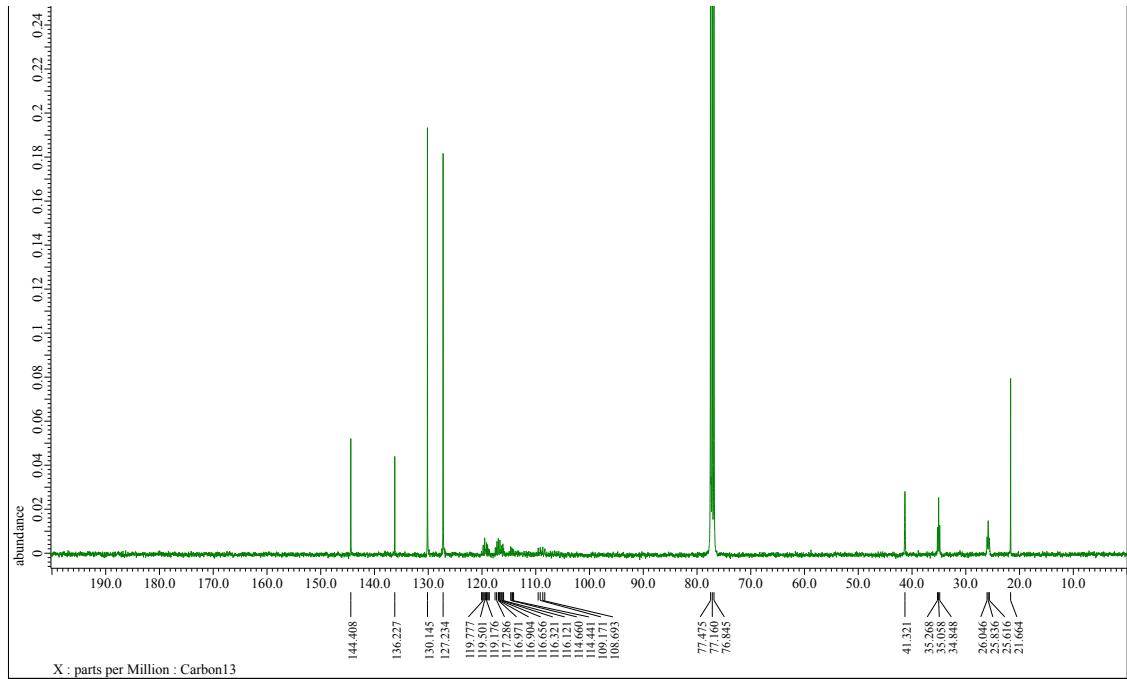
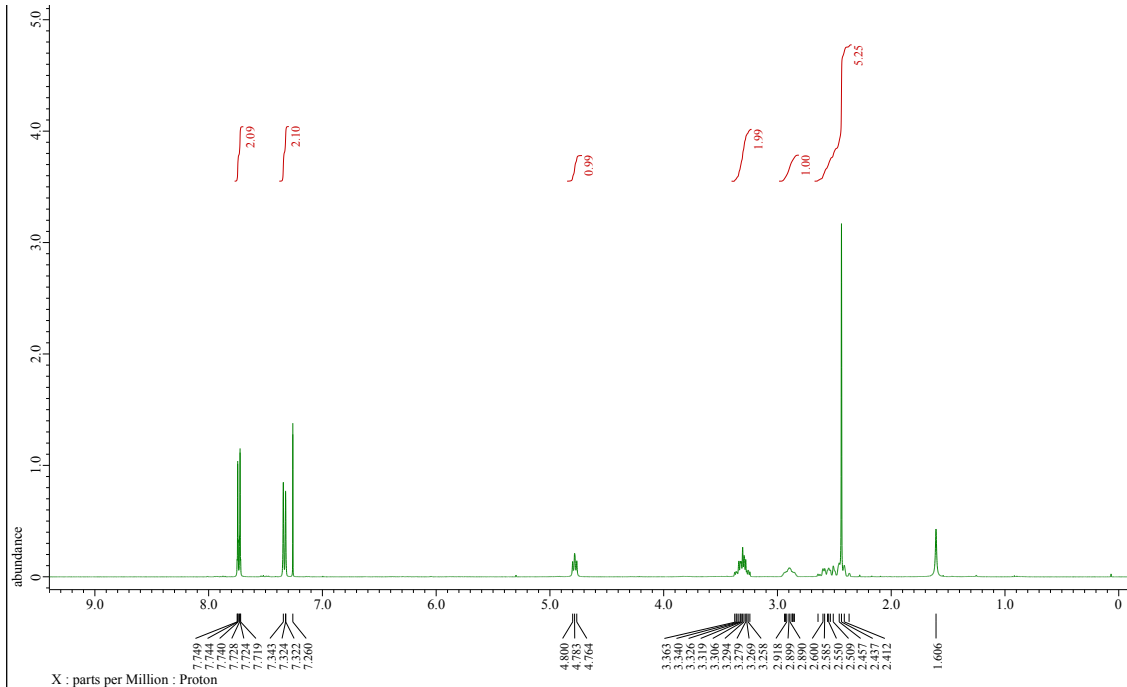
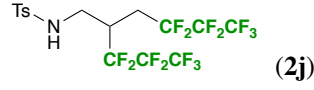


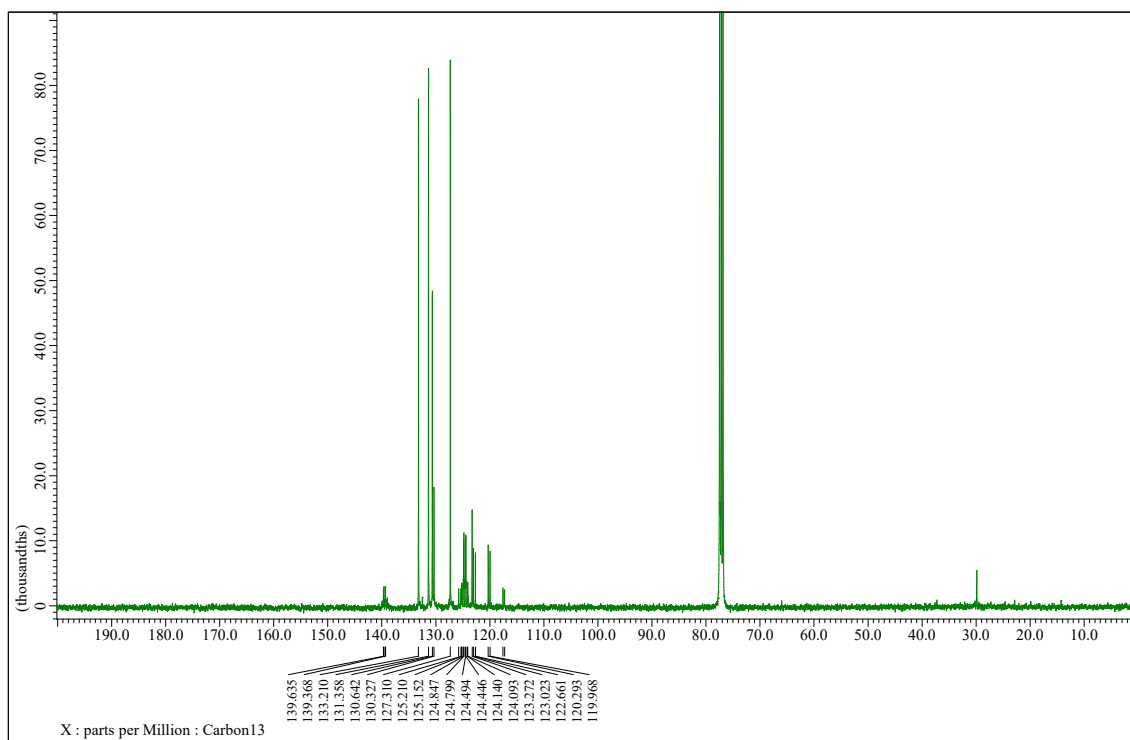
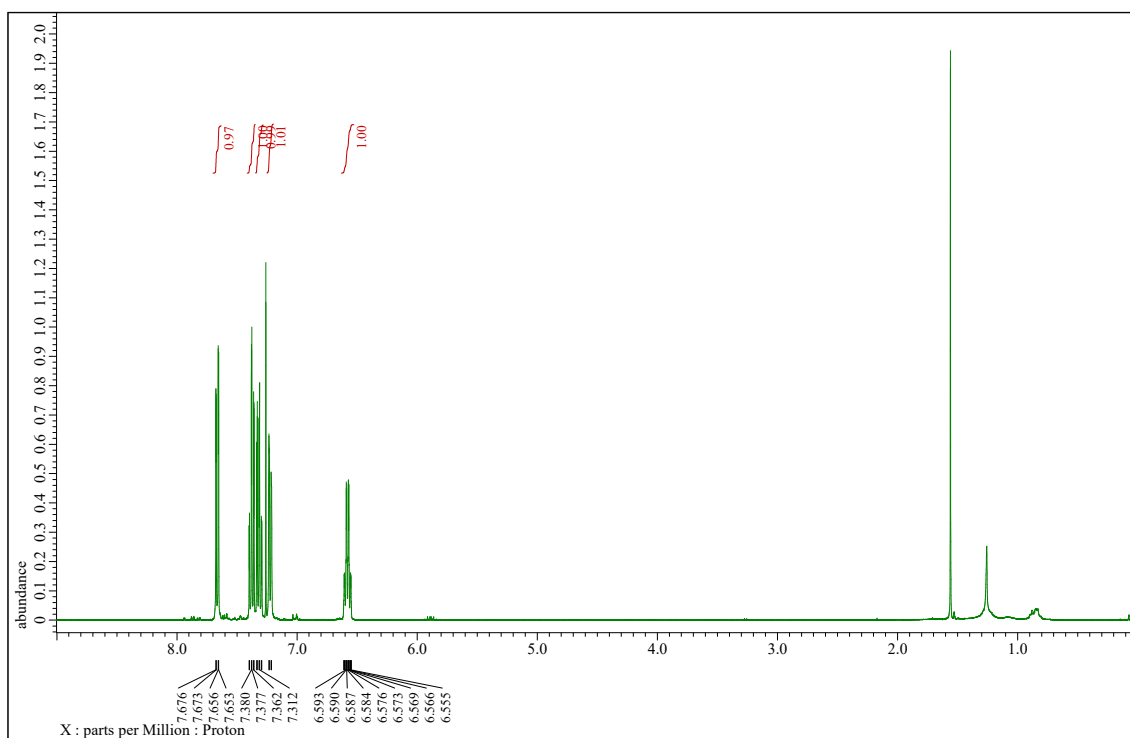
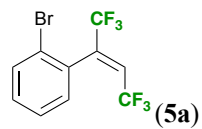


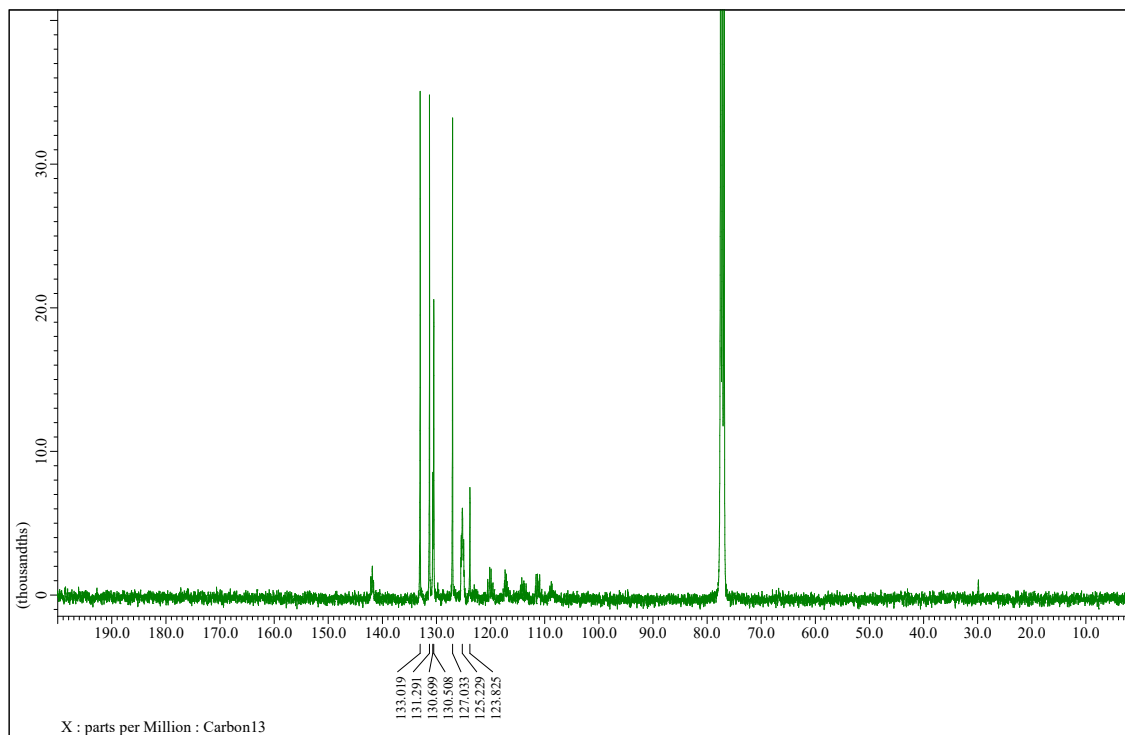
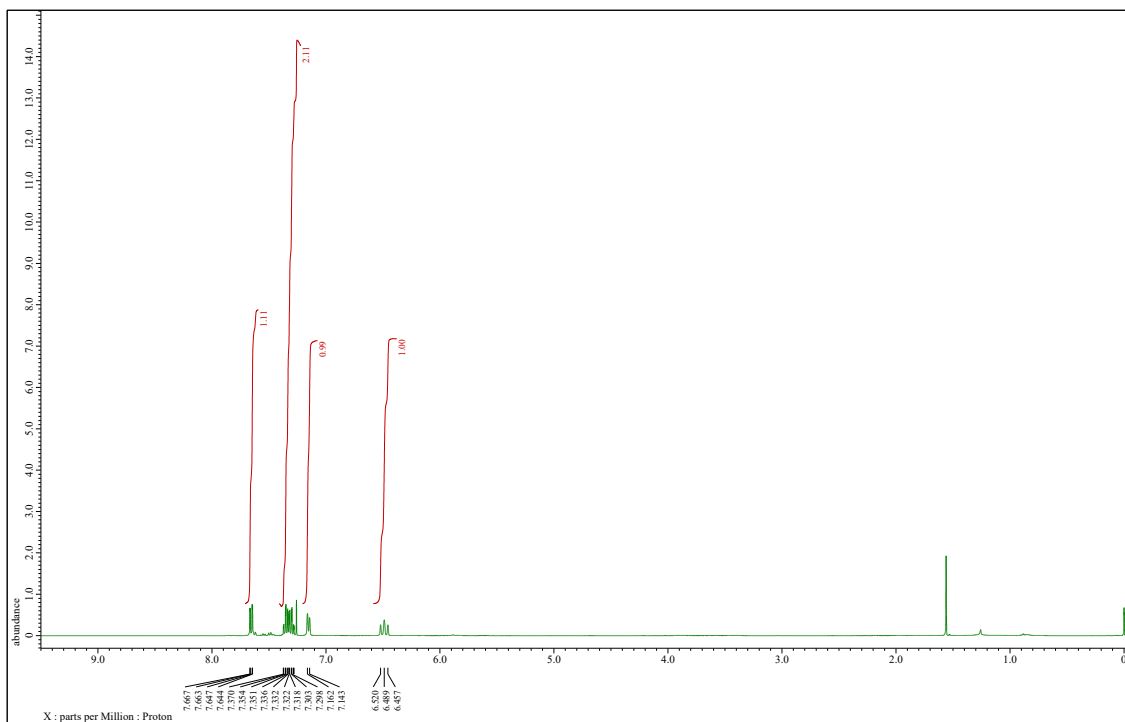
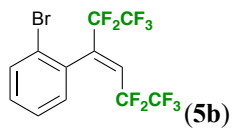


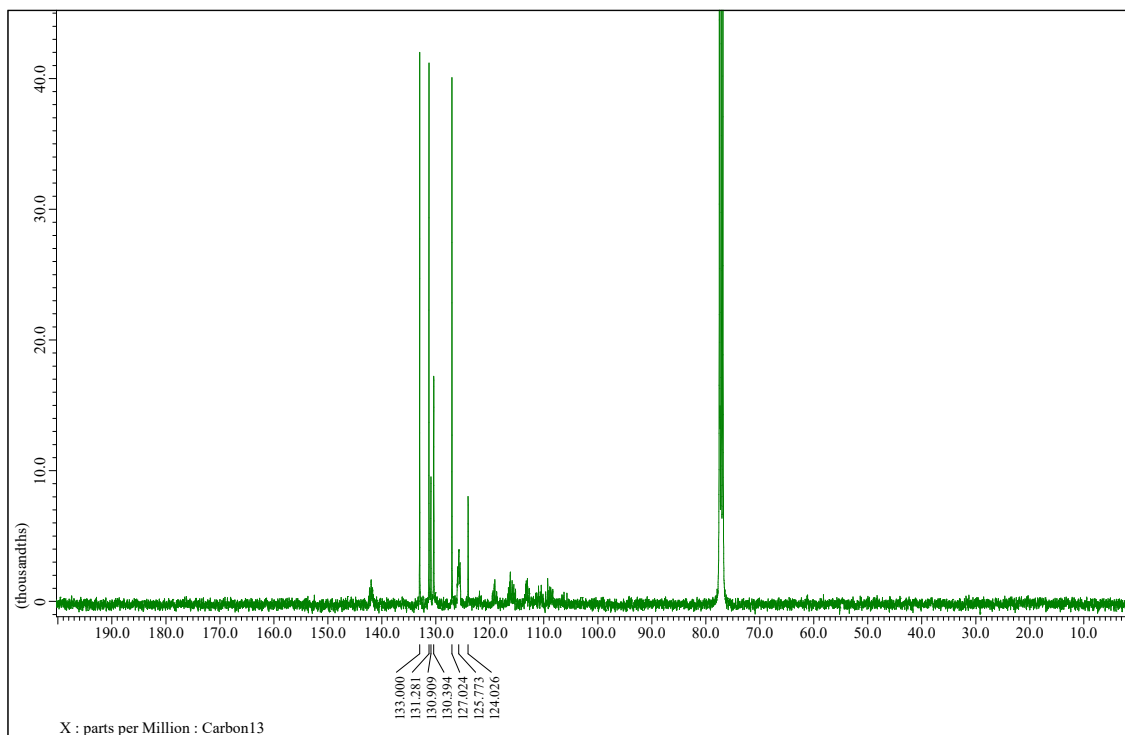
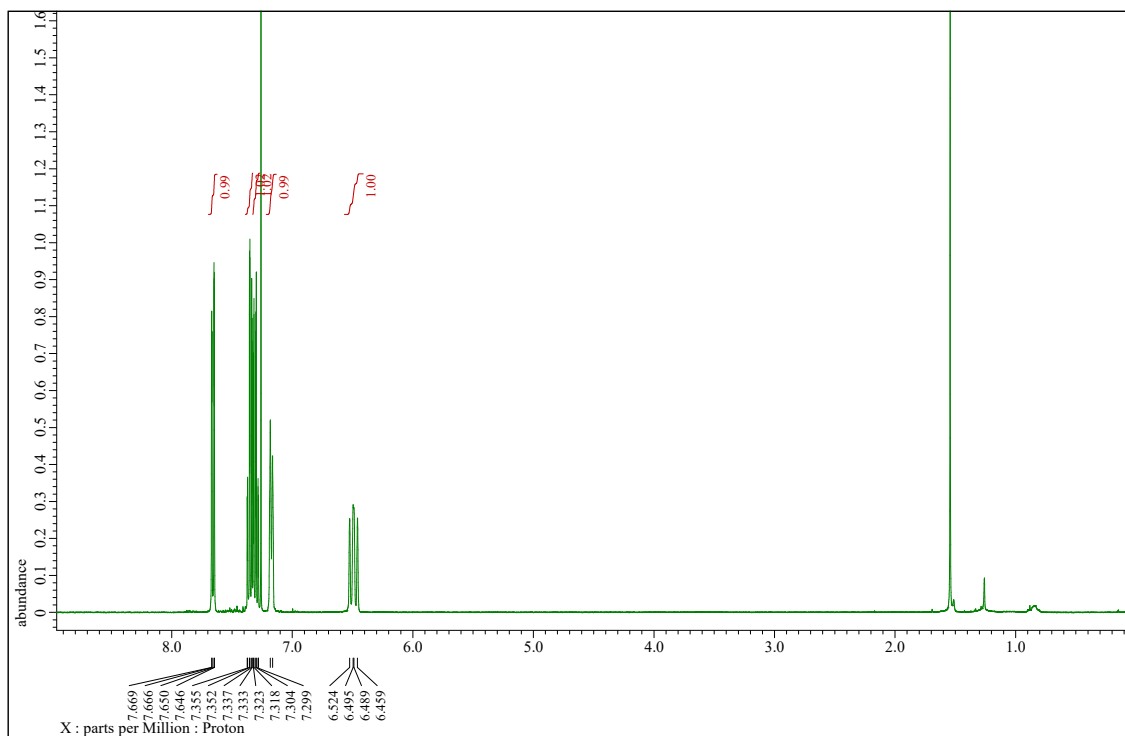
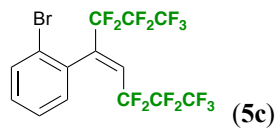


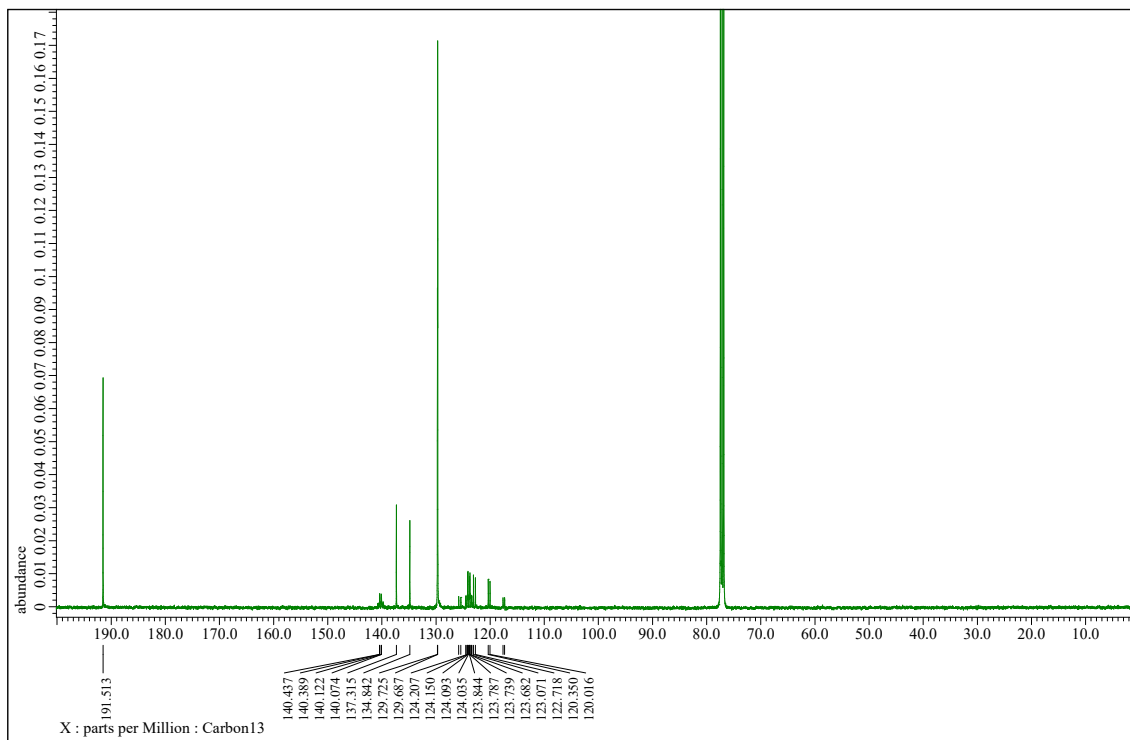
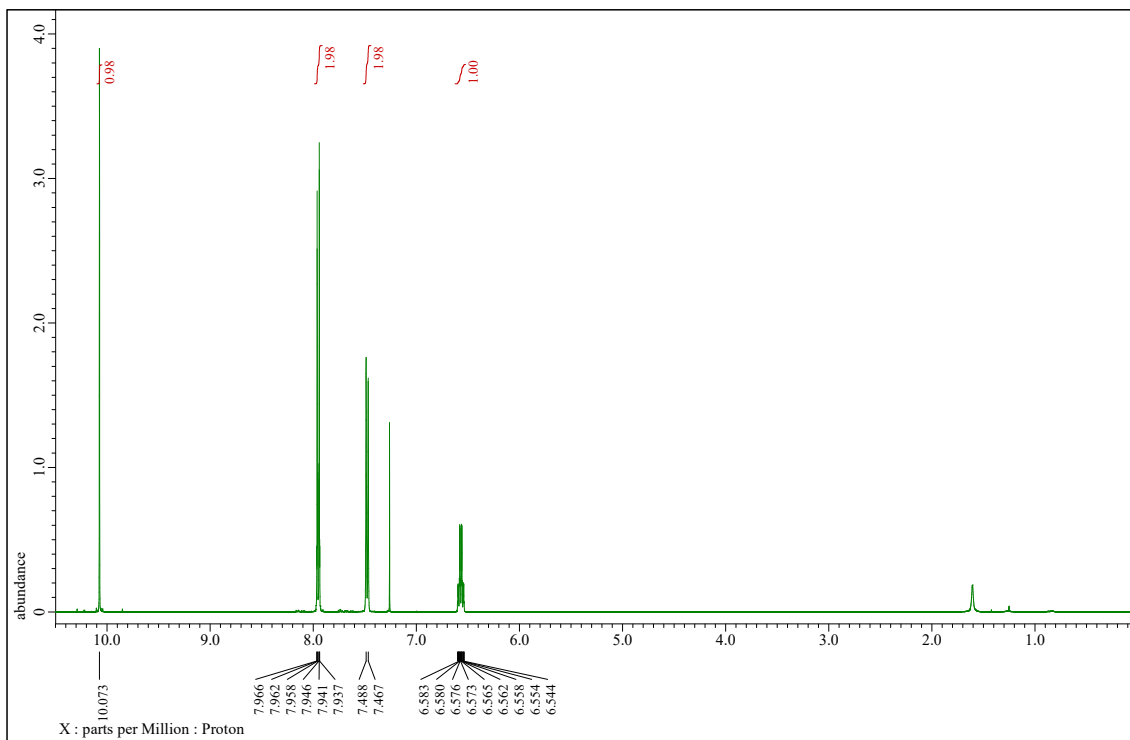
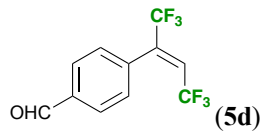


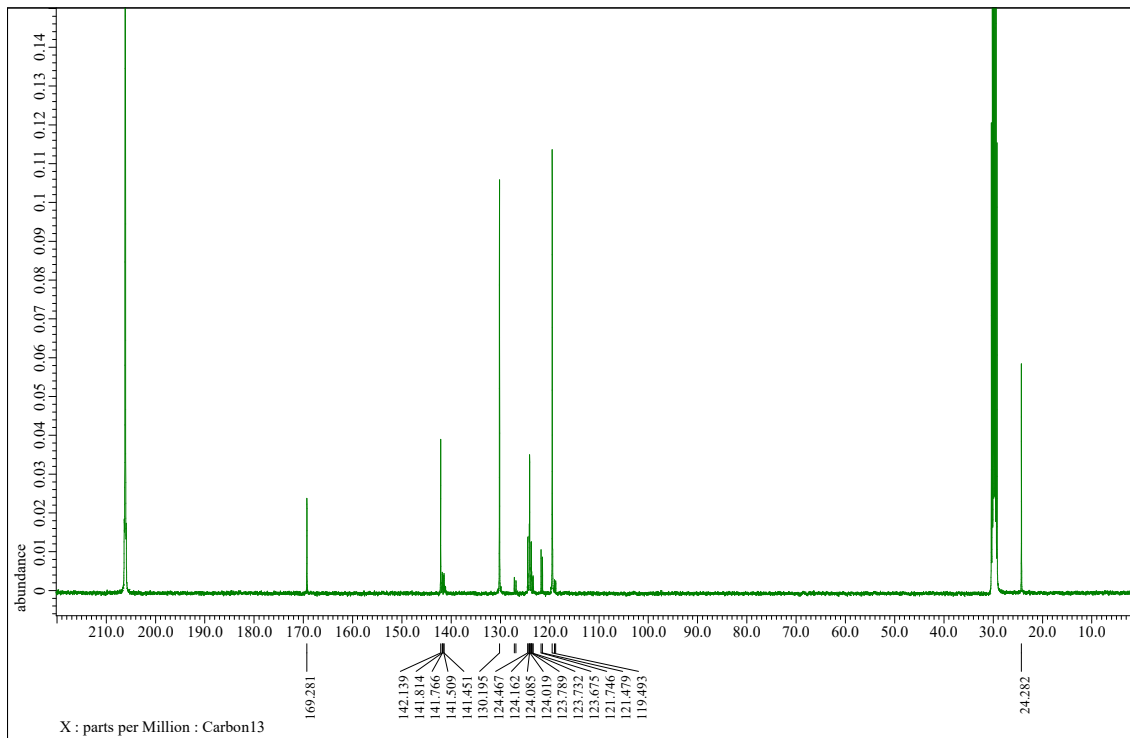
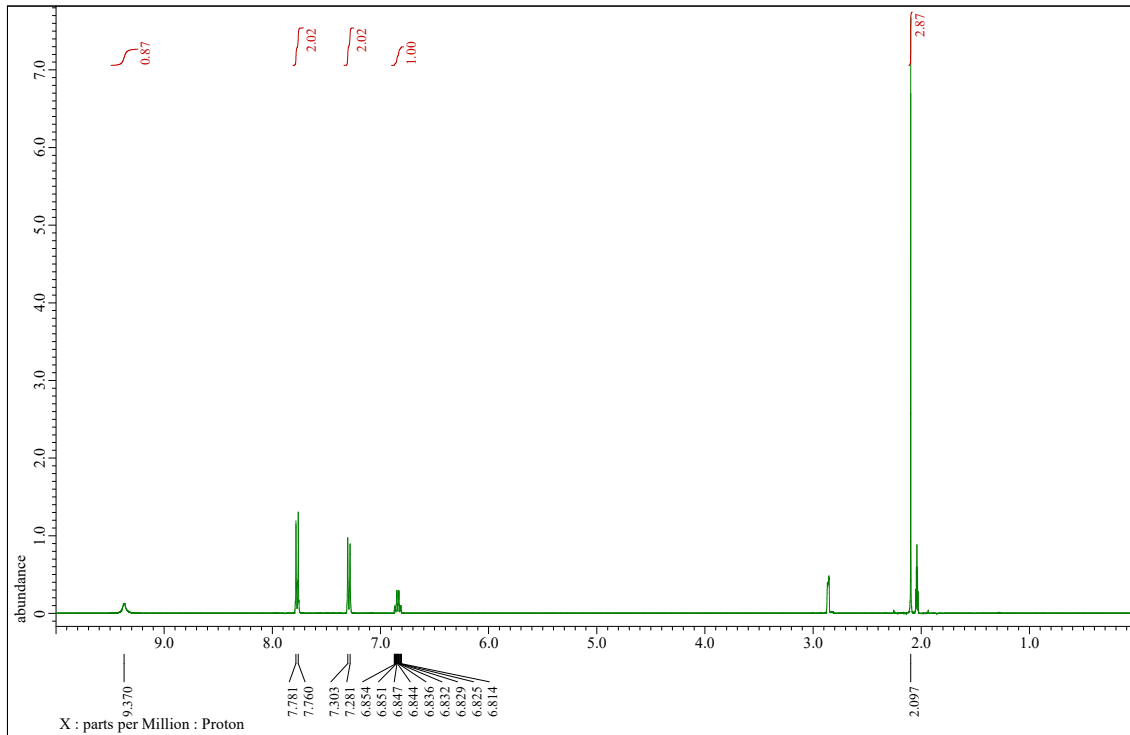
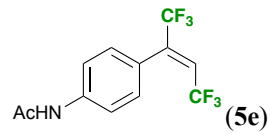


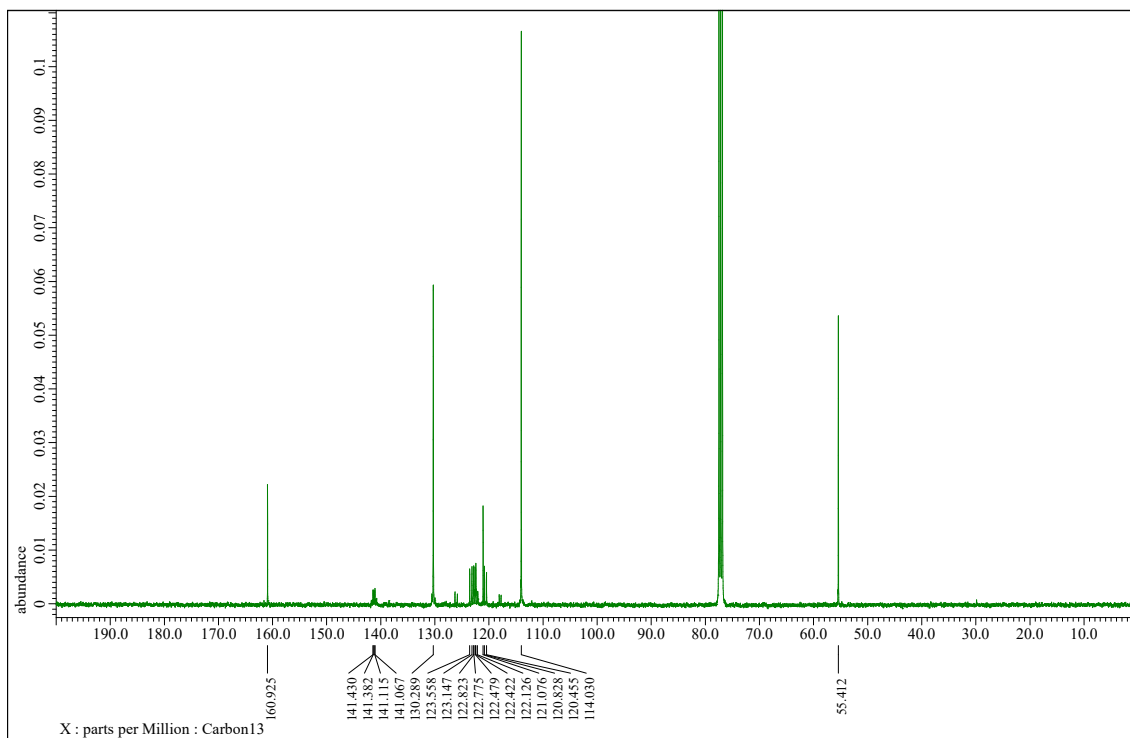
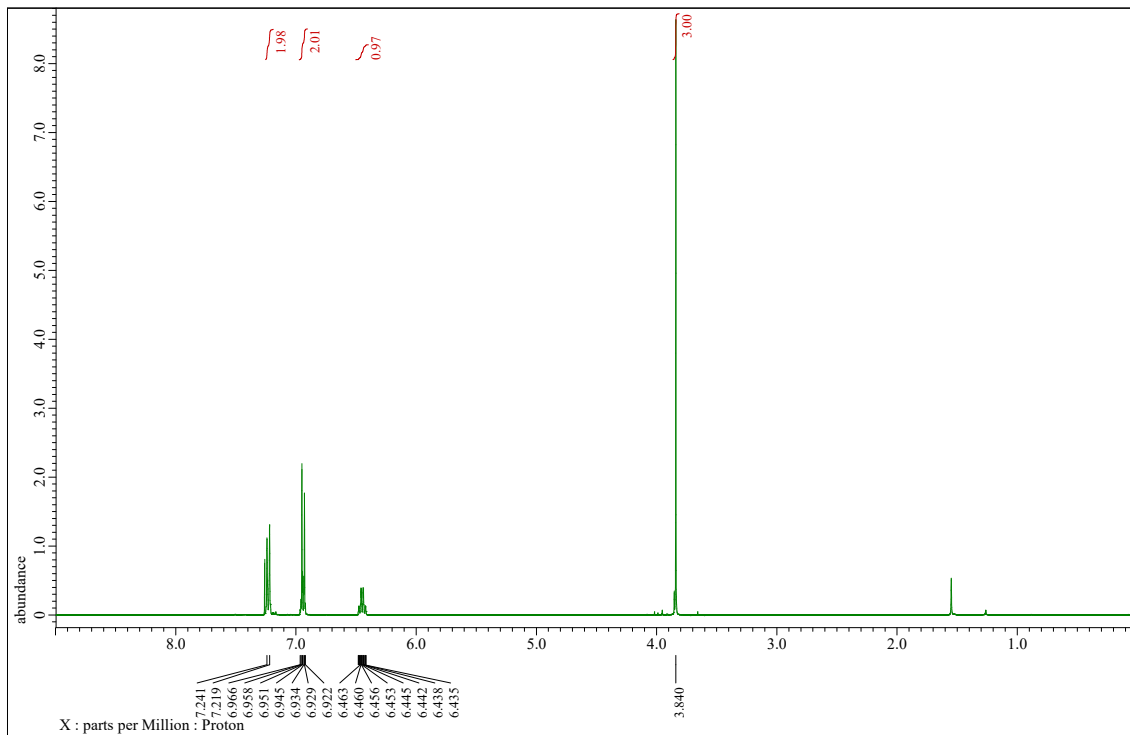
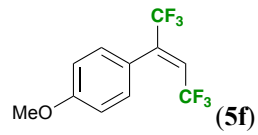


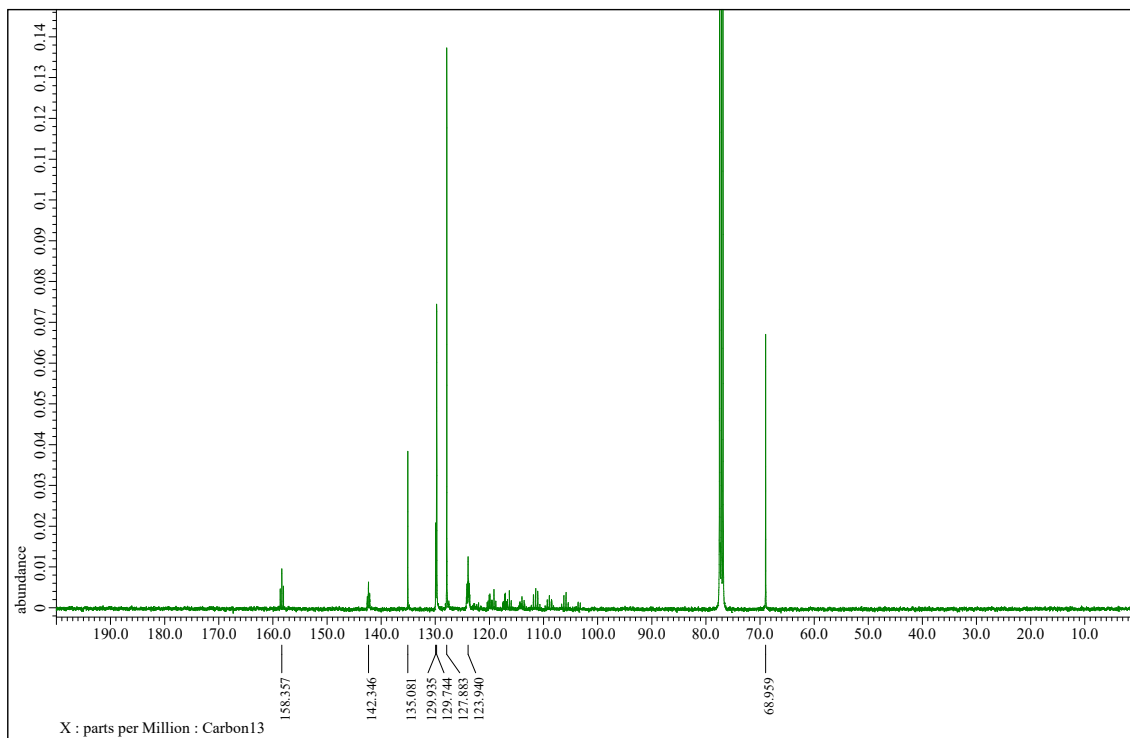
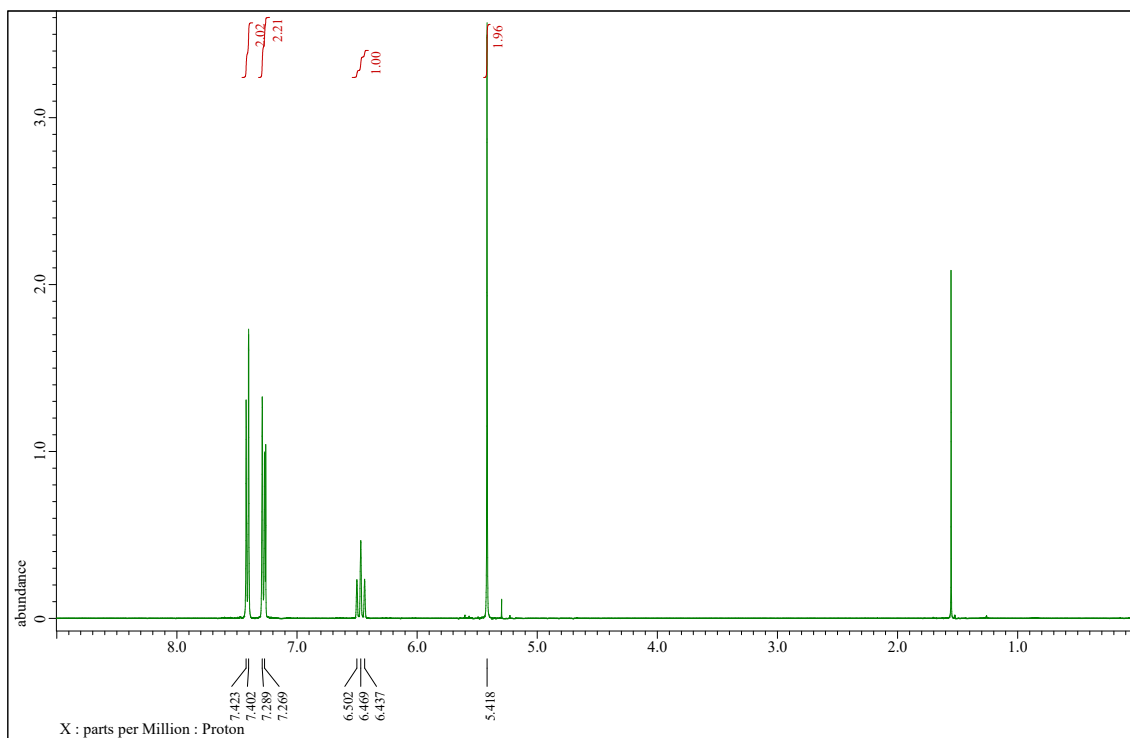
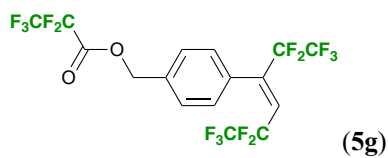


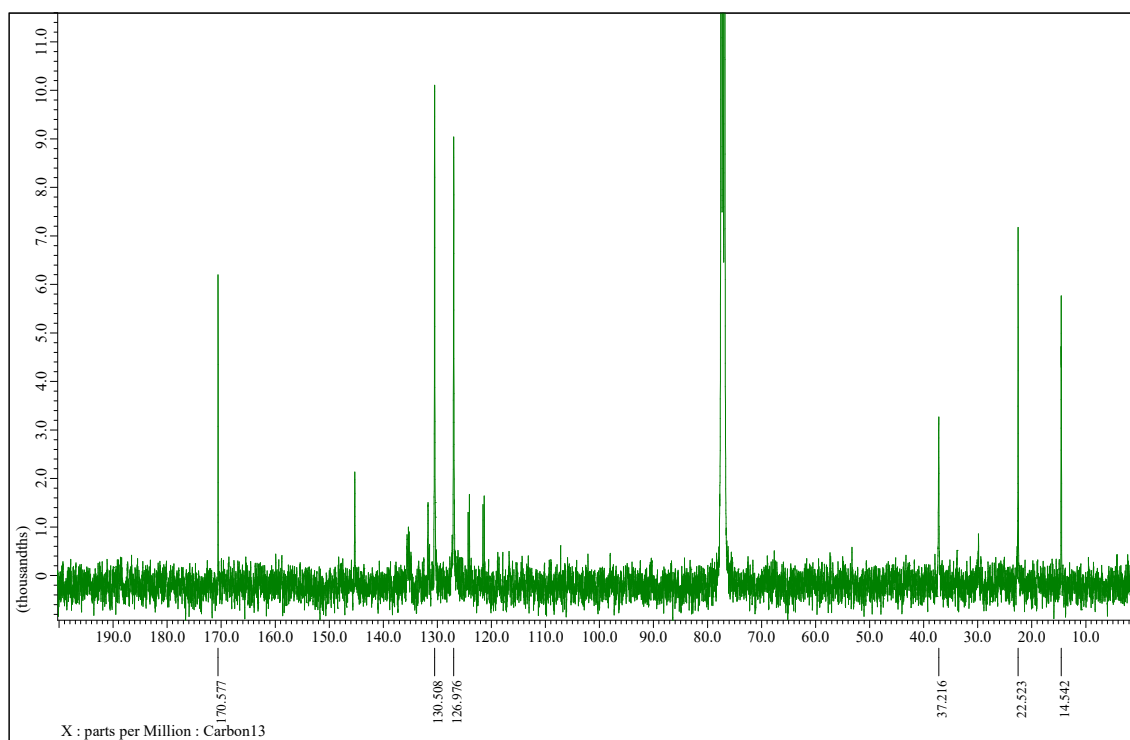
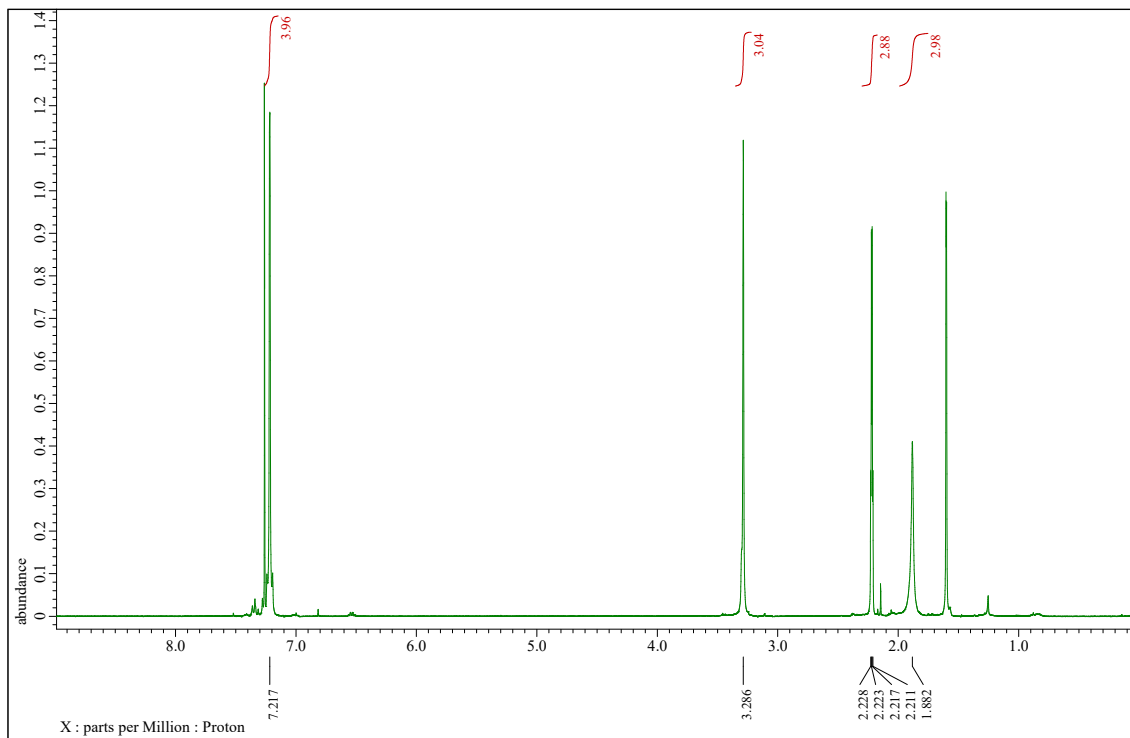
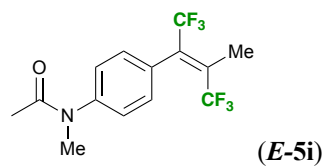


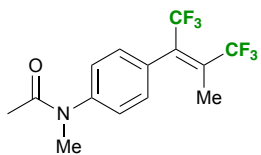




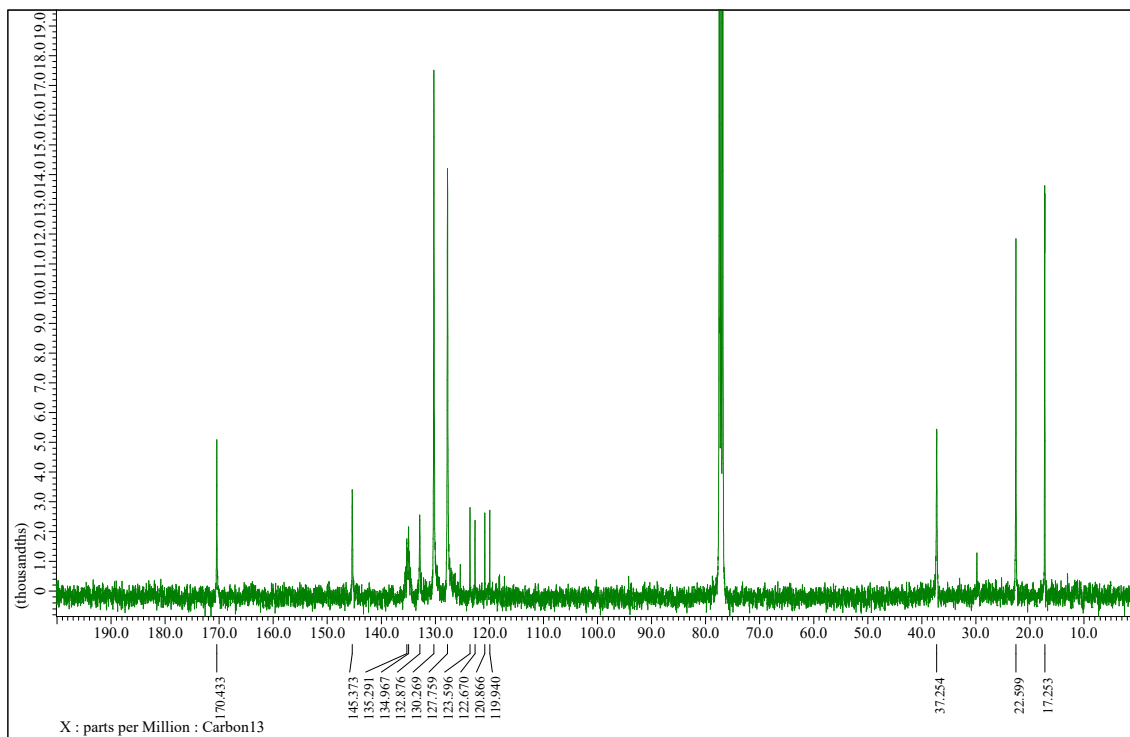
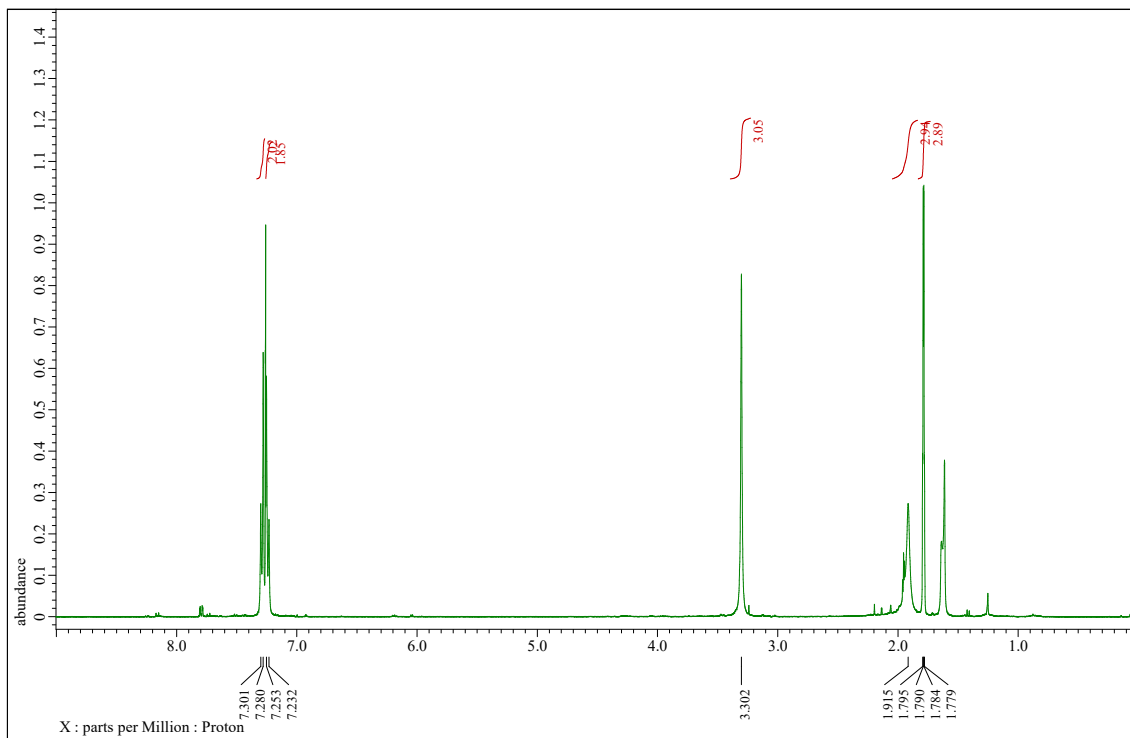


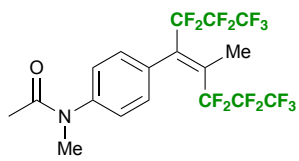




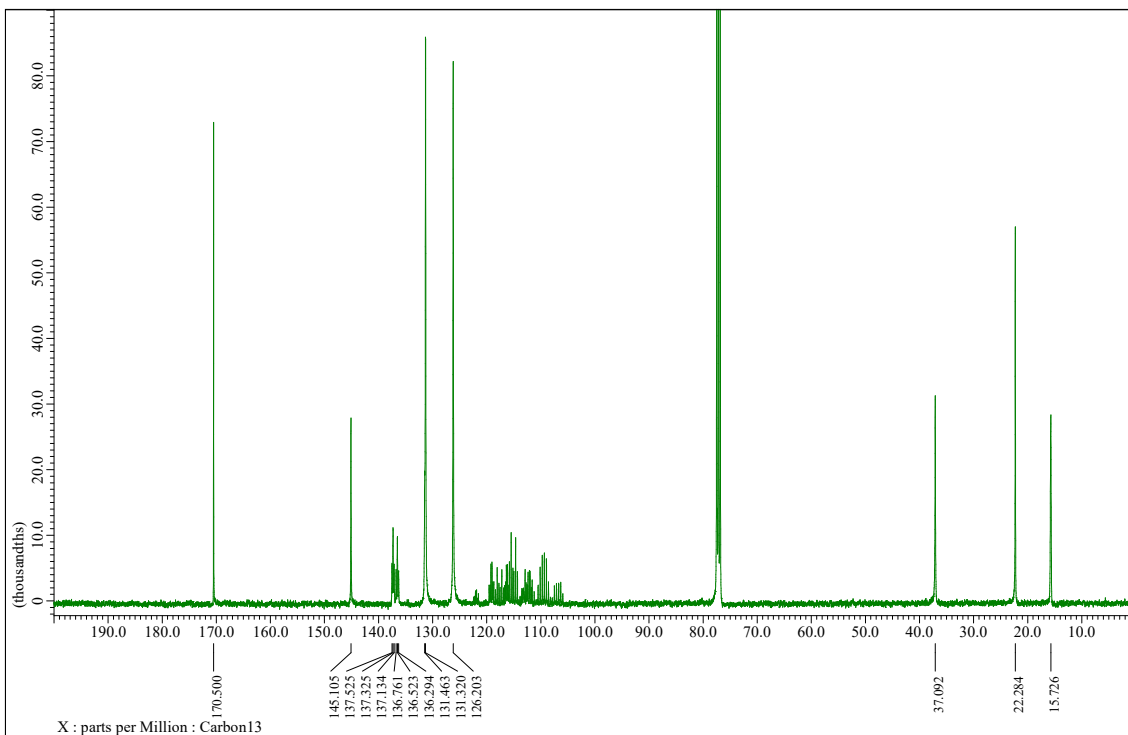
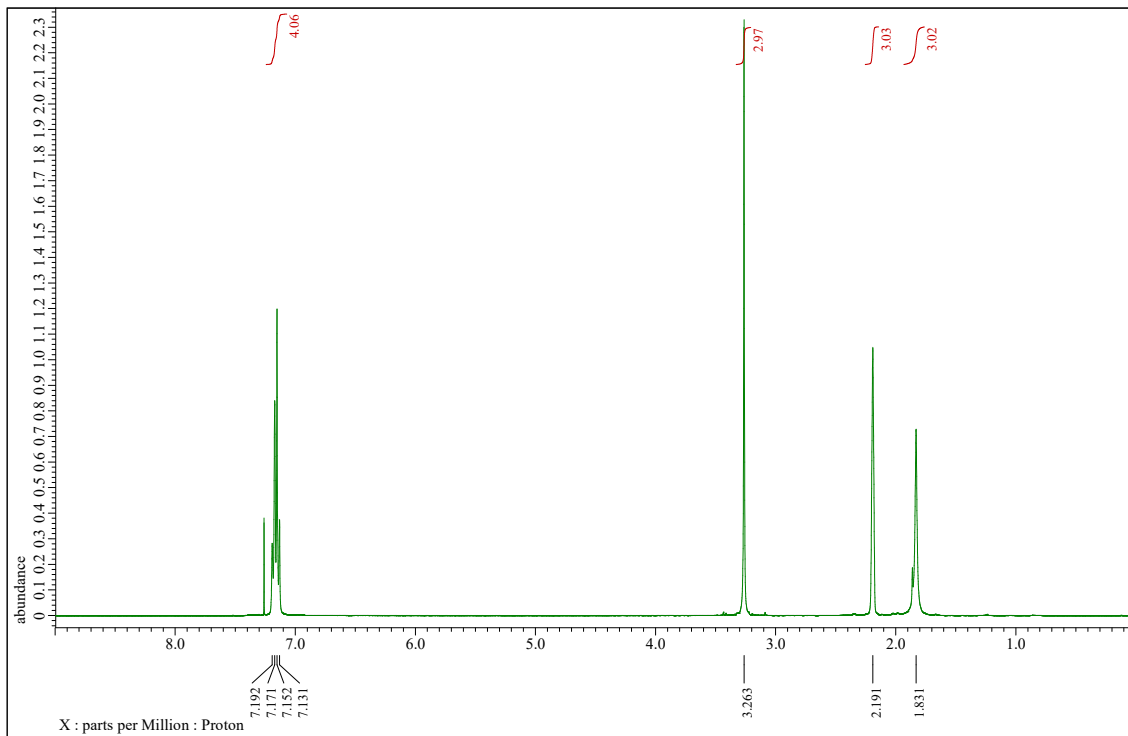


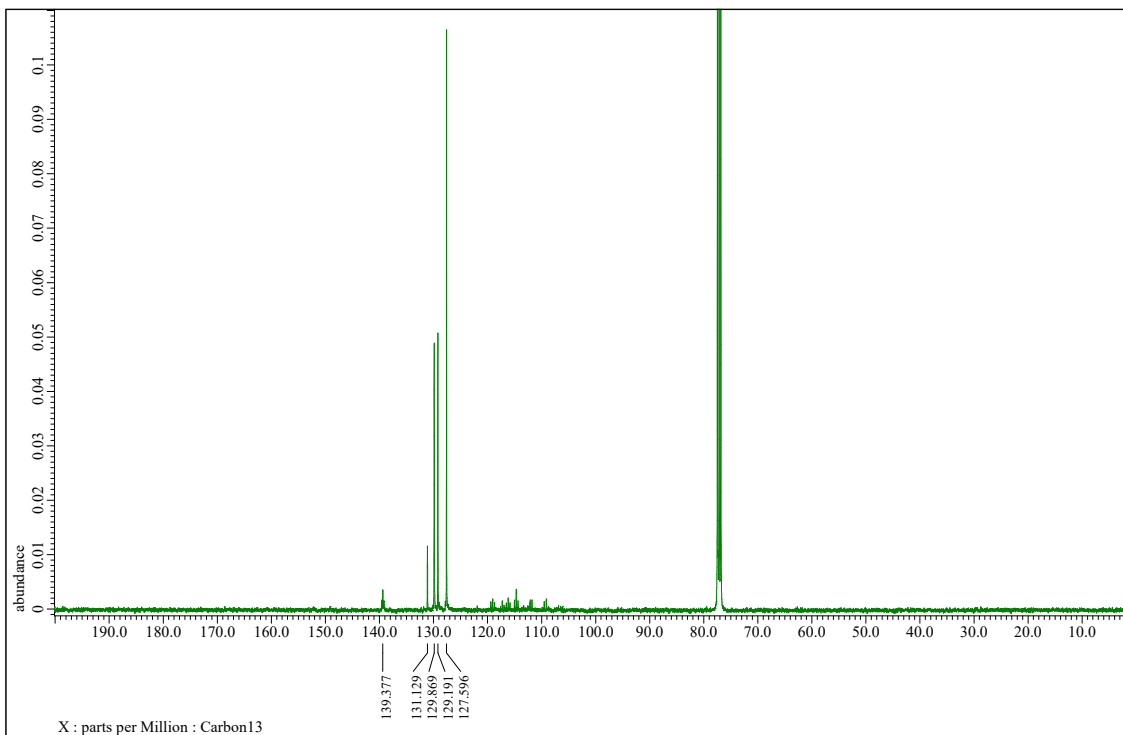
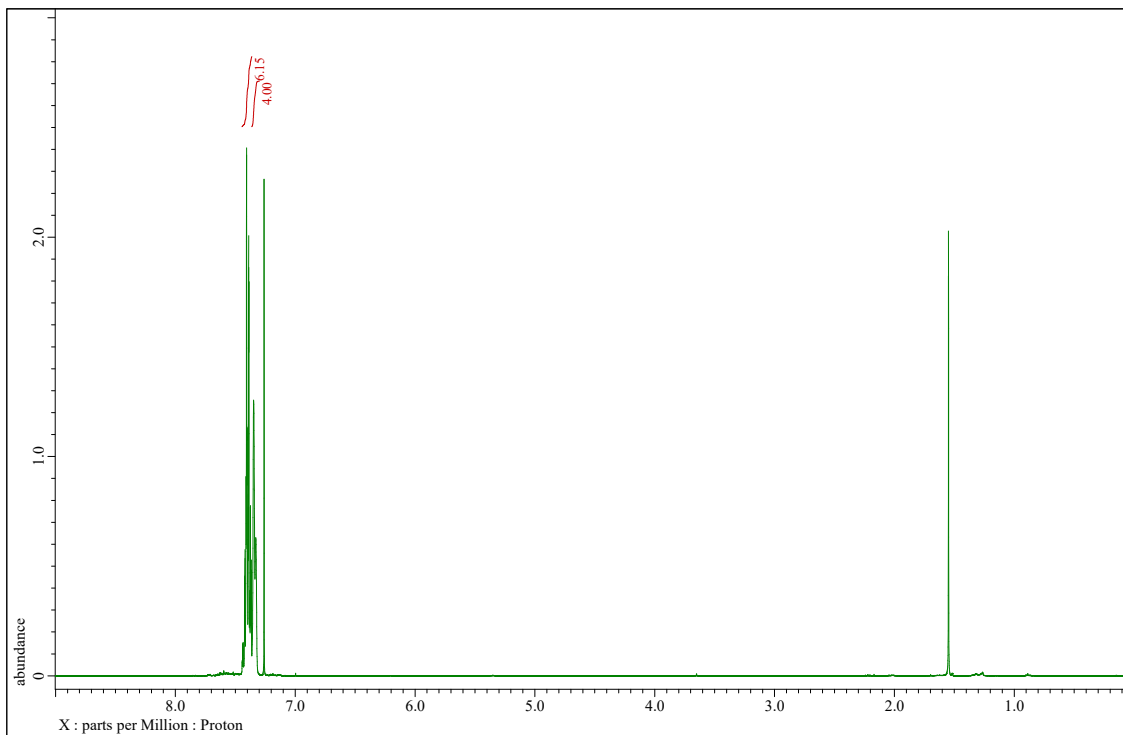
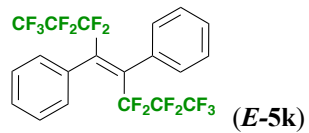
(Z-5i)

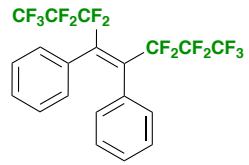




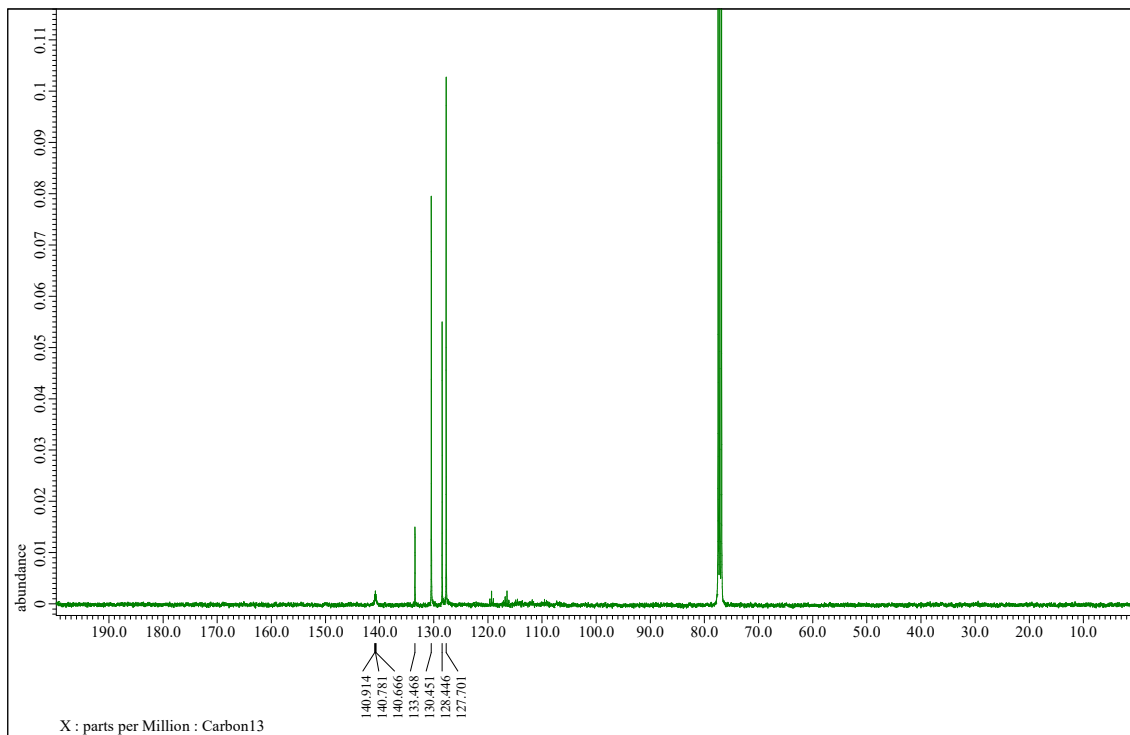
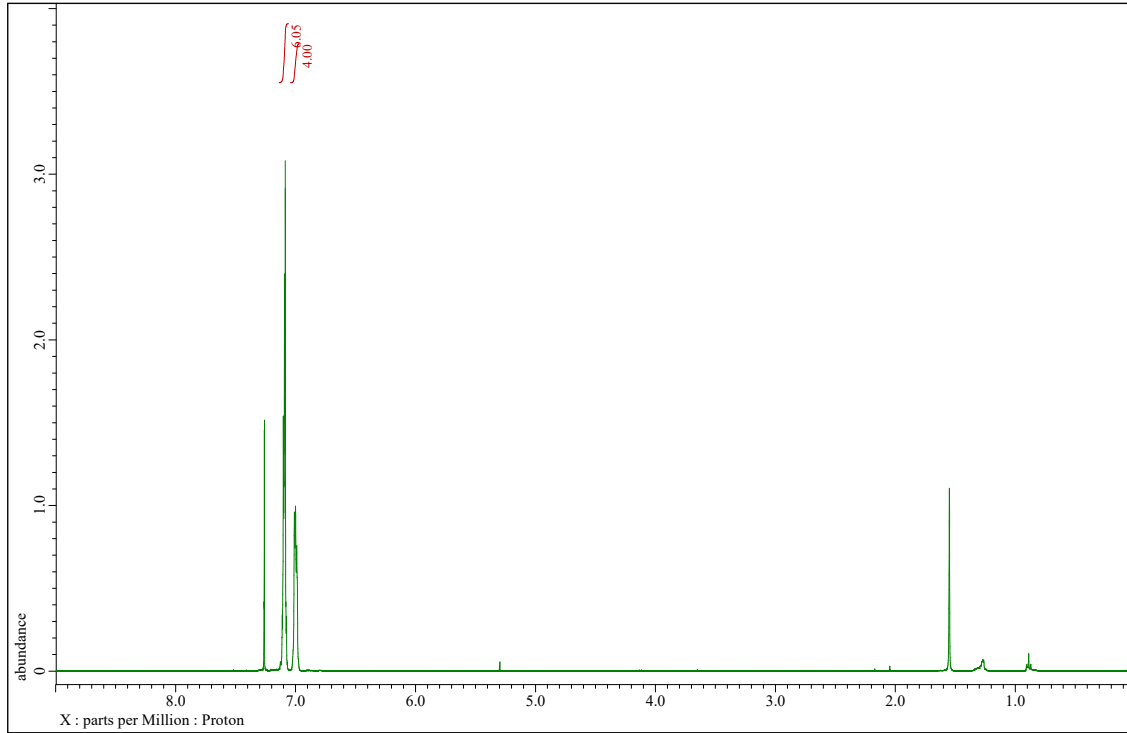
(E-5j)







(Z-5k)



Computational details:

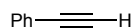
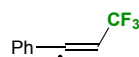
DFT calculations were conducted using Gaussian 16 software. All structures except Cu (optimised by SDD) were optimised using UM06/6-311G+(d,p). The CPCM solvation model (dichloromethane) was used to determine the solvent effect. The free energies described in this work were obtained using vibrational analysis at the UM06 level of theory. No imaginary frequencies were observed for the intermediates, but one imaginary frequency was noted for the transition state. The reaction pathway from the transition state was confirmed by IRC calculations and the vibration mode of the imaginary frequency.

Cartesian coordinates and energies

• CF₃

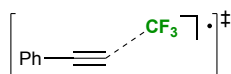
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F 0.0000000444 1.248725998 -0.0719813204
F 1.0814281782 -0.6243626284 -0.0719813204
F -1.0814282226 -0.6243625514 -0.0719813204

H 3.5357962731 2.1448673878 0.5999761158
H 3.5357961898 -2.1448675251 0.5999761158
H 4.6357027244 -0.00000009 1.1700246048

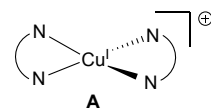


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C 3.2169221889 0.000030717 0.0000042684
C 0.5873826611 -0.0000095105 0.0000111601
H 4.2821022694 0.000040596 -0.0000206594
C -0.1196539442 1.2071833155 0.0000053432
C -0.1196618307 -1.2071978444 0.0000073107
C -1.5054042703 1.2031871605 -0.0000037407
H 0.4292280914 2.1438315325 0.0000083879
C -1.5054120688 -1.2031927066 -0.000001781
H 0.4292142431 -2.1438495545 0.0000118725
C -2.2010195002 -0.0000004763 -0.0000074217
H -2.0459252456 2.1444030741 -0.000008012
H -2.0459392765 -2.144405046 -0.0000045198
H -3.286460922 0.0000029819 -0.0000146379

E(UM06) = -645.840068489
Charge = 0, Multiplicity = 2
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C 1.4833792429 -0.0000051005 -0.9504055841
C -1.1022008805 0.0000021567 -0.3171248451
H 1.8326368835 -0.0000061438 -1.9862664729
C 2.5883746138 -0.0000026833 0.0555375277
C -1.8127329476 -1.2233888855 -0.1557945855
C -1.8127340267 1.2233928098 -0.155796763
F 3.3808265632 1.0743394367 -0.0899937504
F 2.1496852737 0.0000047897 1.3140775253
F 3.3808215234 -1.074349988 -0.0899829011
C -3.15602741 -1.2081967149 0.1470663538
H -1.2787497344 -2.1605149323 -0.2759003599
C -3.15602846 1.2081998826 0.147064243
H -1.2787516415 2.1605191216 -0.2759041967
C -3.8390700453 0.0000014207 0.3012101754
H -3.68658609 -2.1476695058 0.2667156199
H -3.6865879634 2.1476724102 0.2667118501
H -4.8974050233 0.0000011585 0.5402109716

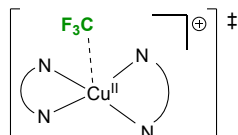


E(UM06) = -645.770641158
Charge = 0, Multiplicity = 2
C -0.0620286276 0.0000000012 -1.260332804
C -1.1925555104 0.0000000232 -1.7060180715
C 1.1975132339 -0.0000000233 -0.6124802549
H -2.043625539 0.0000000397 -2.3511325314
C -2.6008142495 0.0000000505 0.2308469713
C 1.8262935401 1.210004589 -0.2872709063
C 1.8262934931 -1.2100046599 -0.2872709063
F -3.358859682 -1.0807914593 0.2370139763
F -1.8056724799 0.0000000351 1.280230503
F -3.35885964 1.0807915897 0.2370139763
C 3.0552923021 1.2043789834 0.3501398455
H 1.3386671266 2.1462080143 -0.540367371
C 3.0552922553 -1.2043791021 0.3501398455
H 1.3386670432 -2.1462080663 -0.540367371
C 3.6722701433 -0.0000000713 0.6702096359



E(UM06) = -1187.59614284
Charge = 1, Multiplicity = 1
Cu -0.2625505071 -0.3981000749 -0.05272981
N 1.6007507293 -1.245657992 -0.237350358
C 1.8652228733 -2.4999933352 -0.6036618524
H 1.0145320059 -3.1751503634 -0.6530348906
C 3.1436758448 -2.9390362556 -0.9033730214
H 3.3115703383 -3.9698051573 -1.1922227718
C 4.1865232063 -2.028812585 -0.8242980605
H 5.2020451506 -2.3301087184 -1.0576048714
C 3.917176864 -0.7224613734 -0.4511097066
H 4.7186387542 0.0053033339 -0.4038874346

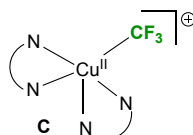
C	2.6072505668	-0.3583315433	-0.1601166158
N	0.9010614657	1.2698596554	0.2360199585
C	2.2207132069	1.0150515454	0.2349727978
C	3.1457546772	1.9870797636	0.5988039987
H	4.2063147123	1.7656172656	0.6124199577
C	2.6940333026	3.2439504937	0.9655705249
H	3.4012162336	4.0137307024	1.2550209053
C	1.3314219355	3.5000849405	0.9659841684
H	0.9369179799	4.4693028171	1.247238414
C	0.4717549156	2.4794858045	0.5966727522
H	-0.6047994991	2.6304796741	0.5831096207
N	-1.6526826818	-1.0851914679	-1.4011297377
C	-1.414515527	-1.4590283941	-2.6584654167
H	-0.4259991899	-1.2293675937	-3.0484368341
C	-2.3598556831	-2.0997035163	-3.4412443394
H	-2.1227274787	-2.3812002903	-4.4603869799
C	-3.6015222761	-2.3664877786	-2.8851854819
H	-4.368237593	-2.8725660288	-3.4618087041
C	-3.8527137794	-1.98665574488	-1.5770615929
H	-4.8118227779	-2.2054985487	-1.1229672301
C	-2.8537103767	-1.3426262352	-0.855590879
N	-1.8980470269	-0.5359369906	1.1825543877
C	-3.0233311251	-0.910765938	0.5503546448
C	-4.258235547	-0.8736111663	1.1881448312
H	-5.1622135487	-1.1609663915	0.6643671845
C	-4.3252490282	-0.4432878537	2.5029709923
H	-5.2805914344	-0.4048275349	3.0151401601
C	-3.1610870368	-0.0562244224	3.1488694939
H	-3.1703134142	0.2875707449	4.1764049111
C	-1.9696511523	-0.1165555278	2.4460445185
H	-1.0305430796	0.1779097852	2.9080003663



E(UM06) = -1525.1477252
Charge = 1, Multiplicity = 2

Cu	-0.4683674	-0.2577415495	0.0525699404
N	-2.3119325697	-1.2479369431	0.1603856081
C	-2.5166883496	-2.5642651019	0.1804988747
H	-1.6474225583	-3.1828089206	0.3909674496
C	-3.7588589025	-3.1331094455	-0.0462680037
H	-3.8796098775	-4.2094917052	-0.0140979576
C	-4.8273185361	-2.2914413958	-0.3159641873
H	-5.8143194863	-2.6969077775	-0.5107942218
C	-4.6201561168	-0.9221913777	-0.3426490856
H	-5.44001238	-0.2518504122	-0.5722923598
C	-3.3442300899	-0.4282100942	-0.0942225276
N	-1.716253352	1.3285572043	-0.1426608313
C	-3.0248650025	1.0163657775	-0.0984420727
C	-4.0031290428	2.0016019271	-0.0320620083
H	-5.0519053264	1.7347015276	0.0232153595
C	-3.6222549728	3.3328105019	-0.0105157612
H	-4.372791013	4.1138572037	0.0446766921
C	-2.2732275255	3.6486904553	-0.0464321378
H	-1.9306115807	4.6763831397	-0.0254290723
C	-1.3563282907	2.6136549589	-0.1088138672
H	-0.2895332021	2.8147805816	-0.1364685955
C	2.2034791483	1.1808171701	-1.6730825201
F	2.0536341146	0.6745703664	-2.8726022433
F	1.6255923987	2.3548700108	-1.5780857732
F	3.472944323	1.2538291275	-1.3479633056

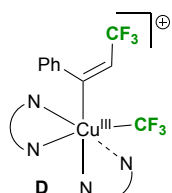
N	1.1566971056	-0.0583945948	1.3142382537
C	2.2426630317	-0.7354060649	0.9040909193
N	0.8626501839	-1.4900078645	-0.8998854115
C	3.4744237642	-0.572409749	1.5274923157
H	4.3499058248	-1.1060486383	1.1770743072
C	2.0434023667	-1.6183567563	-0.2689012409
C	0.6090825218	-2.2413306232	-1.970963565
H	-0.3611501195	-2.0980352932	-2.439807503
C	1.2638474708	0.7883005779	2.3378237682
H	0.3550070915	1.3114386983	2.6253682185
C	3.0070750297	-2.5144164841	-0.7170699832
H	3.9498745244	-2.6238653778	-0.1945729742
C	2.4550979964	1.001901124	3.0109449047
H	2.4955032794	1.6998496544	3.8388088145
C	3.5787622983	0.3050890903	2.5941511214
H	4.5330720696	0.4487755107	3.0891837637
C	1.522861839	-3.1474214121	-2.4823035991
H	1.2782598708	-3.7290534141	-3.3631050216
C	2.7436859274	-3.2822778157	-1.8399925228
H	3.485773514	-3.9838837969	-2.2052879134



E(UM06) = -1525.18612334
Charge = 1, Multiplicity = 2

Cu	0.3995106577	-1.327888663	-1.5708588817
C	1.2511396542	-2.3263032793	1.0247156547
N	1.7857429486	-2.0347105888	-0.172928435
N	-0.0474724505	-3.370682898	-2.3645600074
N	-0.7978727104	-1.5273355486	0.0825838151
C	-0.2023392434	-2.095550614	1.1467800646
C	0.7571573474	-3.7053187561	-3.3815366674
N	1.7119159636	-1.5087006843	-3.127264345
C	2.0313797019	-2.8188887364	2.06282425
H	1.5948868866	-3.0437899233	3.0279225257
C	0.6489929634	-4.9394755833	-4.01411829
H	1.2956937155	-5.2072110224	-4.8406084191
C	1.7514355278	-2.6808735284	-3.7837210213
C	-2.1146122495	-1.3167913222	0.0991993967
H	-2.54742809	-0.868796231	-0.788524454
C	-0.9357420889	-2.4582717981	2.2688464637
H	-0.4525782754	-2.9200614332	3.1208200036
C	3.3864088409	-3.0149920695	1.8533366809
H	4.0108674689	-3.3957273206	2.6540486379
C	3.0876645274	-2.231794571	-0.3717647651
H	3.4743222248	-1.9886441643	-1.3574903431
C	-2.3025634714	-2.2354021492	2.2852908364
H	-2.8887587705	-2.5174776898	3.1529563535
C	2.5682815377	-0.5355596818	-3.4399194621
H	2.4764740361	0.3873001762	-2.8742287607
C	3.9286689097	-2.7196764601	0.6138346923
H	4.9824612374	-2.8601018461	0.4063476263
C	-0.9656336836	-4.2337628341	-1.9451719971
H	-1.591029316	-3.9130842769	-1.1132604749
C	2.6935503653	-2.8947995134	-4.7843165336
H	2.7344359524	-3.8390631855	-5.3124791759
C	-1.1390552526	-5.4829941808	-2.5205961308
H	-1.9026616364	-6.155863791	-2.1490132545
C	-2.9071077756	-1.657106741	1.1818982585
H	-3.9733937757	-1.4697438501	1.1503711805
C	-0.3130844244	-5.8351999679	-3.5753737926

H	-0.4146310747	-6.8014295628	-4.0576116607
C	3.5305995206	-0.6830199646	-4.4216928674
H	4.2116174774	0.1298556155	-4.6418168115
C	3.5905543976	-1.8893353147	-5.1017976718
H	4.331165518	-2.0484402344	-5.8779039695
C	-0.7358965257	0.030687931	-2.5141720325
F	-1.1982989257	1.0381432615	-1.7204320682
F	-1.8669770473	-0.5455540378	-3.0268906627
F	-0.1679925933	0.6634900337	-3.5713424847

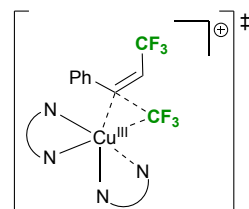


E(UM06) = -2171.06360737

Charge = 1, Multiplicity = 1

Cu	0.387263252	-0.2340181899	-0.2485978944
N	-0.3056713722	-1.0868444712	1.4246692808
C	0.1935088337	-0.7576710901	2.6186844261
H	0.9860803379	-0.0151309552	2.6049313631
C	-0.2636971213	-1.3264417912	3.7931336371
H	0.1635109374	-1.024019032	4.7413839172
C	-1.2613548669	-2.2845299686	3.7158412129
H	-1.6379297209	-2.7649949836	4.6122760008
C	-1.7704189451	-2.6321906048	2.4767805027
H	-2.5326153926	-3.3974581861	2.3984248085
C	-1.2865689733	-2.0063882295	1.3337300678
N	-1.0756507119	-1.889086121	-1.0481044194
C	-1.8148991243	-2.3145804699	-0.0150944702
C	-3.0153583713	-2.990914594	-0.2057985563
H	-3.6281277504	-3.2928792521	0.6354866393
C	-3.434413188	-3.2571546812	-1.49939253
H	-4.3672867271	-3.7834749578	-1.6708434728
C	-2.6541944011	-2.8381387353	-2.5645892947
H	-2.9444892746	-3.0307903738	-3.5906627208
C	-1.4844506795	-2.1475377413	-2.2869018754
H	-0.8465095128	-1.7870075283	-3.0911640607
C	0.7921935519	0.581114357	-1.9809104196
F	1.3054734841	-0.4033083045	-2.7433174886
F	-0.2148024253	1.0918195376	-2.7021986184
F	1.7337334565	1.5297652617	-1.8894692939
C	-0.8474159639	1.2888226102	-0.0475670826
C	-0.3083522319	2.481669915	0.1369677484
C	-2.2515432146	0.9062826251	0.0444885837
H	0.7560560735	2.6683866255	0.0442796797
C	-1.0733714362	3.7106022566	0.5100037547
C	-2.8453866786	0.771765492	1.3049959145
C	-3.0216525904	0.6853138733	-1.1010813154
F	-1.1323812267	3.8643330671	1.8465978863
F	-0.4584728855	4.8008452069	0.029907863
F	-2.3285776866	3.7397070938	0.0624715804
C	-4.1839059504	0.431083191	1.4141064345
H	-2.2499488314	0.9468245565	2.1979469343
C	-4.3578945981	0.3407476251	-0.9846703917
H	-2.5671909557	0.7935292835	-2.0803278876
C	-4.9417561287	0.2096213374	0.2704823829
H	-4.6370526211	0.3386751446	2.3961487569
H	-4.9491044388	0.1741203761	-1.8797889897
H	-5.9890423015	-0.0621516739	0.3568289475
C	3.3070171258	-1.0047809232	-0.0488588948
C	1.9081660659	-2.7316974193	-0.6729329458

C	2.9619922303	-3.6167978231	-0.8014156684
C	4.2427234763	-3.1589088212	-0.5430142787
C	4.4135199656	-1.8405906556	-0.1618342093
H	0.8917023486	-3.0451462275	-0.8823268802
H	2.7713857799	-4.6407263244	-1.0991301085
H	5.098143559	-3.8203923001	-0.6264890405
H	5.3996894802	-1.4605856971	0.0777851556
C	3.4725202279	0.3928271467	0.4059875189
C	4.6227479907	1.1181483818	0.1063852426
C	4.7407716089	2.4088372703	0.5939307219
H	5.4008100184	0.6920596451	-0.5169595188
C	2.6085764366	2.1353305393	1.6110353381
C	3.7218783377	2.9281065538	1.3777341662
H	5.62010299	3.0014713206	0.3650860847
H	1.784143975	2.5091758051	2.2183725782
H	3.7807891444	3.9263563472	1.7956173965
N	2.0652304026	-1.4559675915	-0.3052081374
N	2.4695392075	0.9049312722	1.1230669389

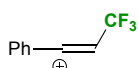


E(UM06) = -2171.05224547

Charge = 1, Multiplicity = 1

Cu	0.3032290322	-0.4239344143	-0.1802861062
N	-0.4733585817	-0.6943845013	1.6991890678
C	0.0846804317	-0.1086006995	2.7599279313
H	1.0120186753	0.4225534664	2.5654266543
C	-0.4677341438	-0.17712023	4.0264309707
H	0.0164827148	0.3205765664	4.8578964903
C	-1.6389779816	-0.8982559401	4.1915638679
H	-2.1034091457	-0.9845469379	5.1679794997
C	-2.2123861634	-1.5170458364	3.0942057318
H	-3.1187241249	-2.0962762921	3.2175249393
C	-1.6130563263	-1.3918292335	1.8450033007
N	-1.4558536535	-1.9289682313	-0.4903060711
C	-2.1955520314	-2.0013512304	0.6241383802
C	-3.4490434425	-2.607687954	0.626541172
H	-4.054861866	-2.6383882641	1.5237302095
C	-3.9289484127	-3.1699201175	-0.5440773413
H	-4.9035223585	-3.6460162733	-0.5590409296
C	-3.1501383694	-3.1143745445	-1.6881492128
H	-3.4827474555	-3.5465591784	-2.6245267117
C	-1.9230135717	-2.4768165762	-1.6105131357
H	-1.2848936098	-2.4006976531	-2.4871292813
C	-0.5252722136	1.3135991335	-0.5363470006
C	0.2416183575	2.3516724263	-0.2164390524
C	-1.9873856414	1.1942792092	-0.5044050547
H	1.3223361481	2.2937447652	-0.2808877629
C	-0.2348550093	3.6870775826	0.2507875824
C	-2.6397720608	1.4675495679	0.7044876648
C	-2.746401831	0.7833120361	-1.6028553798
F	-1.3794363268	4.0828274129	-0.3043817217
F	-0.4126497316	3.7125776291	1.5849842514
F	0.6859745048	4.6191027744	-0.0258840817
C	-4.0170069087	1.3569371901	0.8022146398
H	-2.0604181078	1.7597784244	1.5759344778
C	-4.1233789206	0.6722882905	-1.4977974934
H	-2.2652199096	0.5492519296	-2.5455670455
C	-4.7636664011	0.9583469003	-0.2985329826

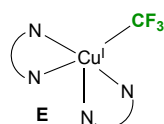
H	-4.50584836	1.5751639422	1.7464429317
H	-4.6999970538	0.3550679259	-2.3609952255
H	-5.8421462468	0.8647561498	-0.2210867798
C	3.1635611266	-1.5125167644	-0.0851394766
C	1.5184035319	-3.0796109595	-0.4651837857
C	2.4378256266	-4.1064643387	-0.5750537406
C	3.7815967668	-3.8048466095	-0.435963004
C	4.1446873015	-2.4934813972	-0.1868553687
H	0.4570893902	-3.2754944467	-0.5713564876
H	2.0966948905	-5.1169813604	-0.7649672133
H	4.5373957667	-4.5794224918	-0.5086224246
H	5.1854068749	-2.2278634855	-0.0408990698
C	3.5541180963	-0.1181775695	0.2261652851
C	4.724419105	0.4259191303	-0.2994824057
C	5.0709612118	1.7211072619	0.0452360849
H	5.3384974031	-0.1457668484	-0.9867004407
C	3.1037305514	1.8049368793	1.3778030933
C	4.2522543721	2.4270717152	0.9140875427
H	5.9692171034	2.1741856299	-0.3607231342
H	2.4305995003	2.3346983642	2.0531262927
H	4.4905827738	3.4383508984	1.2228420887
N	1.8581772325	-1.8070005901	-0.2282174201
N	2.7453033483	0.5687598857	1.0349676509
C	0.5376706885	0.4016881331	-2.0872325304
F	1.8084918903	0.7995144129	-2.0682402348
F	-0.1006621658	1.2088491582	-2.9419330794
F	0.4898947103	-0.808168822	-2.6752496152



E(UM06) = -645.638958676

Charge = 1, Multiplicity = 1

C	0.1785070164	0.000235831	-0.6452917415
C	1.4240823325	0.0003845771	-0.9483333985
C	-1.1267561656	0.000496088	-0.331137333
H	1.7376388044	0.0005970914	-1.9925199478
C	2.5150529761	0.0002376911	0.0911367908
C	-1.8162782743	-1.2436856179	-0.1688036371
C	-1.8165073341	1.2435897278	-0.1682849654
F	3.2803850682	1.0751091775	-0.0529805293
F	2.021874538	-0.0000505823	1.323284607
F	3.2805288989	-1.0744701011	-0.0534276844
C	-3.1474656731	-1.2277925459	0.1441996774
H	-1.2675124757	-2.1695165496	-0.2991455851
C	-3.1476904733	1.2273199497	0.1447166274
H	-1.2679119628	2.1695761893	-0.2982394958
C	-3.8041241924	-0.0003288434	0.2981367499
H	-3.6945292111	-2.1536607626	0.272307269
H	-3.6949230471	2.1530338081	0.2732172504
H	-4.8613488251	-0.000477649	0.5450893458



E(UM06) = -1525.34129933

Charge = 0, Multiplicity = 1

Cu	0.3585084256	-1.7334931769	-1.7818190849
C	0.946055632	-2.3836115213	1.2008715592
N	1.4907605262	-2.3783710887	-0.0246187079
N	0.2200226309	-3.5705274571	-2.7406303166

N	-1.2655650536	-2.5420490856	0.2879848752
C	-0.5055313965	-2.1003198626	1.2945161903
C	1.0332311393	-3.8255082782	-3.779221749
N	2.1240601135	-1.7618011016	-3.2820105925
C	1.7023249381	-2.6545210719	2.3386613682
H	1.2294072513	-2.6728005311	3.3147095015
C	1.0435493317	-5.0673338083	-4.4085993967
H	1.7268198697	-5.2632514254	-5.2271395654
C	1.9260438483	-2.7207388903	-4.1951644195
C	-2.5682572918	-2.2807710328	0.324843765
H	-3.1579410342	-2.6556762651	-0.5115270589
C	-1.0301483425	-1.3889214896	2.370645459
H	-0.3810689633	-1.0251624818	3.1603467729
C	3.0521857659	-2.9310265859	2.203091622
H	3.6564700955	-3.1541908557	3.0763288569
C	2.79072755	-2.6482630298	-0.1449405598
H	3.1829162199	-2.6299395528	-1.1600987535
C	-2.3887842595	-1.1195485726	2.393555759
H	-2.8219628426	-0.5544500392	3.2125657908
C	2.9164420833	-0.7379222368	-3.5868620986
H	3.0461602577	0.0143118151	-2.8105748585
C	3.6120492496	-2.9304984262	0.9346916937
H	4.663089893	-3.1455304105	0.7788781871
C	-0.593796919	-4.5352937986	-2.3065687301
H	-1.2121343488	-4.2712324535	-1.4511418217
C	2.5125104105	-2.666323529	-5.4574404932
H	2.3146328635	-3.4345101431	-6.1965877462
C	-0.647933848	-5.7911474961	-2.8869421187
H	-1.3295144775	-6.539789998	-2.4997061044
C	-3.1801609153	-1.5727899879	1.3493754209
H	-4.2475418453	-1.3835286198	1.3244935649
C	0.189625945	-6.0597919896	-3.9594455189
H	0.1866869894	-7.0349927078	-4.4349577675
C	3.5516123579	-0.6117796525	-4.8125618938
H	4.191852249	0.2396804759	-5.0133166924
C	3.3363186404	-1.5965401408	-5.765751642
H	3.8000721874	-1.529198655	-6.7443730904
C	-0.4847215614	0.031979247	-1.6988542429
F	-0.5040040249	0.6088408352	-0.4346550277
F	-1.8181223968	0.1265635688	-2.0762822256
F	0.1028521254	1.0318255075	-2.463386109

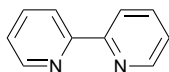
[Cu(CH₃CN)₄]⁺

E(UM06) = -728.119844908

Charge = 1, Multiplicity = 1

Cu	0.0070924327	0.0071104129	0.0004895804
N	-0.3513199901	1.6532869359	-1.1075728905
N	-1.6111974795	-0.3924776437	1.1367466687
N	0.3696449849	-1.5701404961	-1.2033202233
N	1.6132748586	0.3305285453	1.1752687038
C	0.5707981159	-2.4792441236	-1.8768785445
C	2.5371712925	0.5124097025	1.8340020651
C	-2.5421963084	-0.6228667938	1.7698136006
C	-0.5566285838	2.5992104901	-1.7269871231
C	0.821736889	-3.6201645632	-2.7195705563
H	-0.0459288816	-3.8129569276	-3.3535888029
H	1.6901016886	-3.4320216859	-3.3539290019
H	1.0152799759	-4.5015852688	-2.1050031749
C	3.6963627507	0.7395659237	2.6582313859
H	3.5286003791	1.5997542826	3.3092417256
H	3.8928302184	-0.1395477124	3.2751245426
H	4.5677226504	0.9343389517	2.0298603846
C	-0.8137414792	3.7859079264	-2.5017849573
H	0.0774472979	4.0607781469	-3.0694085243
H	-1.6361880871	3.6067136623	-3.1970191914

H	-1.0817860852	4.6117987633	-1.8399437095
C	-3.7103284838	-0.9116990833	2.5615348566
H	-3.5335477116	-1.7945351414	3.1789954734
H	-3.9394120901	-0.0644990735	3.2109183972
H	-4.5650573542	-1.10019323	1.9088893153



E(UM06) = -495.131539831

Charge = 0, Multiplicity = 1

N	1.3569007778	-1.1351053668	0.365446587
C	2.6858923121	-1.1499406138	0.3746593355
H	3.1554286258	-2.0824350718	0.6841815834
C	3.4727572488	-0.0620078331	0.0208838166
H	4.554332092	-0.1353161721	0.0459413946
C	2.8339927848	1.1054052478	-0.3652720096
H	3.4052185482	1.9792539601	-0.662049971
C	1.4491406126	1.1374236535	-0.3754703197
H	0.920885447	2.0302577434	-0.6934030277
C	0.7431617488	-0.0054535471	-0.0002161457
N	-1.3569007778	-1.1351053668	-0.365446587
C	-0.7431617488	-0.0054535471	0.0002161457
C	-1.4491406126	1.1374236535	0.3754703197
H	-0.920885447	2.0302577434	0.6934030277
C	-2.8339927848	1.1054052478	0.3652720096
H	-3.4052185482	1.9792539601	0.662049971
C	-3.4727572488	-0.0620078331	-0.0208838166
H	-4.554332092	-0.1353161721	-0.0459413946
C	-2.6858923121	-1.1499406138	-0.3746593355
H	-3.1554286258	-2.0824350718	-0.6841815834

CH₃CN

E(UM06) = -132.701263999

Charge = 0, Multiplicity = 1

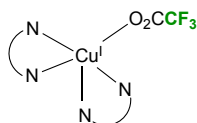
C	-0.0000356171	0.0000140303	0.2735580482
N	0.0000298536	-0.0000563631	1.4258254902
C	0.0000019173	0.0000375147	-1.1709132004
H	-0.0000067133	1.0250432957	-1.5467072212
H	0.8877350721	-0.512521884	-1.5465693812
H	-0.8877245127	-0.5125155937	-1.5465957356

CF₃CO₂⁻

E(UM06) = -526.311698489

Charge = -1, Multiplicity = 1

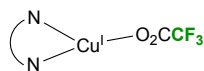
O	0.0440918997	-0.8800585852	0.3468334588
C	0.0651959577	-0.0632447926	1.2776931835
O	0.992269338	0.5670056663	1.7970703316
C	-1.3535544425	0.1904015969	1.8855266691
F	-1.880230436	-0.9444804427	2.3818671432
F	-2.2153747777	0.6341525531	0.9525388145
F	-1.3770045392	1.0850700043	2.8790413992



E(UM06) = -1713.92363168

Charge = 0, Multiplicity = 1

Cu	0.3905512822	-2.4017181884	-1.4653360984
C	0.9751230936	-2.0495117784	1.3796175455
N	1.6003641048	-2.1631104541	0.1958666632
N	0.2845374177	-4.0168567819	-2.6722517713
N	-1.0546707238	-2.246174812	0.1314204484
C	-0.5071261298	-2.0099217383	1.3309882397
C	0.8948828684	-4.0381947592	-3.8678368465
N	2.457889558	-2.3356976318	-3.2063504251
C	1.6912738672	-1.9854260049	2.5712818285
H	1.1789945377	-1.9101781591	3.5231251499
C	0.7186115694	-5.0934089906	-4.7574297417
H	1.2432230014	-5.0944388306	-5.7067335384
C	1.754732069	-2.8786649515	-4.2058795567
C	-2.3784839936	-2.2153773729	-0.0027778616
H	-2.7532681472	-2.3888454277	-1.0102175443
C	-1.2943879906	-1.7342127104	2.4455774108
H	-0.8459461341	-1.5257187554	3.4098763044
C	3.0746633362	-2.0320939501	2.533140613
H	3.6472319207	-1.9832084327	3.4533218418
C	2.9317136377	-2.2191618393	0.1661075068
H	3.3732914243	-2.3348739599	-0.8213734646
C	-2.6725361182	-1.713940584	2.305117972
H	-3.3031083949	-1.5001618882	3.1618090388
C	3.195535212	-1.2640979049	-3.4755968557
H	3.7576565587	-0.8406093278	-2.6438018061
C	3.7125146097	-2.151429294	1.3078254425
H	4.7928236434	-2.1973205657	1.233211937
C	-0.5185254201	-5.0328072737	-2.3434404522
H	-1.0004707972	-4.9627692638	-1.3710383511
C	1.7784926522	-2.3717392007	-5.5016088803
H	1.1771274585	-2.8268312035	-6.2816342893
C	-0.7460335082	-6.1156459297	-3.1744758195
H	-1.4070141998	-6.9138282326	-2.8574729761
C	-3.2313751105	-1.9595829261	1.0601922262
H	-4.3047886617	-1.9474521386	0.9095574051
C	-0.1100208965	-6.145557173	-4.4060975404
H	-0.25337665	-6.9804226201	-5.0839420841
C	3.27492474	-0.6800777572	-4.7330273456
H	3.8884485615	0.1999438536	-4.8903844698
C	2.5515103249	-1.2519442342	-5.7662981592
H	2.5752520235	-0.8251726373	-6.7637452939
O	-0.1306491317	-0.6924856035	-2.6128189668
C	-1.2225934298	-0.7268997454	-3.2213161176
O	-2.1129032059	-1.5734352839	-3.2355683555
C	-1.430583997	0.5311929596	-4.1143186775
F	-2.6448795965	0.60016571	-4.6619872819
F	-0.5452308854	0.5438440623	-5.1257485041
F	-1.2492303503	1.6671357316	-3.4254044983



E(UM06) = -1218.76866197

Charge = 0, Multiplicity = 1

Cu	-0.0681515222	-0.5703197628	0.0114103314
N	1.7900332103	-1.3016231534	0.0170557955
C	2.0913116824	-2.602012929	0.0123523488
H	1.2520114655	-3.2902831351	0.0289937524
C	3.3943156328	-3.0680550662	-0.0117441702
H	3.5898711762	-4.1335666761	-0.0142205529
C	4.4226038864	-2.1400949404	-0.0337003742
H	5.4582003693	-2.4619327562	-0.0555624536
C	4.115207689	-0.7897535938	-0.028657397
H	4.9107727345	-0.0550633463	-0.0493818559

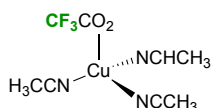
C	2.7831329112	-0.3944294156	-0.0011571776
N	1.0440026848	1.2456935602	-0.020839181
C	2.3658846428	1.0299766787	0.0063823641
C	3.2705197043	2.0845872632	0.0416012812
H	4.3388423171	1.907919905	0.0702083695
C	2.7847546084	3.3831233344	0.0442563692
H	3.4742476248	4.2202287014	0.0719179837
C	1.4165208588	3.5967110142	0.0124549916
H	0.9999039989	4.5971769001	0.0126692146
C	0.5780446756	2.4917597277	-0.0183276543
H	-0.5054531749	2.5860397224	-0.0434751154
O	-1.9637068906	-0.8465116856	0.0337171176
C	-2.7300378107	0.1559951494	-0.0372923548
O	-2.4725076595	1.3446335595	-0.1273303282
C	-4.2197498873	-0.2739422045	0.0083241843
F	-4.5076719923	-1.12596042	-0.9837252924
F	-5.0558249289	0.7548997835	-0.098349404
F	-4.5013690065	-0.8982632147	1.1599652076

[Cu(CH₃CN)₃]⁺

E(UM06) = -932.970559034

Charge = 1, Multiplicity = 2

Cu	-0.6185107628	-0.1178388448	-0.2242299991
N	-0.5895487117	1.6376264193	-1.1686840563
N	-2.105308033	-0.4537645496	1.0596391491
N	0.1143903763	-1.6920420224	-1.2039489496
C	0.614947947	-2.5923009952	-1.7102587277
C	-2.9007178324	-0.641474139	1.8654963853
C	-0.5126076831	2.6651763453	-1.6741436329
C	1.2398347129	-3.7197068805	-2.345032645
H	0.6130529528	-4.0767698349	-3.1644385904
H	2.2144340361	-3.4270215362	-2.7404817954
H	1.373919415	-4.5241092837	-1.6192737504
C	-0.4199838023	3.9492889472	-2.3120236108
H	0.5436363477	4.042030535	-2.8166803204
H	-1.2211347507	4.0543238006	-3.0463062614
H	-0.5119708626	4.7405996041	-1.5656212678
C	-3.8994021675	-0.877639233	2.8712616002
H	-3.5788227834	-1.6907092455	3.5256358234
H	-4.045716219	0.0258055637	3.4663741548
H	-4.8436143223	-1.1510179259	2.3962141764
C	0.877246166	0.184236626	1.07412064
F	1.0607077008	-0.8857231108	1.8527087581
F	0.6186527582	1.2285850373	1.8659009744
F	2.0245910879	0.4279899731	0.4345511255

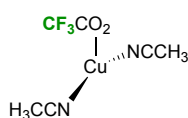


E(UM06) = -1121.742477030

Charge = 0, Multiplicity = 1

Cu	-0.4322072821	-0.0941508838	-0.0469937392
N	-0.5554623788	1.6010247818	-1.0930967674
N	-2.0066978364	-0.425436495	1.1430823399
N	0.1811013743	-1.6768318869	-1.0920046854
C	0.6530063187	-2.5632578576	-1.6511525224
C	-2.8701847374	-0.5883889179	1.8840168611
C	-0.5218084089	2.6022450833	-1.656572516
C	1.2480034874	-3.673093221	-2.3508983848
H	0.8717527362	-3.7145850575	-3.3749481472
H	2.333359872	-3.5566206652	-2.3766388599

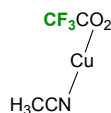
H	1.0038839277	-4.6090863703	-1.8445599438
C	-0.4776884015	3.8572904234	-2.362530069
H	0.53501641	4.0446073447	-2.7251397894
H	-1.1605114871	3.8317038302	-3.2140391013
H	-0.7714922291	4.6709443341	-1.696456407
C	-3.9512925403	-0.7895761203	2.8149762111
H	-3.712466629	-1.6116148407	3.4926020819
H	-4.1116760827	0.1174236036	3.40121076
H	-4.8695014447	-1.0301135136	2.2755154114
O	1.0780271311	0.2362130035	1.412022509
C	2.2422238548	0.5024890655	1.0372252286
O	2.721764703	0.618538677	-0.0854675328
C	3.2016846687	0.7094050158	2.245676349
F	3.2655261031	-0.3948852767	3.0068336783
F	2.7754724296	1.7043008379	3.0398455853
F	4.4515964414	1.0068161058	1.8886834502



E(UM06) = -989.030908474

Charge = 0, Multiplicity = 1

Cu	1.2972584509	-0.1240429484	-0.1648940247
O	-0.7241175355	0.0489364396	-0.803363273
C	-1.4022482137	0.1316251428	0.2465253728
O	-1.0336210999	0.1103759825	1.4179195943
C	-2.9211495751	0.2797246781	-0.0350850695
F	-3.1690345678	1.3695730676	-0.7756210514
F	-3.6556315232	0.3824907203	1.0710402454
F	-3.3863253572	-0.7744344735	-0.7212801504
C	1.8678233918	-3.1077286912	0.0300864556
C	2.3108590942	2.739902174	0.0539273405
C	2.0822453481	-4.5272733342	0.1189950328
H	1.3102870149	-4.9799289302	0.7445195011
H	2.0371556707	-4.9709032073	-0.8776836177
H	3.0616252684	-4.730593662	0.5564662115
C	2.7340605396	4.111054274	0.1540818011
H	3.0729599754	4.4652301995	-0.8215862911
H	1.9017402756	4.733374549	0.4888080294
H	3.5546439611	4.196671596	0.8690899448
N	1.6971844972	-1.9742235045	-0.0412405787
N	1.9745123844	1.6447089278	-0.0264544727



E(UM06) = -856.319746698

Charge = 0, Multiplicity = 1

Cu	0.8662935346	0.0547639739	0.7007321155
O	-0.9558370405	-0.2978775402	0.7841010548
C	-1.6516881161	-0.1787240381	-0.2735701818
O	-1.315684868	0.1482185568	-1.3937825375
C	-3.1370386781	-0.5237139699	-0.0004477922
F	-3.2621481597	-1.7834912567	0.4329803631
F	-3.8933818006	-0.3973228565	-1.0848500457
F	-3.6489417046	0.2749351166	0.9427635282
C	3.7968678648	0.5828069433	0.6902664405
C	5.2103418134	0.8362747602	0.6751532578
H	5.4567178429	1.6012148391	1.4141732082

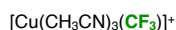
H	5.7525474677	-0.08088184	0.9136659492
H	5.5119378418	1.1840434381	-0.3149693201
N	2.6676440024	0.3797938734	0.70122296



E(UM06) = -1065.69005012

Charge = 1, Multiplicity = 2

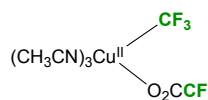
Cu	0.0028300682	-0.0808633392	0.1933526124
C	0.0093939624	-2.0315136453	-0.2497427965
F	0.0112289022	-2.266376234	-1.5810243555
F	-1.0677319732	-2.6850820663	0.2401009077
F	1.0898334194	-2.6782023773	0.2418500699
N	-1.8093246986	0.1467229367	-0.816570255
N	-0.0037965633	1.9429903322	0.6504737566
N	0.0014011335	-0.5341387107	2.2320588768
N	1.8151894038	0.1586696093	-0.8131701809
C	-0.0061814662	3.0618626588	0.9044668248
C	-2.8018899702	0.1738351001	-1.3926474357
C	-0.0036383766	-0.8786820396	3.3270809054
C	2.8087511134	0.1924457746	-1.3871720335
C	-4.0457830384	0.2115212302	-2.1148605876
H	-4.7803812157	0.7970199068	-1.5587892867
H	-3.8912750785	0.6688938583	-3.0939682294
H	-4.4255978869	-0.802894405	-2.2507415744
C	-0.0088466855	4.4650352239	1.2229797836
H	0.9362821112	4.7395699646	1.6952629031
H	-0.136215517	5.051730846	0.3112906137
H	-0.8286531169	4.6879935589	1.908448579
C	-0.0091771989	-1.3068873358	4.7007393255
H	0.994711277	-1.2176465192	5.1202215411
H	-0.6952535014	-0.6862493076	5.280150899
H	-0.3303512125	-2.3484265386	4.7621689659
C	4.0537863775	0.2387622906	-2.1068984911
H	3.8939028725	0.6751322582	-3.0946881762
H	4.7763601522	0.847411515	-1.5600342572
H	4.4518697066	-0.7710655457	-2.2230399047



E(UM06) = -932.970304439

Charge = 1, Multiplicity = 2

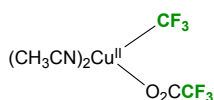
Cu	-0.0778857376	0.1230866127	0.3222159642
N	-0.6630402496	2.0336902856	0.2538418166
N	-1.6861168669	-0.5571284694	1.3459419419
N	0.1171082236	-1.46987546	-0.8697784873
C	0.2867037811	-2.359143754	-1.5744403892
C	-2.582314424	-0.9349599321	1.9547730701
C	-0.939440095	3.1459926908	0.203649132
C	0.4911009036	-3.4718996274	-2.4598676983
H	-0.2318851926	-3.4293611584	-3.2768084169
H	1.501290417	-3.4350143731	-2.8720850338
H	0.3599743874	-4.4076915004	-1.9131442282
C	-1.292027865	4.5371520788	0.1390705205
H	-0.4054718903	5.1322535899	-0.0881400916
H	-2.038492144	4.6917809819	-0.6424685101
H	-1.7043674187	4.857802809	1.0977068977
C	-3.7050272714	-1.4063307582	2.7178700092
H	-3.4912514244	-2.4006574203	3.1145049551
H	-3.9008731218	-0.7234523477	3.5467862478
H	-4.5889722437	-1.4577690629	2.0791288954
C	1.8444520888	0.6083695895	0.1436363684
F	2.6642020211	-0.436540151	0.3474409343
F	2.2193622736	1.5669402191	1.0075390786
F	2.1081192689	1.0735767575	-1.0903529666



E(UM06) = -1459.31846019

Charge = 0, Multiplicity = 2

Cu	0.4965864916	-1.4891009974	-1.7280225349
C	-0.8714578543	-0.6588347703	-2.8976494865
F	-0.9966327354	0.6735807072	-2.6815462771
F	-2.1177483661	-1.1721344122	-2.7237591338
F	-0.6153977917	-0.7940530036	-4.218078074
O	1.9770660774	-0.5318809616	-2.807106477
C	2.7985566716	0.3698157127	-2.5103671571
O	3.7853589319	0.747355898	-3.1269646728
C	2.5697221239	1.1067896907	-1.1571648382
F	1.3633436407	0.8919103277	-0.6192984258
F	3.4772177033	0.6943069913	-0.2547387315
F	2.7124968781	2.4259789807	-1.2828301297
C	-0.0333984563	-4.3847456348	-3.1929614691
C	2.8932865036	-2.4567445096	0.1610085797
C	-1.502167164	-0.9915338834	0.7820222772
C	-0.3011438243	-5.589204571	-3.9350812019
H	0.5131435425	-6.3022310307	-3.7932895184
H	-1.2336453669	-6.0391822563	-3.5893591686
H	-0.3907358879	-5.3569168469	-4.9979596257
C	4.0390124948	-2.766923954	0.9740089256
H	4.626787841	-1.8610518422	1.1378380267
H	3.7161622744	-3.1634725313	1.938362332
H	4.6613345801	-3.5093197457	0.4709130047
C	-2.4280634539	-0.6602863795	1.8332793567
H	-2.531013889	-1.5037145404	2.5185594517
H	-2.0640407675	0.2071511167	2.3871672107
H	-3.4047832426	-0.4257722491	1.4057327645
N	0.182133485	-3.42521677	-2.5996788022
N	1.9819957883	-2.2039647081	-0.4886508718
N	-0.7629172283	-1.2557558268	-0.0556213332

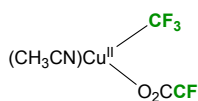


E(UM06) = -1326.60704759

Charge = 0, Multiplicity = 2

Cu	0.2556429261	-0.4107601346	-0.0018742164
C	-0.1835185556	-2.3256247794	0.3430796081
F	0.2297338256	-3.1139130764	-0.6814312148
F	0.4506099571	-2.8049579088	1.4432338068
F	-1.4860368835	-2.6179419847	0.5223654752
O	-1.5439289032	-0.0218714869	-0.7405068159
O	-2.1825789597	0.4642867232	1.3560553788
C	-2.3621182736	0.3293006679	0.1586513915
C	-3.7703325926	0.5998588515	-0.4284448458
F	-4.2630537723	-0.5032806102	-1.0024353963
F	-3.7238862394	1.5519028701	-1.3681134826
F	-4.6404978231	0.9932085762	0.4951905544
C	0.7648860108	2.7264352936	0.1594701743
C	3.3240954333	-1.1758568318	0.0448272613
C	0.9118908677	4.1541397147	0.2484744412
H	-0.0719472932	4.6273182126	0.240397289
H	1.4278831467	4.415871983	1.1741786796
H	1.4924074679	4.5200479044	-0.6005606361
C	4.6980344705	-1.5970422274	0.0760395634
H	5.131135073	-1.5147569032	-0.9227068224
H	5.2628344941	-0.9659708056	0.7647377314

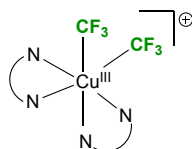
H	4.75812499	-2.6351617395	0.4083649398
N	0.6461781961	1.5877472954	0.0877649872
N	2.2281794372	-0.837937604	0.0177721485



E(UM06) = -1193.88639055

Charge = 0, Multiplicity = 2

Cu	0.1962892064	-0.8643302502	-0.3625014321
C	-0.307554591	-2.6173209809	0.495076227
F	0.3524360509	-3.6345429368	-0.0815218485
F	0.0421384379	-2.6055078313	1.7896429451
F	-1.6094249969	-2.9035826451	0.4328879982
O	-1.4589526442	-0.1117780991	-0.8471037514
O	-2.0321375402	0.1981866379	1.3039506678
C	-2.2251731238	0.2470512924	-0.1084198575
C	-3.5615961583	0.8090244215	-0.4344839801
F	-4.1970167805	-0.1064153953	-1.171454879
F	-3.3450942153	1.8731973119	-1.2144200562
F	-4.3802968666	1.1827114021	0.5401850195
C	3.2213602585	-1.1800760038	-0.1403058415
C	4.6375745569	-1.3712277002	-0.014603219
H	5.1050471934	-1.3070389362	-0.9992670862
H	5.0561751442	-0.5998337166	0.6347048966
H	4.8385285217	-2.353939758	0.4166919158
N	2.0899935469	-1.0234828124	-0.2438394336

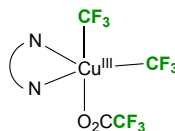


E(UM06) = -1862.77134244

Charge = 1, Multiplicity = 1

Cu	0.0000004468	-0.3466445289	0.0000009048
N	-0.8536983996	1.0546022053	-1.1543503257
C	-0.1048039345	1.7727505393	-1.9956559722
H	0.9430346652	1.4938321564	-2.053180929
C	-0.6255409354	2.8019783094	-2.7556174093
H	0.0198270146	3.3582243434	-3.4241607502
C	-1.9740326804	3.0955906177	-2.6319170892
H	-2.4191718206	3.9033480111	-3.2024298714
C	-2.7496612753	2.3498740289	-1.7625076951
H	-3.8009832323	2.5772803228	-1.6344907044
C	-2.1678360218	1.321025694	-1.0303925949
N	-2.2492926161	-0.1108091138	0.8829069141
C	-2.9491892742	0.4974428049	-0.082868996
C	-4.3256243272	0.3456687644	-0.2065357219
H	-4.8679728541	0.8165821298	-1.018059513
C	-4.992593991	-0.4488415683	0.7122312743
H	-6.0649147596	-0.5910194699	0.6323293851
C	-4.2716984545	-1.0615869507	1.7239215912
H	-4.7553104535	-1.6868584421	2.4651011682
C	-2.89955969	-0.8651496693	1.7646608792
H	-2.2972740231	-1.3341537893	2.5392405569
C	0.42844208	-1.7665144311	1.2892494973
F	0.2859360354	-1.2426262327	2.5145069642
F	-0.3592731835	-2.8415045643	1.2594851198
F	1.6897832938	-2.1757690944	1.1740664544
C	2.1678359015	1.3210308235	1.0303884399
C	0.1048032725	1.7727587094	1.9956492404
C	0.6255396581	2.8019894648	2.7556070649

C	1.9740313467	3.0956017545	2.6319061519
C	2.7496605161	2.3498821996	1.7624998195
H	-0.9430353014	1.4938403139	2.053174646
H	-0.0198287391	3.3582378204	3.4241480409
H	2.4191700073	3.9033614506	3.202416046
H	3.8009823697	2.5772885884	1.6344823393
C	2.9491893957	0.4974445675	0.0828680583
C	4.32562458	0.3456712831	0.2065347747
C	4.9925938714	-0.4488430683	-0.7122289969
H	4.8679735712	0.8165881702	1.0180561824
C	2.8995588997	-0.8651568121	-1.7646551004
C	4.2716977915	-1.0615934041	-1.7239159177
H	6.0649147249	-0.5910203543	-0.6323271139
H	2.2972727573	-1.3341648045	-2.5392320572
H	4.7553094537	-1.686868276	-2.4650928606
N	0.8536982807	1.0546074473	1.1543465913
N	2.249292254	-0.1108121597	-0.8829043912
C	-0.4284422759	-1.7665201138	-1.2892411147
F	0.3592718292	-2.8415109184	-1.2594719114
F	-1.6897838617	-2.1757731147	-1.1740560609
F	-0.2859359125	-1.2426376397	-2.5145010075

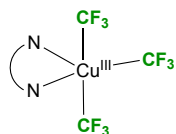


E(UM06) = -1893.94778556

Charge = 0, Multiplicity = 1

Cu	-0.3826894374	-0.7054297645	-0.338826477
N	-0.2139898651	1.1090695777	-1.0796609395
C	0.4668475697	1.3226599318	-2.2074344765
H	0.7514250276	0.4425130894	-2.7758734146
C	0.8011164189	2.5933502627	-2.6319291943
H	1.3609470075	2.7274314852	-3.5490471589
C	0.4032634425	3.6706059184	-1.8547968296
H	0.649530936	4.684284014	-2.1514094574
C	-0.3022814863	3.4437836411	-0.6866982444
H	-0.5969475798	4.2760954972	-0.0599682717
C	-0.5954730823	2.1400214955	-0.3060595353
N	-1.2340733187	0.5165740473	1.3251006052
C	-1.2811223516	1.8059763039	0.9586769498
C	-1.9313316038	2.7608499426	1.7301877117
H	-1.9822584807	3.7952950663	1.412635811
C	-2.5327401184	2.3678841635	2.9152553927
H	-3.0468556542	3.096855811	3.532209104
C	-2.4715531657	1.0382215921	3.295127466
H	-2.9257154125	0.6891805615	4.2147629295
C	-1.8148131904	0.145687848	2.4612488627
H	-1.7501617226	-0.9073063698	2.7214147582
C	-0.5813549406	-2.4314520717	0.5057449913
F	0.0922734557	-2.3426107123	1.655239311
F	-1.831374812	-2.7656709365	0.8289656405
F	-0.0500134246	-3.4133909809	-0.208534889
O	1.5680687636	-0.8381959302	-0.0855242108
C	2.2777190203	0.0721752992	0.4404466172
O	1.9579969449	1.0705423383	1.05424416
C	3.7842733931	-0.1760033555	0.1607793476
F	4.5700639442	0.6331267367	0.8629207201
F	4.1501176216	-1.4300260089	0.4319761232
F	4.0393183944	0.043749119	-1.1384869552
C	-1.9409177842	-1.1348560681	-1.4698276871
F	-3.0287624087	-0.6009130557	-0.9085244226
F	-2.206918793	-2.4130553989	-1.7319742704

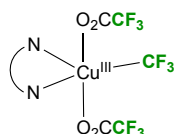
F -1.7723083076 -0.5423060889 -2.6586800675



E(UM06) = -1705.38587253

Charge = 0, Multiplicity = 1

Cu	-0.6986213541	-0.2823872189	0.0000010895
N	1.0567139747	-1.2239801553	0.0000129349
C	1.1219625374	-2.5547534813	0.0000277847
H	0.1749295748	-3.0873088347	0.0000280171
C	2.3299633744	-3.2276998592	0.0000423575
H	2.3469702853	-4.3104815429	0.0000543967
C	3.4964065524	-2.4797344723	0.0000416001
H	4.4642396975	-2.9690661949	0.0000532867
C	3.4205801132	-1.0969780373	0.0000261244
H	4.327284327	-0.5052115857	0.0000262786
C	2.1754809393	-0.4814432009	0.0000117245
N	0.7258464598	1.416212636	-0.0000057411
C	1.9942546796	0.9893273035	-0.000005018
C	3.0576698065	1.8840058701	-0.0000206705
H	4.0841955144	1.538317702	-0.0000210898
C	2.7855156278	3.2432721027	-0.0000373922
H	3.6004321486	3.9591240015	-0.0000504629
C	1.469259088	3.6752407548	-0.0000376265
H	1.2186061945	4.7293265955	-0.0000504431
C	0.4655029475	2.718329229	-0.0000213216
H	-0.5847831472	3.0002967167	-0.0000209112
C	-0.7026626351	-0.3068329595	-1.9863085471
C	-2.6127424401	0.1329083438	-0.0000129932
C	-0.7026795883	-0.306801931	1.9863110164
F	-1.2181429633	-1.4495197231	-2.4842399784
F	0.5498126637	-0.2332975035	-2.4940373811
F	-1.3664512059	0.7103979627	-2.5675186922
F	-2.7288269492	1.4766515484	-0.0000545533
F	-3.2997519234	-0.310533642	-1.0621397328
F	-3.2997583486	-0.3104663319	1.0621371435
F	-1.3664382793	0.7104654663	2.5674926481
F	-1.2182049579	-1.4494597794	2.4842612145
F	0.5497932859	-0.2332997793	2.4940509378

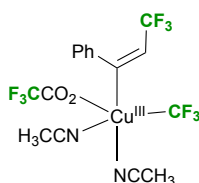


E(UM06) = -2082.50075338

Charge = 0, Multiplicity = 1

Cu	0.0000433789	-0.0822957401	-0.5060192517
N	0.0000195755	0.5317742763	1.3390032175
C	0.0000429457	-0.2888193462	2.3860295971
H	0.0001054984	-1.3527007768	2.1660702859
C	-0.0000126155	0.2001265652	3.6805705087
H	0.0000084159	-0.4867902623	4.5175598729
C	-0.0000967557	1.5736756374	3.8670506463
H	-0.0001434485	1.9903695252	4.8681521115
C	-0.0001227336	2.4184536171	2.768304356
H	-0.0001892473	3.4926090773	2.9058057174
C	-0.0000634436	1.8645507052	1.4971356115
N	-0.0000185901	1.9023646929	-0.8948914196
C	-0.0000781678	2.6317181155	0.2446512271

C	-0.0001394083	4.0165519788	0.2083047713
H	-0.0001881897	4.5866450721	1.1290840714
C	-0.0001369319	4.6651821618	-1.0152423614
H	-0.0001847964	5.748487584	-1.0580707678
C	-0.0000709256	3.9114318506	-2.1744801515
H	-0.0000637638	4.3720039069	-3.1545139101
C	-0.0000134134	2.5308925132	-2.0702204613
H	0.000037549	1.9206971337	-2.9640565402
C	0.0000763563	-0.6971915378	-2.3300180371
F	-1.0795024643	-0.2221437013	-2.9284178238
F	1.0796799484	-0.2221357249	-2.9283655104
F	0.0000797478	-2.0011594604	-2.3905922656
O	-1.5394334108	-1.3277211093	-0.2223436053
C	-2.6338239438	-0.7142126921	-0.0181123131
O	-2.8874022354	0.4694889981	-0.1174850268
C	-3.7349337856	-1.6865802033	0.4779676494
F	-4.931676491	-1.1141263606	0.5135732873
F	-3.8259370413	-2.7731095767	-0.2885728266
F	-3.4414753835	-2.0922209301	1.7210961907
O	1.5394655351	-1.3277417239	-0.2222954521
C	2.6338954418	-0.714249928	-0.0182121298
O	2.8875087532	0.4694286458	-0.1177495516
C	3.7350010244	-1.6866081342	0.4778941075
F	3.8259521909	-2.7731825257	-0.2885894436
F	3.4415793716	-2.0921712442	1.7210552402
F	4.9317554538	-1.1141760794	0.5134223796

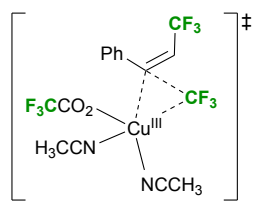


E(UM06) = -1972.49499366

Charge = 0, Multiplicity = 1

N	-2.2426333682	0.5139209908	-1.1791790873
C	-3.1966044019	0.8888856061	-1.6917521841
C	-4.3931684719	1.3614877922	-2.3338651037
H	-5.1553159936	1.5755884966	-1.5822327856
H	-4.1751559098	2.2743421597	-2.8916069084
H	-4.770575376	0.6020036381	-3.0210771377
O	-0.2754583002	2.9238957722	-1.2768852292
C	-0.3656882903	2.8021263224	-0.0710189442
O	-0.4668837918	1.7556233189	0.6405212244
C	-0.3655287002	4.0760112837	0.8153983204
F	-1.5011107487	4.1691192351	1.518036348
F	-0.2454887968	5.1890658319	0.1001701753
F	0.6445819208	4.0522648967	1.6927548347
Cu	-0.5201866183	0.0316648965	-0.2820200573
C	1.3445299873	-0.2142809594	0.1797043708
C	1.5854323244	-0.9501227056	1.2485252512
C	2.1759326476	0.7178757962	-0.5628583006
H	0.8045997523	-1.5142574648	1.7506769978
C	2.9238377138	-1.1067499199	1.8894080209
C	2.6688730818	1.8457774681	0.1073373717
C	2.4663110715	0.5461528184	-1.9198264169
F	3.9536194374	-0.8559733148	1.0809635422
F	3.0589235933	-0.299104887	2.9571381458
F	3.0772159555	-2.3604678179	2.3430644103
C	3.4419137858	2.7753763639	-0.5656256869
H	2.4309841176	1.9844500661	1.1579407572
C	3.2437501141	1.4793840664	-2.5854783858
H	2.0821963579	-0.3195821825	-2.4466166658

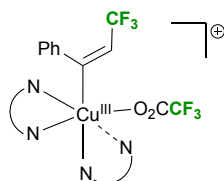
C	3.7277439286	2.5963789784	-1.9144434756
H	3.8195248709	3.6452561439	-0.0374444482
H	3.4706405384	1.337042437	-3.6371468846
H	4.3282247051	3.32938566	-2.4438470473
C	-0.3804098571	-1.7515133809	-1.0969710719
F	0.1021966481	-2.735642258	-0.3381244633
F	0.3176237866	-1.7507471767	-2.2427020267
F	-1.6314853213	-2.1223850318	-1.4147357099
C	-3.1022655753	-1.633237142	3.6473759667
H	-3.5318311369	-2.6237080363	3.4856051721
H	-3.9097890685	-0.920330853	3.8246126419
H	-2.4583123266	-1.6653487226	4.5283436931
C	-2.3366494309	-1.2333867495	2.4930382816
N	-1.7250588544	-0.9143264367	1.5724404948



E(UM06) = -1972.48620155
Charge = 0, Multiplicity = 1

N	-2.3447039716	0.1572667794	-1.1580402377
C	-3.3573159122	0.3743846334	-1.6509729046
C	-4.6259614793	0.6483057931	-2.2717428268
H	-4.7471145593	1.725309183	-2.403157437
H	-4.6732631928	0.1619535884	-3.2479489065
H	-5.4359984564	0.2714096917	-1.6445609753
O	-0.2902082013	2.7192691722	-1.4263686114
C	-0.3356697673	2.7159107575	-0.2068226274
O	-0.4750461385	1.7524869195	0.5972919843
C	-0.2252440603	4.073455733	0.5363677486
F	-1.3872441005	4.3766597528	1.1341713123
F	0.07688828	5.0808081573	-0.2781303681
F	0.712176161	4.0396629743	1.4905967902
Cu	-0.5462843524	-0.0517744864	-0.2886739443
C	1.3058839502	-0.5425290501	-0.0248504811
C	1.5147996657	-1.3076106849	1.0416647453
C	2.1645293573	0.4591854264	-0.659658806
H	0.7417067574	-1.9680928137	1.4236838625
C	2.7898998836	-1.3791943191	1.8126889554
C	2.5868121394	1.5382958532	0.1263269703
C	2.5378220921	0.4105292264	-2.005187729
F	3.8784553053	-1.1274248672	1.0843168778
F	2.8056012557	-0.5232805347	2.8492004154
F	2.9398027802	-2.6063443968	2.3323621496
C	3.3766075418	2.5361201515	-0.419133957
H	2.2702606763	1.5992149799	1.1630430222
C	3.3302077977	1.4119886479	-2.5432475166
H	2.2216632019	-0.4121169804	-2.6362852387
C	3.7493670675	2.4768239586	-1.7560291078
H	3.6935244202	3.3685303985	0.2012935342
H	3.6192297697	1.3607846221	-3.5879804893
H	4.361769565	3.2629191311	-2.186071521
C	0.165168622	-1.6823400579	-1.3740651333
F	-0.6948134519	-2.5835626278	-0.8984545603
F	1.2860526981	-2.3583442397	-1.6525813187
F	-0.2737201166	-1.2417354303	-2.5597021513
C	-2.8684494915	-1.4130074963	3.7915197394
H	-3.4169579999	-0.5216400869	4.1021033307
H	-2.1593180089	-1.6835122389	4.5762152199
H	-3.5742998176	-2.2340469918	3.6524447935

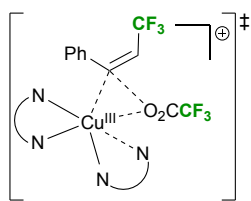
C	-2.1646741745	-1.1528032123	2.5605649342
N	-1.6022627351	-0.9452700161	1.5790614632



E(UM06) = -2359.59643366
Charge = 1, Multiplicity = 1

Cu	0.3680075727	-0.2002623104	-0.4113244138
N	-0.9209734929	-1.4208794751	-1.5554286268
C	-0.6033965058	-2.70614208	-1.7274838501
H	0.3038536723	-3.0485861602	-1.2406844326
C	-1.3676317075	-3.5863416036	-2.4719905349
H	-1.064676829	-4.6222390192	-2.565516452
C	-2.5075594878	-3.100186722	-3.0895910951
H	-3.1313528683	-3.7482296158	-3.6957539698
C	-2.8335017908	-1.7647728233	-2.9344844256
H	-3.7009310261	-1.3577540586	-3.4395769904
C	-2.0286160081	-0.9431283303	-2.1499538064
N	-1.3760608623	1.2838040721	-1.5452569042
C	-2.3674478237	0.4866691467	-1.9478121604
C	-3.6618412206	0.9635641194	-2.1499731479
H	-4.4673809211	0.2947278846	-2.4301571908
C	-3.9163647075	2.3110448527	-1.9595371249
H	-4.9162054105	2.7040837877	-2.1114188639
C	-2.8820432227	3.141369867	-1.5582595689
H	-3.0356504284	4.2019294313	-1.3954789172
C	-1.6339442223	2.5742259315	-1.3521565951
H	-0.8020519208	3.1875881695	-1.0094673872
C	-0.500844789	-0.2520269504	1.4965552015
C	0.2892192784	-0.7617075479	2.4279148659
C	-1.9247139909	-0.1551877423	1.3323025922
H	1.368889559	-0.6713459302	2.3914838078
C	-0.2497624277	-1.4962264649	3.6141728033
C	-2.6285106574	-1.3356653008	1.0492381357
C	-2.6182146067	1.0427828639	1.5444886663
F	-1.4106086482	-1.0164554217	4.0603852161
F	-0.4442572061	-2.8007342007	3.3517696616
F	0.6247620977	-1.4320680604	4.6217260656
C	-4.0106009257	-1.3191275087	1.0082082451
H	-2.0802894973	-2.2590261574	0.8808905117
C	-3.9987592752	1.0500414488	1.4778621315
H	-2.0640381095	1.9498226539	1.760434658
C	-4.694925153	-0.1261873188	1.2141024887
H	-4.5555805481	-2.2353778477	0.8070471173
H	-4.5399763884	1.9764973515	1.6395521354
H	-5.7792634327	-0.1118124188	1.1687345197
C	3.0427441068	-0.1280473659	-1.6784473846
C	1.7376756753	1.6167871775	-2.4388677836
C	2.7965187433	2.1813981062	-3.1304778815
C	4.0271072883	1.5487943653	-3.074293231
C	4.1535763918	0.3801425176	-2.3415933908
H	0.7499542382	2.0670926574	-2.4508789937
H	2.6526709203	3.0955096236	-3.693932072
H	4.8859486905	1.9611424439	-3.592770712
H	5.113636694	-0.1172027571	-2.2795556951
C	3.0920219061	-1.3698912796	-0.8742775184
C	4.1827878542	-2.233916885	-0.9007648232
C	4.1540481842	-3.384120522	-0.1313544857
H	5.0436669498	-2.0215841438	-1.5227935359

C	1.9922055136	-2.7423736662	0.6125100809
C	3.0366030639	-3.6503720846	0.6438996495
H	4.9954850605	-4.0683816647	-0.143342488
H	1.09110718	-2.9158424074	1.1991557004
H	2.9676353351	-4.5405817561	1.2574140632
N	1.8552345852	0.4959483935	-1.7293106158
N	2.0142059974	-1.6314171625	-0.1206134651
O	0.2291326857	1.4179937586	0.8417597589
C	1.3329637464	1.884507611	1.3300599459
O	2.3380154036	1.305309879	1.6494375926
C	1.2426079254	3.4290341949	1.4273989412
F	1.321036438	3.9517978777	0.1967658753
F	2.2311945404	3.9286188751	2.1488846077
F	0.0895248139	3.8246757023	1.9618484954

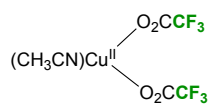


E(UM06) = -2359.59643029

Charge = 1, Multiplicity = 1

Cu	0.4295729358	-0.1017254609	-0.4285331758
N	-0.6741745248	-1.0266291376	-1.969231869
C	-0.2785598381	-2.2199200719	-2.4185514004
H	0.5992354132	-2.6474441001	-1.9448928134
C	-0.9303981891	-2.908172456	-3.4258359467
H	-0.5688511155	-3.8798512217	-3.7401445571
C	-2.0354613723	-2.3153529261	-4.0133619256
H	-2.570547224	-2.8101499137	-4.8167305192
C	-2.4391969432	-1.068747083	-3.5700154499
H	-3.2777829611	-0.5708427363	-4.0415594012
C	-1.7472073025	-0.4461241932	-2.5347400239
N	-1.2533293981	1.5884220613	-1.3663861644
C	-2.1714293721	0.8812257827	-2.0276394775
C	-3.4690350868	1.3527654964	-2.2210776345
H	-4.2166362393	0.745073025	-2.7178406331
C	-3.8038494669	2.6069561634	-1.7399116268
H	-4.8080262736	2.9940839872	-1.8778004574
C	-2.8444175715	3.3489650576	-1.0695857975
H	-3.061944954	4.3352301111	-0.6760421184
C	-1.5881224772	2.7878875658	-0.8992191603
H	-0.8139525021	3.3293112854	-0.3575770348
C	-0.6289445291	-0.6455523206	1.3050583038
C	0.0952153486	-1.3430763709	2.1650768976
C	-2.0316820308	-0.5491869378	1.0129301973
H	1.1670734507	-1.2132447698	2.2636325469
C	-0.5049155082	-2.3607610228	3.0820696469
C	-2.6386903073	-1.6368395777	0.3665061896
C	-2.8074430673	0.534216568	1.4441397884
F	-1.7544433636	-2.0830681256	3.4515848614
F	-0.5260564772	-3.5848227908	2.5260565947
F	0.2305281641	-2.4560964886	4.1935511292
C	-4.0087327596	-1.6490111192	0.1808749184
H	-2.0268920815	-2.4701418962	0.0302510277
C	-4.1732725125	0.5193023827	1.2324732485
H	-2.3277586257	1.3708153226	1.9407144692
C	-4.7744226801	-0.5688381253	0.6061965201
H	-4.4802785936	-2.4975802739	-0.3034939386
H	-4.7779833271	1.3571972291	1.5635356806
H	-5.8482606648	-0.573875397	0.4484220358
C	3.2269244464	0.3619652615	-1.2736298046

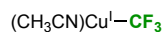
C	1.9176091844	2.1970710954	-1.7662045108
C	3.0181805951	2.9543015109	-2.1319677069
C	4.271419091	2.3709888242	-2.0487196172
C	4.3792716234	1.0590690724	-1.6171024837
H	0.9106916029	2.599136488	-1.8185684192
H	2.8881171736	3.9755396911	-2.4694955719
H	5.1615690038	2.930959925	-2.3143413554
H	5.3545679719	0.5948236735	-1.5369998709
C	3.2517982822	-1.0427921512	-0.8079802303
C	4.3876615936	-1.8411579192	-0.9031368759
C	4.3327319163	-3.1513554763	-0.4602005868
H	5.3045769698	-1.4528584498	-1.3293072197
C	2.0601574924	-2.7815918223	0.1208310579
C	3.1456624583	-3.638558957	0.0634694115
H	5.2087457514	-3.7870146409	-0.5299826625
H	1.1052643622	-3.1237504185	0.5176144848
H	3.0552308752	-4.658478324	0.4172599821
N	2.0166460091	0.9382696439	-1.3430405876
N	2.1062293401	-1.5187767594	-0.2988535963
O	0.0685804739	1.1562493052	1.1525556033
C	1.0847534062	1.5249619291	1.8635147161
O	2.081875933	0.9170178532	2.1535581107
C	0.8987760185	2.9986078456	2.3089518685
F	1.09529432	3.8027599035	1.2558717098
F	1.7663538169	3.3348106902	3.2481500314
F	-0.3290776831	3.2276746842	2.7687231927



E(UM06) = -1382.44298387

Charge = 0, Multiplicity = 2

Cu	0.3260837312	-0.3915615834	-0.1549333126
O	0.4169179504	1.4572014709	-0.3033934112
O	1.205600923	1.6835755932	1.7850153758
C	0.8528200824	2.1110733346	0.7115433635
C	0.8977239994	3.6281064647	0.4124689706
F	-0.3134223613	4.0810301759	0.0835376176
F	1.7168958389	3.8795059067	-0.6112246453
F	1.3246789076	4.3215146614	1.4572482459
C	3.3335076622	-1.1260116271	0.0115256346
C	4.725896094	-1.4653955576	0.0796984695
H	5.1650400452	-1.4061708945	-0.9181621441
H	5.2417204146	-0.7686963616	0.7432487175
H	4.8377525054	-2.481250538	0.4633931312
N	2.2218033379	-0.8549404611	-0.0448733983
O	-0.4638840657	-2.0679305179	-0.047462424
C	-0.251662099	-2.896780888	-1.0043891314
O	0.39467641	-2.7333840662	-2.0116710621
C	-0.9485559471	-4.2493568815	-0.7250684333
F	-2.2574050611	-4.0793916575	-0.5322858766
F	-0.4456016299	-4.8124048785	0.3765068905
F	-0.7891827382	-5.1000636944	-1.7280265778

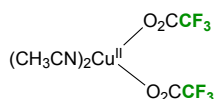


E(UM06) = -667.747922302

Charge = 0, Multiplicity = 1

Cu	0.9035671747	0.0616466945	0.7150405152
C	3.8697155962	0.5953240687	0.6993823659
C	5.2842152242	0.8454131407	0.6897761979
H	5.5210230629	1.6570924386	1.3804433651
H	5.8204737855	-0.0545681249	0.9971052846
H	5.6027540986	1.1263621293	-0.3160847936

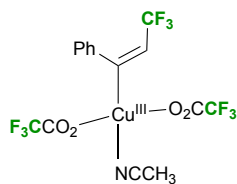
N	2.7397650698	0.3947267285	0.7063774394
C	-0.9809063243	-0.2850312054	0.7235221105
F	-1.7753250964	0.8219076273	0.5611478759
F	-1.4580820697	-0.855042494	1.8769554033
F	-1.4163195214	-1.1383190033	-0.2588887642



E(UM06) = -1515.17595483

Charge = 0, Multiplicity = 2

Cu	0.3266709817	-0.3769633876	-0.2060077388
O	-1.5108897386	-0.0206327892	-0.7504473815
O	-1.8860114818	0.156299674	1.4498938312
C	-2.2275698176	0.1595627835	0.2817736664
C	-3.7087546292	0.4167616958	-0.0864223236
F	-4.2146268655	-0.611812141	-0.7716867109
F	-3.8210851321	1.5057446951	-0.8547591879
F	-4.4676896466	0.600929556	0.9864009419
C	0.8024030433	2.7116495345	-0.1031606205
C	3.3287747908	-1.1128489161	0.2682671473
C	0.9544204088	4.1390761958	-0.0544857462
H	-0.0288770689	4.6133946762	-0.0651858078
H	1.4815448725	4.4226047776	0.8584546947
H	1.5267965678	4.4779274673	-0.9201533082
C	4.6919568319	-1.5146311132	0.4763273769
H	5.1601850271	-1.733859584	-0.4852403877
H	5.2431675137	-0.7123750626	0.970341267
H	4.7195804247	-2.4095025529	1.1009659805
N	0.6789787335	1.57294548	-0.1422451955
N	2.2406145279	-0.7941940211	0.1016107853
O	-0.1064935543	-2.2691830686	-0.0333118634
C	0.042129018	-2.8404768568	-1.1571925924
O	0.412691498	-2.3549567429	-2.2098163588
C	-0.3045698084	-4.3469938415	-1.083932308
F	-0.1655205797	-4.9518676095	-2.2568528082
F	0.4924694619	-4.970286248	-0.2091146521
F	-1.5640853789	-4.5277456009	-0.6788126996

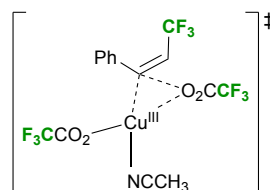


E(UM06) = -2028.33292410

Charge = 0, Multiplicity = 1

N	-2.1995547865	0.6039955419	-1.1456138254
C	-3.25180496	0.7841328671	-1.5645623945
C	-4.5704861336	1.010021621	-2.0902769565
H	-5.3171070057	0.6326810698	-1.3889210004
H	-4.7288455055	2.0793578597	-2.2421219833
H	-4.6805848084	0.4916093259	-3.0446478035
O	-0.1041898005	3.0085249904	-1.3691723021
C	-0.231954509	2.9392613474	-0.1661214631
O	-0.3031838184	1.8998428347	0.5751892389
C	-0.3070533948	4.2334269439	0.6825494688
F	-1.4125516903	4.2560428248	1.4287656332
F	-0.3041874291	5.3201525342	-0.0760472758
F	0.74091672	4.3092933781	1.5093239096
Cu	-0.3196738203	0.2989567938	-0.4550021678
C	1.5366420497	0.0363008571	0.1850493477

C	1.5574259079	-0.8433944257	1.1552083625
C	2.3857145536	0.9407180261	-0.5109364847
H	0.6678978213	-1.345167968	1.5273549413
C	2.8175390508	-1.2746160312	1.8396820838
C	2.847903933	2.0881840184	0.1602291549
C	2.7302931477	0.7243364851	-1.8556191178
F	3.917828076	-0.7414805075	1.318536261
F	2.7823509639	-0.9406081157	3.1357799649
F	2.9467818578	-2.6044971309	1.7834668774
C	3.6547866748	2.9891527177	-0.502990427
H	2.5689773295	2.2416744156	1.1981474236
C	3.5355072309	1.6366658905	-2.5075982218
H	2.3522184932	-0.1505398751	-2.3736909271
C	3.9915897619	2.7682236327	-1.8366734343
H	4.0226531393	3.8689791724	0.0138151573
H	3.8071462098	1.4736845978	-3.5446687673
H	4.6164630702	3.4860034087	-2.3582885106
O	-0.2217387662	-1.4631671181	-1.1453695322
C	-0.1643614501	-1.5330375061	-2.4196930754
O	-0.0341822099	-0.6395492187	-3.2273656623
C	-0.2690432051	-3.004243295	-2.8946841717
F	-1.4019442388	-3.5640531697	-2.4648081611
F	0.7470275811	-3.7255929787	-2.4148728978
F	-0.24553704	-3.0960698142	-4.2166642612



E(UM06) = -2028.31623784

Charge = 0, Multiplicity = 1

N	-0.5777070188	-2.5103703127	-1.1766059561
C	-0.846297299	-3.5645355859	-1.5420886377
C	-1.1839077349	-4.8851331412	-1.9992202805
H	-1.3676832533	-5.5360602313	-1.1422242469
H	-2.0830600202	-4.8437616606	-2.6169495878
H	-0.3617398265	-5.2937747632	-2.5897465355
O	1.8004276217	-1.9095460024	1.273511684
C	2.3869549432	-1.347220069	0.3645894643
O	1.9059018524	-0.6837264083	-0.6016495375
C	3.9348234364	-1.3610575402	0.3458119929
F	4.4138710455	-1.7163443717	-0.8482226437
F	4.4475969023	-2.1892076187	1.2481697131
F	4.401778179	-0.1325584665	0.6149039788
Cu	-0.0580202872	-0.7012335498	-0.509715979
C	-0.2984871159	1.3188275592	-0.1701701485
C	-0.3322164076	1.872819561	-1.3698906954
C	0.1921072457	1.6155178082	1.1433209623
H	-0.7658467983	1.3767073409	-2.2327814436
C	0.2558834976	3.2189655884	-1.6467899933
C	1.5808916794	1.7392097321	1.3067974848
C	-0.6671554074	1.8248591249	2.2302971175
F	0.3269734817	3.9997879887	-0.5706720011
F	1.4956029698	3.1157455757	-2.1448499538
F	-0.4788225713	3.858926331	-2.5616183032
C	2.0972814472	2.0811208754	2.541933927
H	2.2339325789	1.5652957044	0.4577060731
C	-0.1352945472	2.155976609	3.4621409126
H	-1.7380482941	1.7293987688	2.0946752547
C	1.2416348663	2.2825011471	3.61961702
H	3.1699655031	2.1830911645	2.6672276973

H	-0.7958468854	2.3207248791	4.3064681809
H	1.650505362	2.5402923143	4.5913020869
O	-1.7404455091	0.145603282	0.1329993371
C	-2.7473456887	0.142198857	-0.6995209666
O	-2.7218071503	0.0876991137	-1.8969173456
C	-4.0742835917	0.2485479454	0.0882154741
F	-4.1911203223	-0.7523652644	0.957325079
F	-5.1155235937	0.2207458379	-0.7245997477
F	-4.1041427592	1.3933819768	0.7724456429