Electronic Supplementary Information

The Lewis Superacidic Aluminum Cation: $[(NHC)Al(C_6F_5)_2]^+$

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Table of Contents

General Considerations

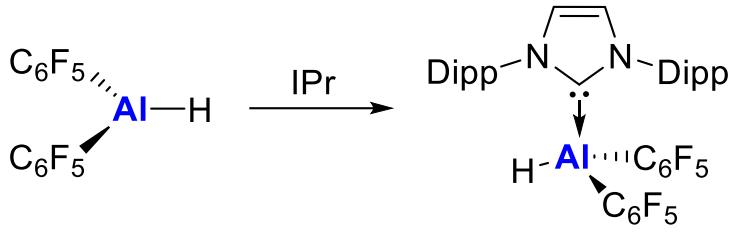
All experiments were carried out under inert gas atmosphere by using Schlenk-type glassware or in an Ar-filled glove box. Toluene, n-hexane and Deuterated solvents (C_6D_6) were dried with sodium/potassium alloy prior to use and stored with 3Å molecular sieves. C_6H_5F was dried by refluxing with CaH_2 and stored with 3Å molecular sieves. 1,2-dichlorobenzene ($C_6H_4Cl_2$) was stored with 3Å molecular sieves. All solvents were stored under argon atmosphere.

$[HAl(C_6F_5)_2]_2$[S1], ^{i}Pr-NHC[S2](IPr) and Cp*Al[S3] were synthesized according to the literature methods. NMR spectra were recorded on a Bruker Advance 500 (^{1}H: 500 MHz, ^{13}C: 125 MHz, ^{19}F: 470 MHz, ^{11}B: 160 MHz) spectrometer at 298 K. Data are presented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), integration, coupling constant in hertz (Hz).

HRMS were recorded on a Thermo Scientific TM Q-Exactive PlusTM mass spectrometer. Single-crystal X-ray diffraction data were collected on a Bruker D8 QUEST diffractometer using Cu (60W, Diamond, μKα = 12.894 mm^{-1}) micro-focus X-ray sources. Using Olex2[S4], the structure was solved with the XT[S5] structure solution program using Intrinsic Phasing and refined with the XL[S6] refinement package using Least Squares minimization.

Experimental Procedures

Synthesis of compound 1



Scheme S1-1：Synthesis of 1

In the glovebox, a toluene solution (5 mL) of $[HAl(C_6F_5)_2]_2$ (362 mg, 1 mmol) was added dropwise into a toluene solution (5 mL) of IPr (388 mg, 1 mmol) at room temperature and the reaction mixture was stirred for 30 min. After removing the solvent under vacuum, the resulting solid was washed with hexane (3×2 mL). After evaporation to dryness, **1** was obtained as white solids (675 mg, 90% yield). **NMR** data of compound **1** were obtained from a solution of the isolated colorless solid in toluene. **Single crystals** (colorless) suitable for X-ray analysis were obtained from the toluene solution at room temperature for 2 hours.

^{1}H NMR (500 MHz, C_6D_6, ppm): δ 0.84 (d, *J*=6.8 Hz, 12H, CH(C*H*$_3$)$_2$), 1.20 (d, *J*=6.8 Hz, 12H, CH(C*H*$_3$)$_2$)，2.74 (sept, *J*=6.8 Hz, 4H, C*H*(CH$_3$)$_2$), 4.35 (s, 1H, Al*H*), 6.48 (s, 4H, N-C*H*-), 6.86 (d, *J*=7.8 Hz, 4H, Ar-*H*), 7.06 (t, *J*=7.8 Hz, 2H, Ar-*H*).

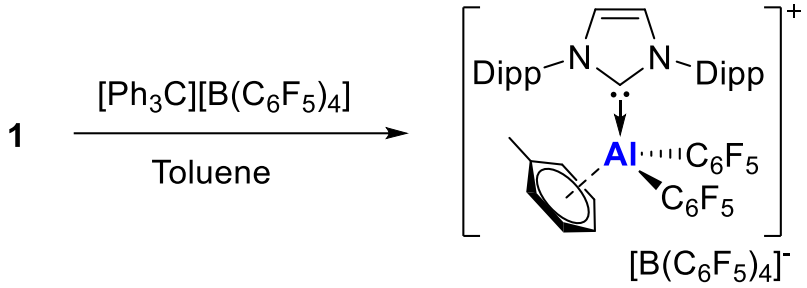
^{13}C{^{1}H} NMR (125 MHz, C_6D_6, ppm): IPr: δ 21.6, 26.4 (CH(*C*H$_3$)$_2$), 28.9 (*C*H(CH$_3$)$_2$), 124.1 (Ar*C*), 125.6 (Ar*C*), 128.3 (Ar*C*), 131.2 (Ar*C*), 133.7 (-N-*C*H-), 145.7 (N*C*N); Al(C_6F_5)$_2$: δ 137.8-135.9 (m, *m*-C_6F_5), 142.0-140 (m, *p*-C_6F_5), 150.9-148.9 (m, *o*-C_6F_5).

$^{19}F\{^1H\}$ NMR (470 MHz, C_6D_6, ppm): δ -118.4 (m, *o*-C_6F_5), -155.8 (tm, *p*-C_6F_5), -162.6 (m, *m*-C_6F_5).

HRMS(m/z): $[M]^-$ calcd. for $C_{39}H_{37}AlF_{10}N_2^-$, 750.2617; found: 750.2588.

FT-IR (solid, cm^{-1}): 2962.83, 1831.39(Al-H), 1638.04, 1508.39, 1437.32, 1054.24, 953.60, 646.46.

Synthesis of compound 2



Scheme S1-2: Synthesis of 2

In the glovebox, a toluene solution (5 mL) of $[Ph_3C][B(C_6F_5)_4]$ (461 mg, 0.5. mmol) was added dropwise into a toluene solution (5 mL) of **1** (375 mg, 0.5 mmol), and the reaction mixture was stirred at room temperature for 1 h. n-Hexane (15 mL) was slowly added into the solution while stirring. The precipitate was collected and washed with n-Hexane (3×2.0 mL). After drying under vacuum, white solids of **2** (684 mg, 90% yield) were obtained.

NMR data of compound **2** were obtained from a solution of the isolated colorless solid in a mixed solvent of C_6D_6 and 1,2-dichlorobenzene. **Single crystals** (colorless) suitable for X-ray analysis were obtained by storing a toluene solution of **2** at -30 °C for 2 hours.

^1H NMR (500 MHz, C_6D_6+1,2-dichlorobenzene, ppm): δ 0.87 (d, *J*=6.7 Hz, 12H,

CH(CH_3)$_2$), 0.98 (d, *J*=6.7 Hz, 12H, CH(CH_3)$_2$)，2.12 (s, 3H, PhCH_3)，2.48 (sept, *J*=6.7 Hz, 4H, C*H*(CH$_3$)$_2$), (6.5-7.11 were overlap with 1,2-dichlorobenzene).

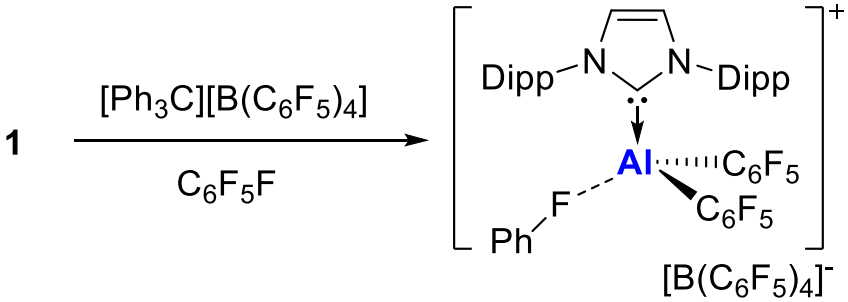
^{13}C{^{1}H} NMR (125 MHz, C_6D_6+1,2-dichlorobenzene, ppm): IPr: δ 21.3, 26.6 (CH(*C*H$_3$)$_2$), 29.2 (*C*H(CH$_3$)$_2$), 125.4 (Ar*C*), 127.6 (Ar*C*), 128.5 (Ar*C*), 130.4 (Ar*C*), 133.4 (-N-*C*H-), 146.0 (N*C*N); Tol: δ 21.5 (C_6H_5-*C*H$_3$); Al(C_6F_5)$_2$ and [B(C_6F_5)$_4$)]$^-$ not listed.

^{11}B{^{1}H} NMR (160 MHz, C_6D_6+1,2-dichlorobenzene, ppm): δ -17.3 [*B*(C_6F_5)$_4$]$^-$.

^{19}F{^{1}H} NMR (470 MHz, C_6D_6+1,2-dichlorobenzene, ppm): Al(C_6F_5)$_2$: δ -119.5 (m, *o*-C_6F_5), -146.8 (tm, *p*-C_6F_5), -159.6 (m, *m*-C_6F_5); [B(C_6F_5)$_4$]$^-$: δ -132.8 (m, *o*-C_6F_5), -163.5 (t, p-C_6F_5), -167.5 (m, *m*-C_6F_5).

HRMS(m/z): [M]$^+$ calcd. for $C_{46}H_{44}AlF_{10}N_2^+$, 841.3155; found: 841.3157.

Synthesis of compound 3



Scheme S1-3: Synthesis of 3

In the glovebox, a fluorobenzene solution (5 mL) of [Ph$_3$C][B(C_6F_5)$_4$] (461 mg, 0.5. mmol) was added dropwise into a fluorobenzene solution (5 mL) of **1** (375 mg, 0.5 mmol) and the reaction mixture was stirred at room temperature for 1 h. n-Hexane (15 mL) was slowly added into the solution while stirring. The

precipitate was collected and washed with n-Hexane (3×2.0 mL). After drying under vacuum, white solids of **3** (685 mg, 90 % yield) were obtained.

NMR data of compound **3** were obtained from a solution of the isolated colorless solid in mixed solvents C_6D_6 and fluorobenzene. **Single crystals** (colorless) suitable for X-ray analysis were obtained by storing a fluorobenzene solution of **3** at -30 °C for 1 hours.

^{1}H NMR (500 MHz, C_6D_6+fluorobenzene, ppm): δ 0.90 (d, *J*=6.7 Hz, 12H, CH(C*H*$_3$)$_2$), 1.01(d, *J*=6.7 Hz, 12H, CH(C*H*$_3$)$_2$), 2.57 (sept, *J*=6.8 Hz, 4H, C*H*(CH$_3$)$_2$), (6.5-7.2 were overlap with fluorobenzene).

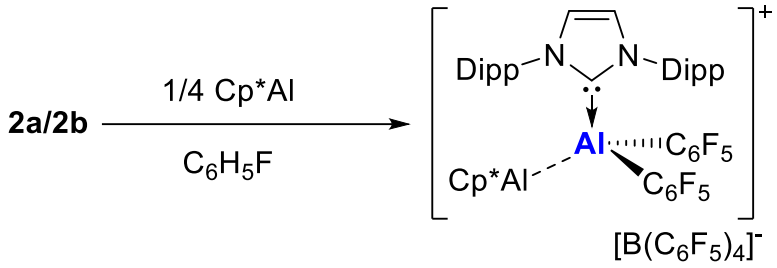
^{13}C{^{1}H} NMR (125 MHz, C_6D_6+fluorobenzene, ppm): IPr: δ 21.3, 26.1 (CH(*C*H$_3$)$_2$), 29.3 (*C*H(CH$_3$)$_2$), 125.1 (Ar*C*), 128.5 (Ar*C*), 128.7 (Ar*C*), 131.6 (Ar*C*), 132.9 (-N-*C*H-), 146.2 (N*C*N); fluorobenzene was overlap with fluorobenzene; Al(C_6F_5)$_2$ and [B(C_6F_5)$_4$)]$^-$ not listed.

^{11}B{^{1}H} NMR (160 MHz, C_6D_6+fluorobenzene, ppm): δ -15.9 [*B*(C_6F_5)$_4$)]$^-$.

^{19}F{^{1}H} NMR (470 MHz, C_6D_6+fluorobenzene, ppm): Al(C_6F_5)$_2$: δ -119.6 (m, *o*-C_6F_5), -146.0 (tm, , *p*-C_6F_5), -158.8 (m, *m*-C_6F_5); [B(C_6F_5)$_4$]$^-$: δ -132.1 (m, *o*-C_6F_5), -163.1 (t, *p*-C_6F_5), -166.9 (m, *m*-C_6F_5).

HRMS(m/z): [M]$^+$ calcd. for $C_{45}H_{41}AlF_{11}N_2^+$, 845.2904; found: 845.2857.

Synthesis of compound 4



Scheme S1-4: Synthesis of 4

Compound **3** (608 mg, 0.4 mmol) and $[Cp^*Al]_4$ (65.2 mg, 0.1mol) were dissolved in 5 mL of fluorobenzene. The resulting solution was stirred at room temperature for 6 hours. The solvent was evaporated under vacuum, resulting in the formation of pale-yellow solids. The residue was washed with n-hexane (3×2 mL), and the remaining material was dried under vacuum. White solids of **4** as pale-yellow solids (26.0 mg, 90 % yield) were obtained.

NMR data of compound **4** were obtained from a solution of the isolated colorless solid in a mixed solvent of C_6D_6 and fluorobenzene. **Single crystals** (colorless) suitable for X-ray analysis were obtained by storing a mixed solvent of toluene and fluorobenzene of **4** at -30 °C for 5 hours.

^{1}H NMR (500 MHz, C_6D_6+fluorobenzene, ppm): δ 0.85 (dd, *J*=6.7 Hz, 24H, $CH(CH_3)_2$), 1.42(s, $(CH_3)_5Cp$), 2.42 (sept, *J*=6.8 Hz, 4H, $CH(CH_3)_2$); (6.5-7.2 were overlap with fluorobenzene).

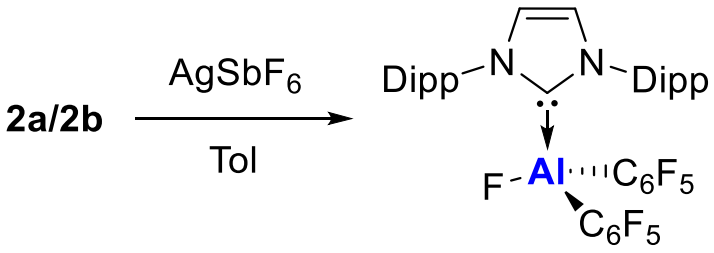
^{13}C{^{1}H} NMR (125 MHz, C_6D_6+fluorobenzene, ppm): IPr: δ 8.76 $(CH_3)_5Cp$), 21.9, 25.5 ($CH(CH_3)_2$), 28.7 ($CH(CH_3)_2$), 117.2 (Ar*C*), 125.0 (Ar*C*), 128.5 (Ar*C*), 132.5 (Ar*C*), 132.7 (-N-*C*H-), 146.0 (N*C*N); $Al(C_6F_5)_2$ and $[B(C_6F_5)_4]^-$ not listed.

$^{11}B\{^1H\}$ NMR (160 MHz, C_6D_6+fluorobenzene, ppm): δ -16.0 $[B(C_6F_5)_4)]^-$.

$^{19}F\{^1H\}$ NMR (470 MHz, C_6D_6+fluorobenzene, ppm): $Al(C_6F_5)_2$: δ -118.1 (m, *o*-C_6F_5), -150.4 (tm, *p*-C_6F_5), -160.3 (m, *m*-C_6F_5); $[B(C_6F_5)_4]^-$: δ -131.8 (m, *o*-C_6F_5), -162.9 (t, *p*-C_6F_5), -166.7 (m, *m*-C_6F_5).

HRMS(m/z): $[M]^+$ calcd. for $C_{49}H_{51}Al_2F_{10}N_2^+$, 911.3518; found: 911.3468.

Synthesis of compound 5



Scheme S1-5: Synthesis of 5

Mixture of **2** (152.6 mg, 0.1 mmol) (or **3**) and $AgSbF_6$ (34.3mg, 0.1mmol) were combined in toluene (5 mL). The mixture was stirred for 30 minutes yielding a turbid solution. the mixture was filtered off and vacuumed to give a white solid of **5** in 90% yield (69 mg).

[Caution] Extra caution should be exercised when handling $AgSbF_6$, due to the potential oxidizing properties of Ag^+ ions.

NMR data of compound **5** were obtained from C_6D_6. **Single crystals** (colorless) suitable for X-ray analysis were obtained by storing a mixed solvent of toluene and n-hexane of **5** at -30 °C for 2 hours.

^1H NMR (500 MHz, C_6D_6, ppm): δ 0.85 (d, *J*=6.8 Hz, 12H, $CH(CH_3)_2$), 1.22 (d, *J*=6.8 Hz, 12H, $CH(CH_3)_2$), 2.76 (sept, *J*=6.8 Hz, 4H, $CH(CH_3)_2$), 6.46 (s, 2H,

-N-C*H*-), 6.87 (d, *J*=7.8 Hz, 4H, Ar-*H*), 7.04 (t, *J*=7.8 Hz, 2H, Ar-*H*).

$^{13}C\{^1H\}$ NMR (125 MHz, C_6D_6, ppm): IPr: δ 21.7, 26.5 (CH(*C*H_3)$_2$), 29.0 (*C*H(CH$_3$)$_2$), 124.0 (Ar*C*), 125.7 (Ar*C*), 128.3 (Ar*C*), 131.3 (Ar*C*), 133.4 (-N-*C*H-), 145.9 (N*C*N); Al(C_6F_5)$_2$ not listed.

$^{19}F\{^1H\}$ NMR (470 MHz, C_6D_6, ppm): (C_6F_5)$_2$AlF: δ -119.6 (m, *o*-C_6F_5), -154.7 (tm, *p*-C_6F_5), -162.2 (m, *m*-C_6F_5), 170.9 (s, Al-*F*); [B(C_6F_5)$_4$]$^-$: -131.8 (m, *o*-C_6F_5), -162.5 (t, *p*-C_6F_5), -166.3 (m, *m*-C_6F_5).

HRMS(m/z): [M]$^-$ calcd. for $C_{39}H_{36}AlF_{11}N_2^-$,768.2523; found: 768.2501.

Spectroscopic Data

Spectra of 1

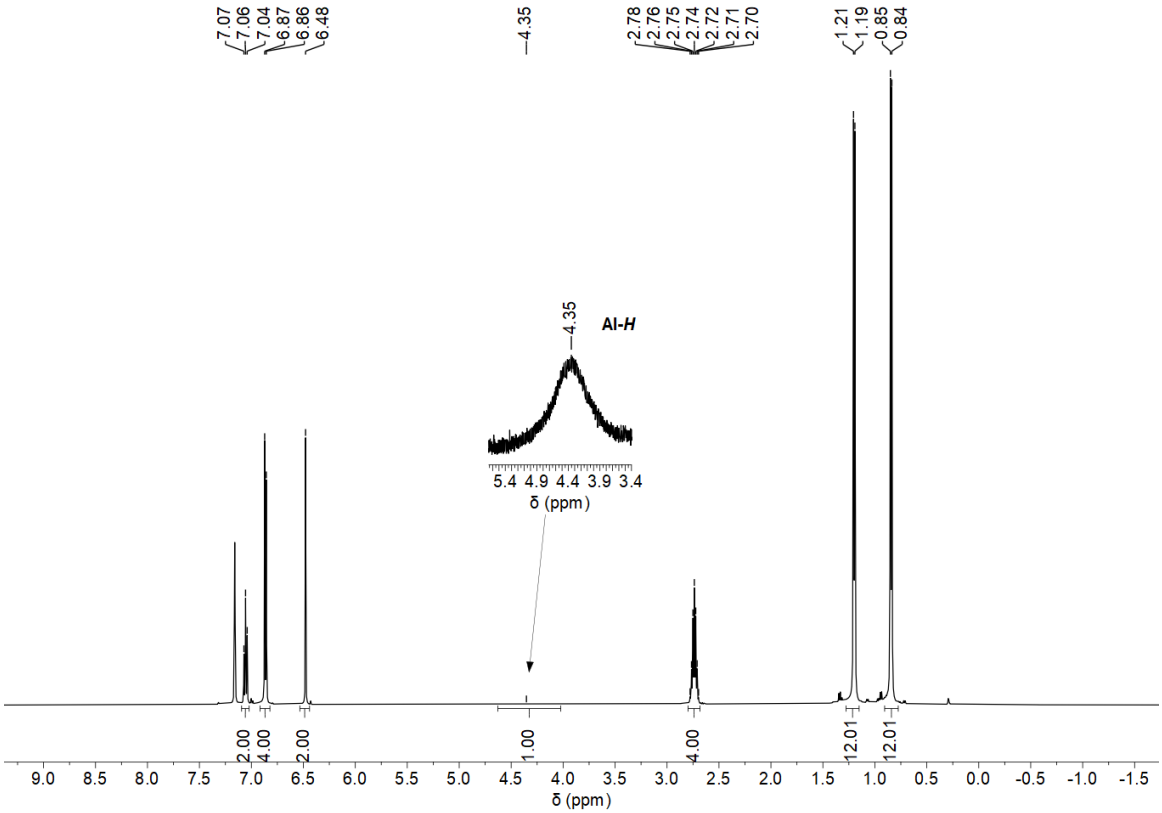


Figure S2-1. ^{1}H NMR spectrum of **1** in C_6D_6

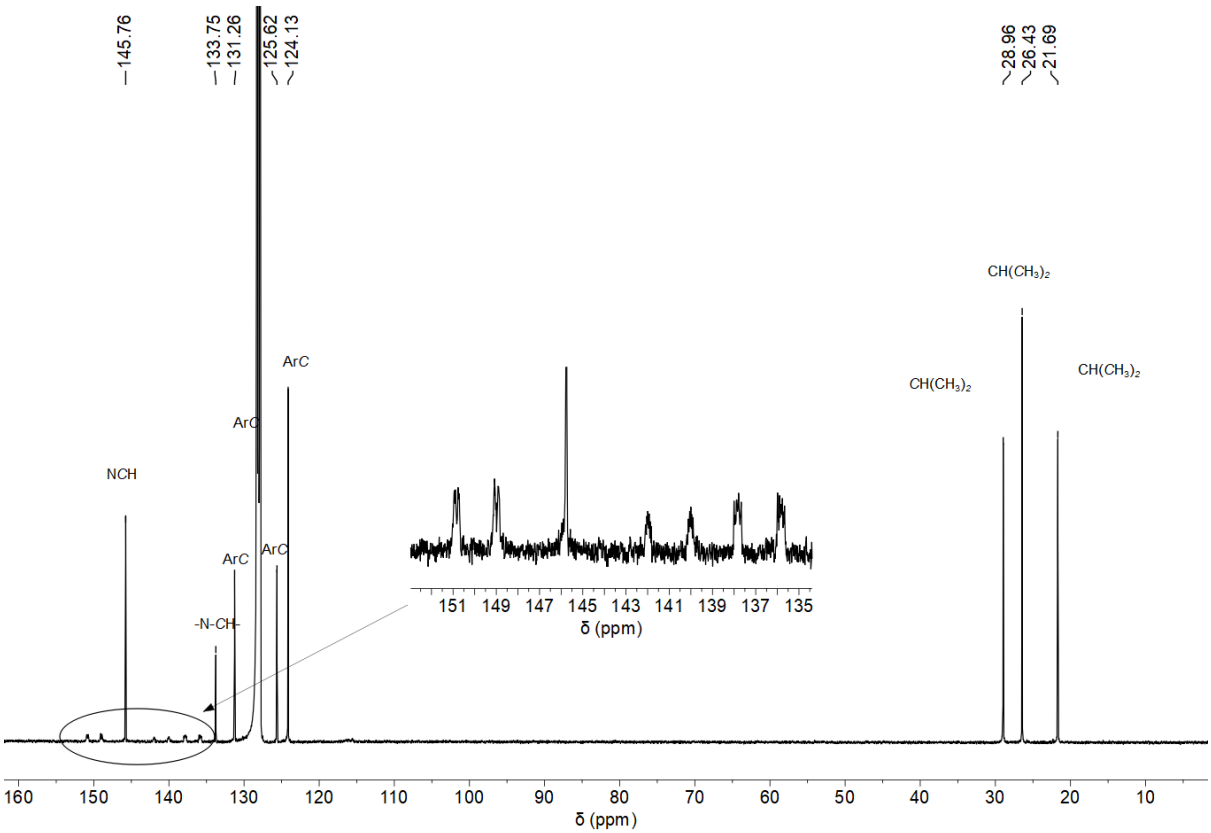


Figure S2-2. ^{13}C NMR spectrum of **1** in C_6D_6

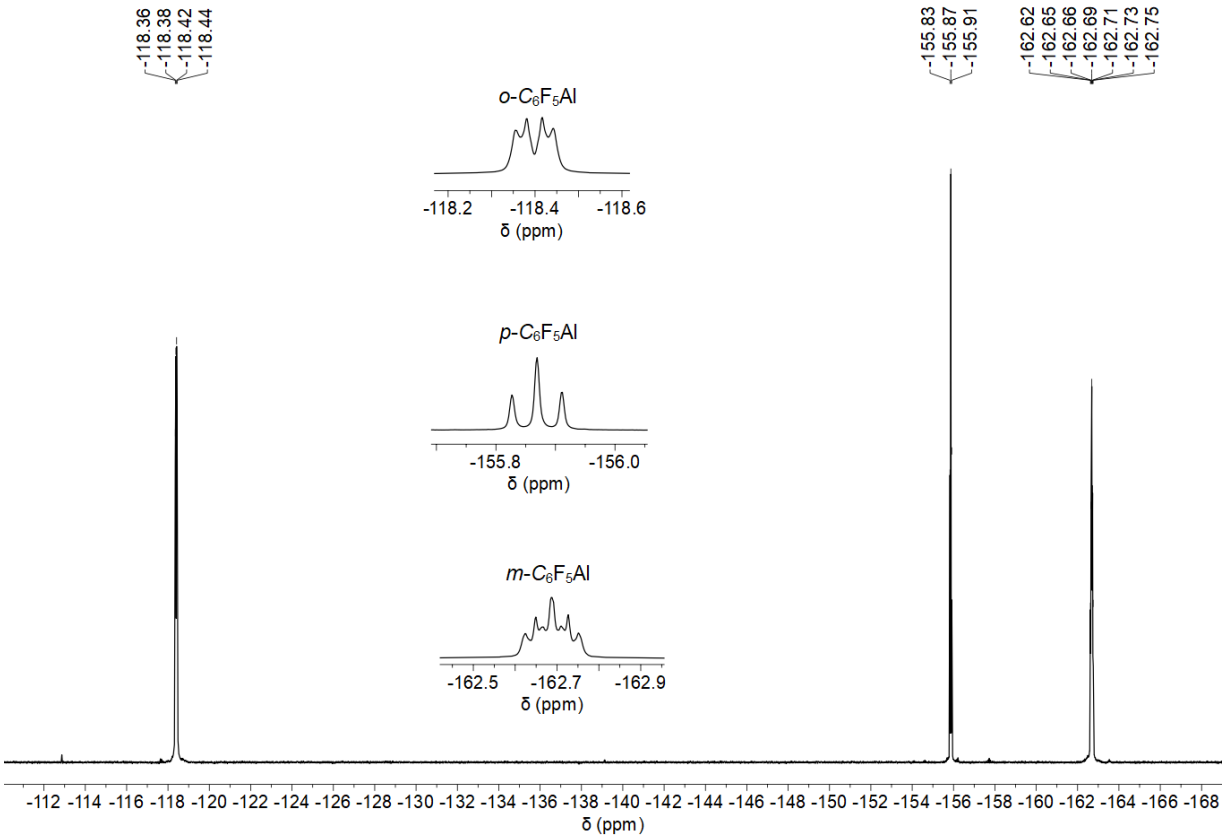


Figure S2-3. ^{19}F NMR spectrum of **1** in C_6D_6

Spectra of 2

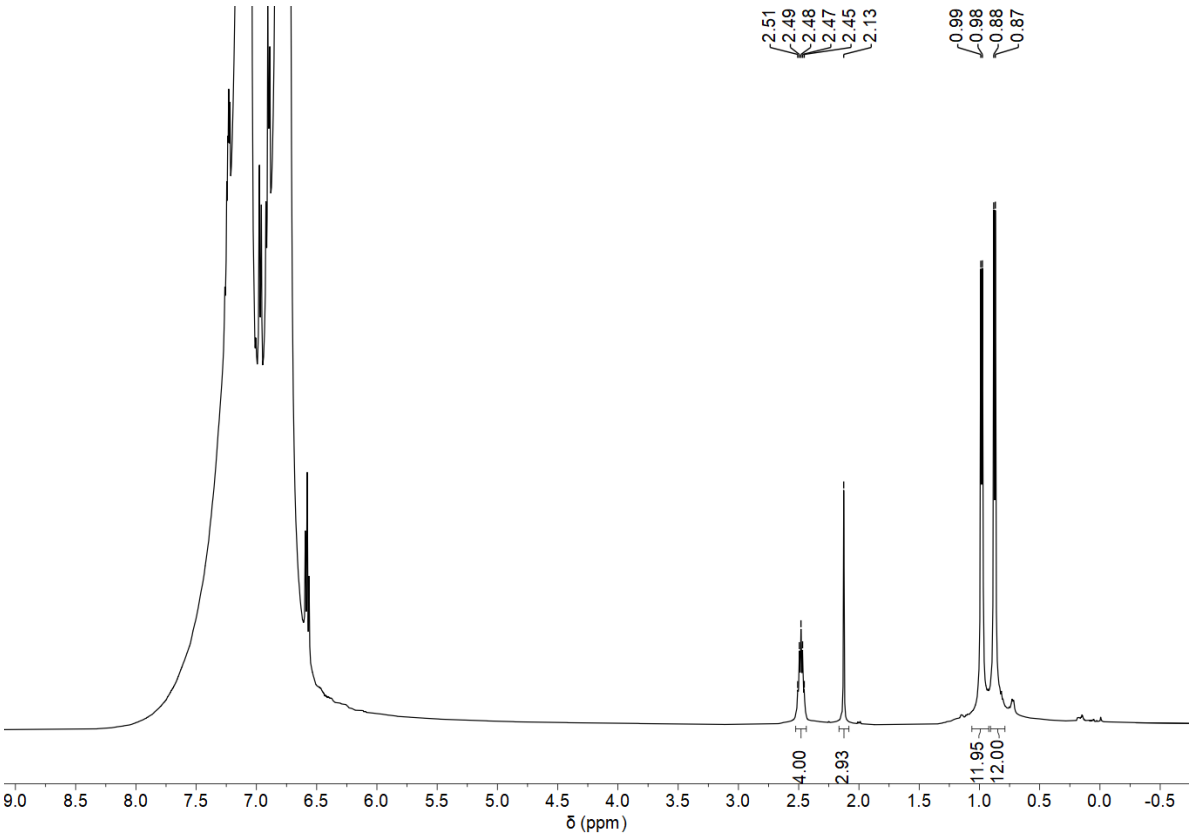


Figure S2-4. ^{1}H NMR spectrum of **2** in C_6D_6+1,2-dichlorobenzene

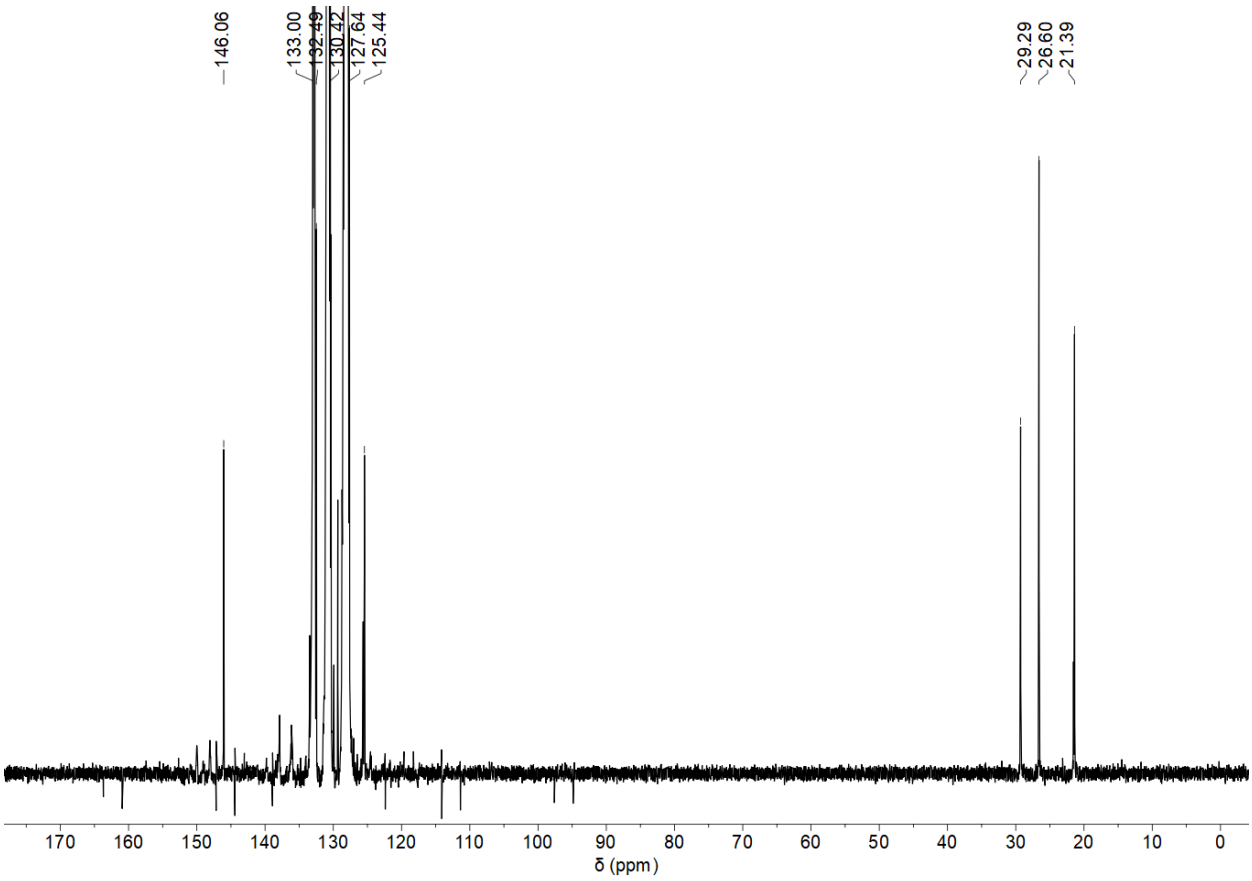


Figure S2-5. ^{13}C NMR spectrum of **2** in C_6D_6+1,2-dichlorobenzene

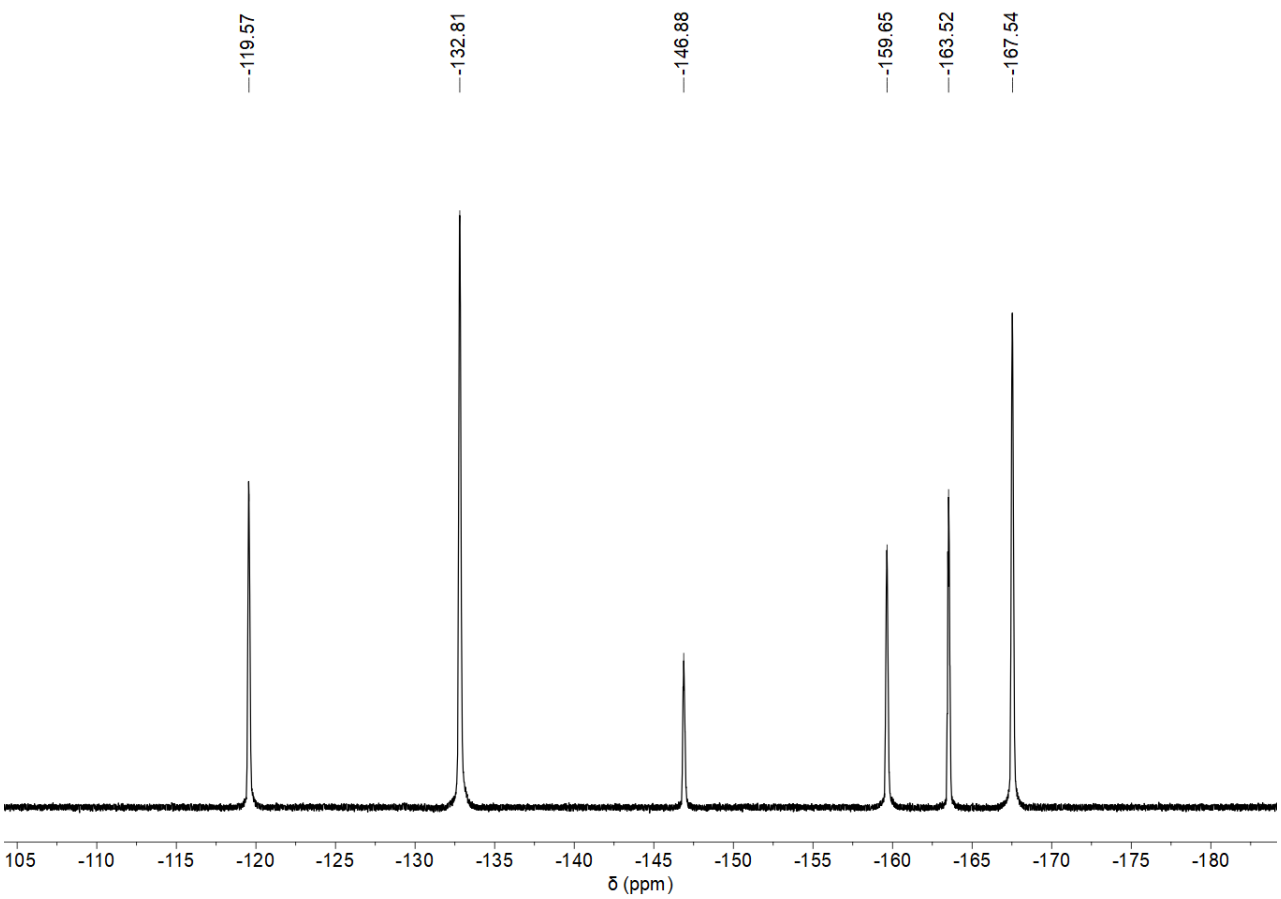


Figure S2-6. ^{19}F NMR spectrum of **2** in C_6D_6+1,2-dichlorobenzene

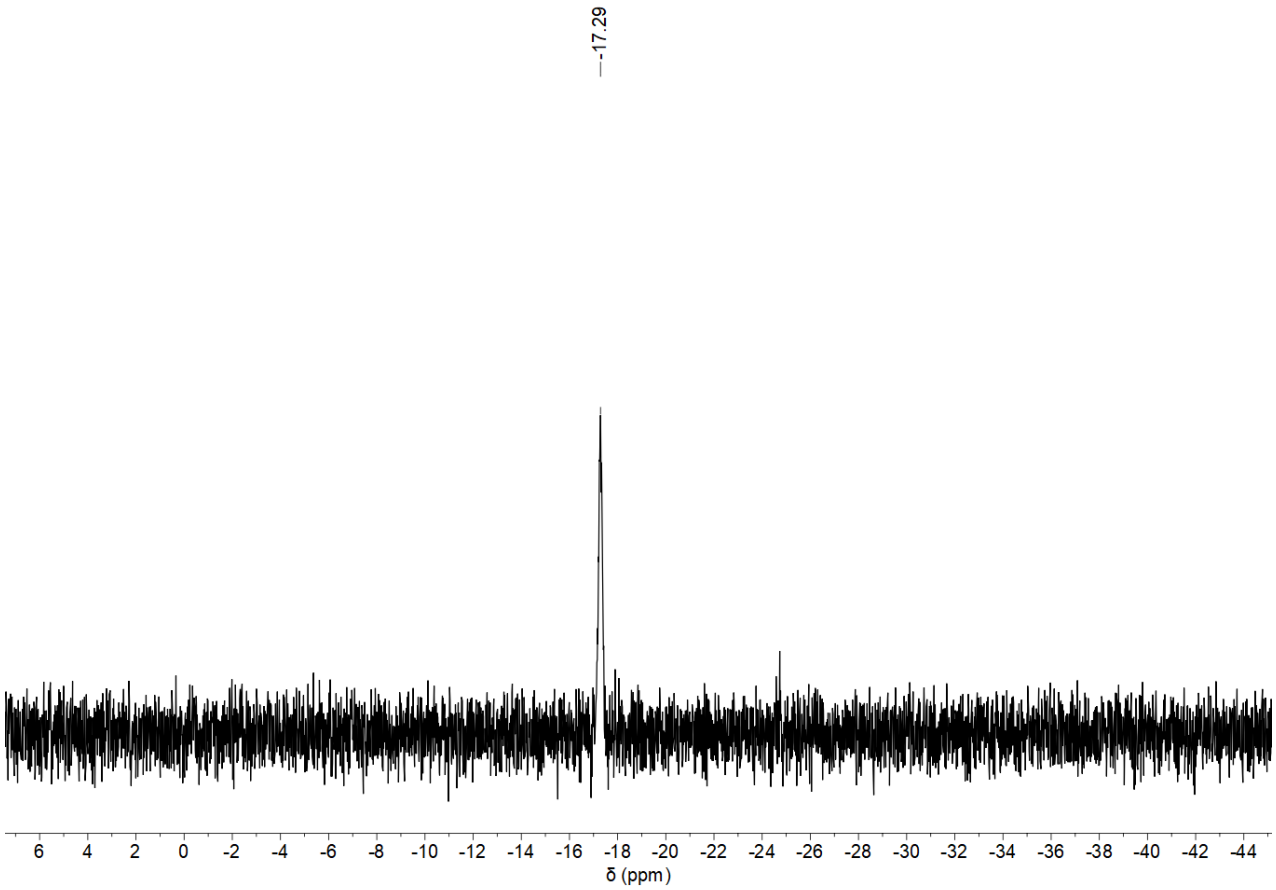


Figure S2-7. ^{11}B NMR spectrum of **2** in C_6D_6+1,2-dichlorobenzene

Spectra of 3

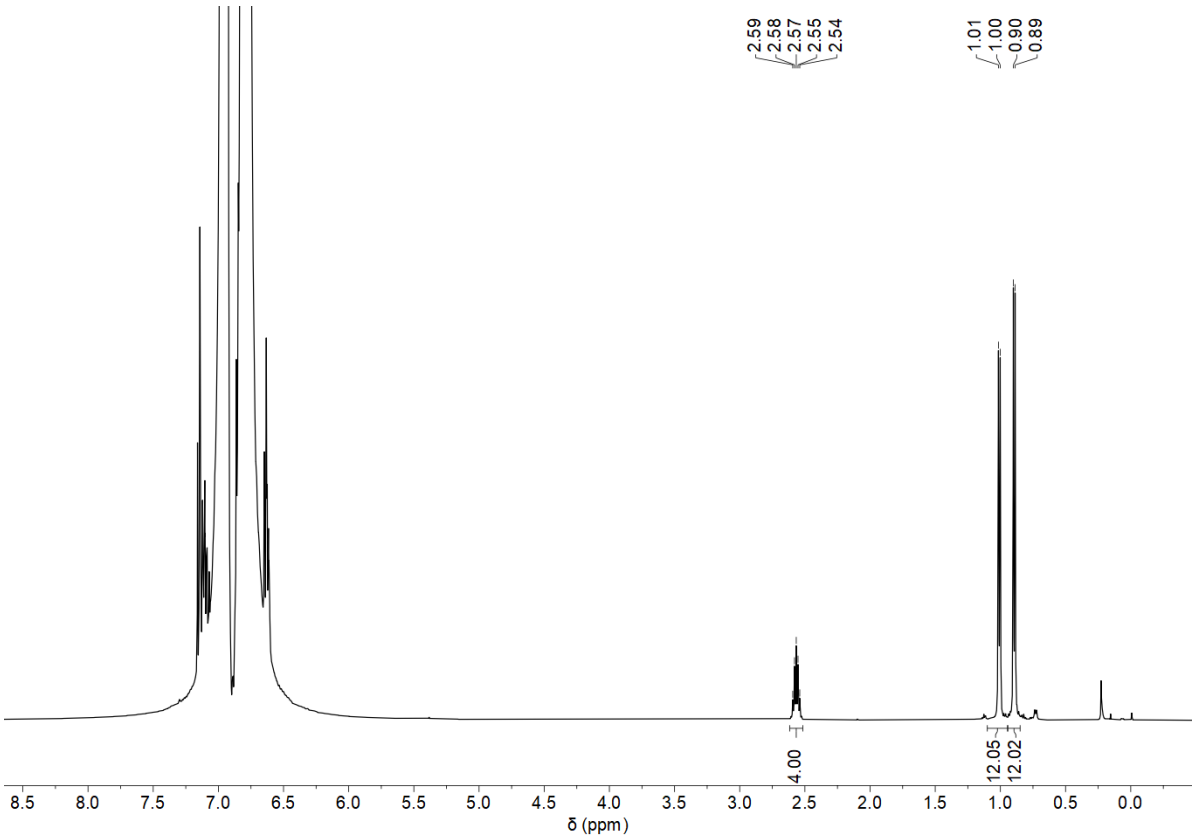


Figure S2-8. ^{1}H NMR spectrum of **3** in C_6D_6+fluorobenzene

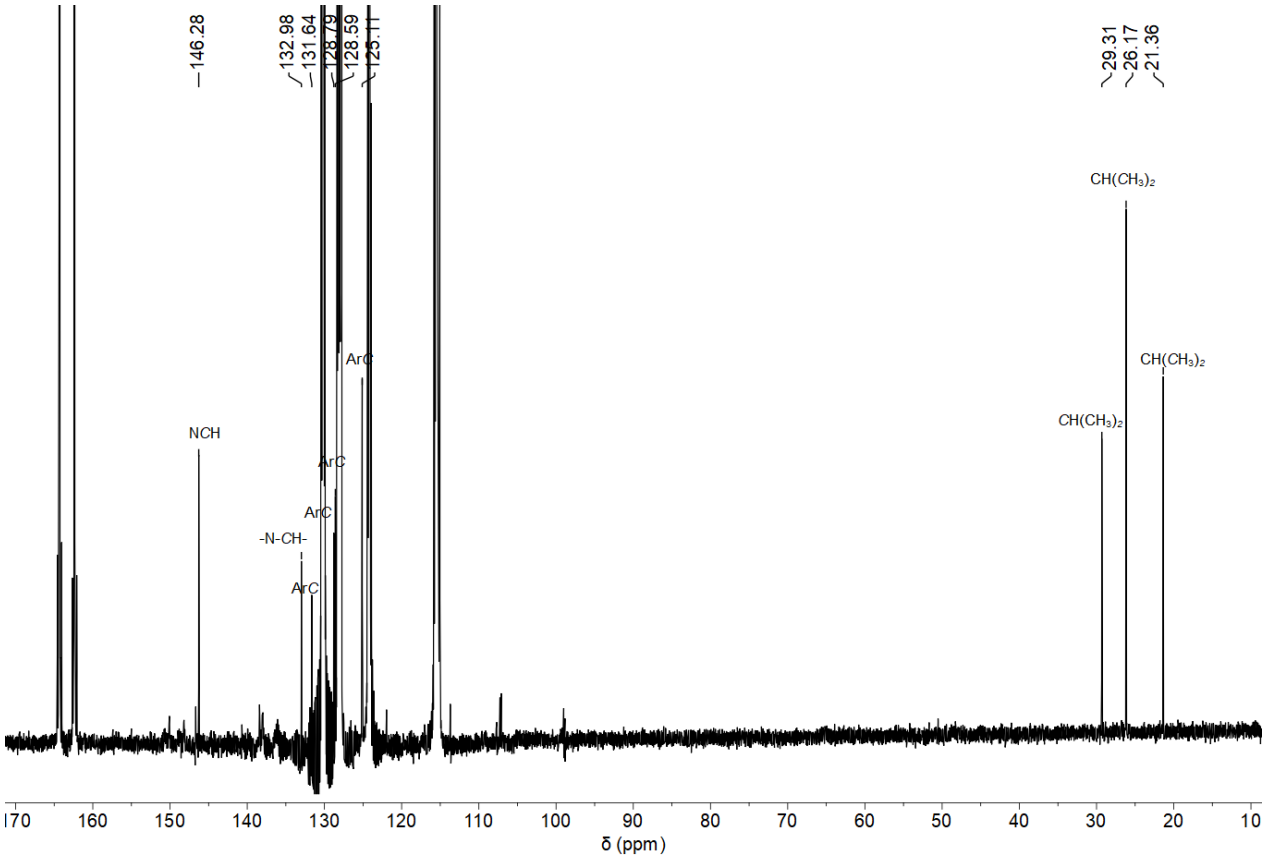


Figure S2-9. ^{13}C NMR spectrum of **3** in C_6D_6+fluorobenzene

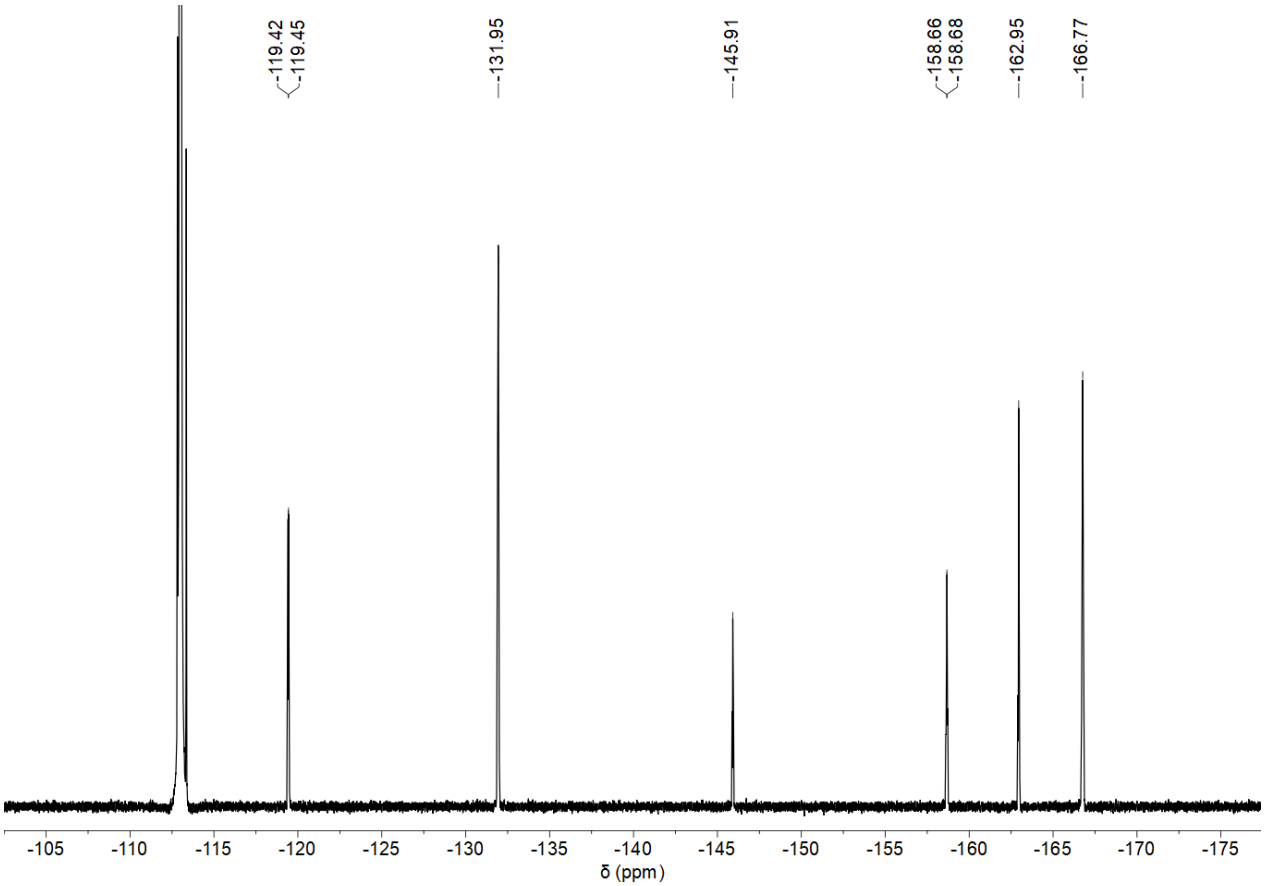


Figure S2-10. ^{19}F NMR spectrum of **3** in C_6D_6+fluorobenzene

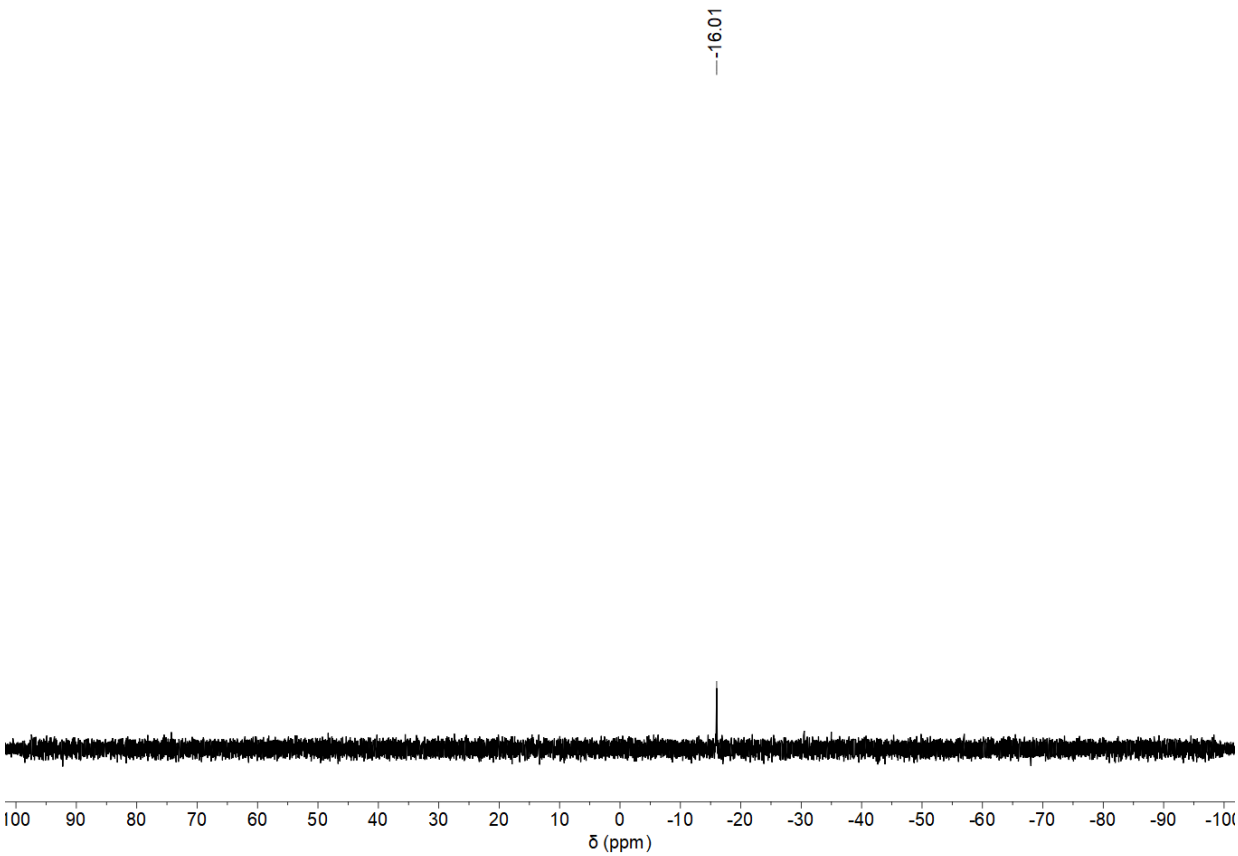


Figure S2-11. ^{11}B NMR spectrum of **3** in C_6D_6+fluorobenzene

Spectra of 4

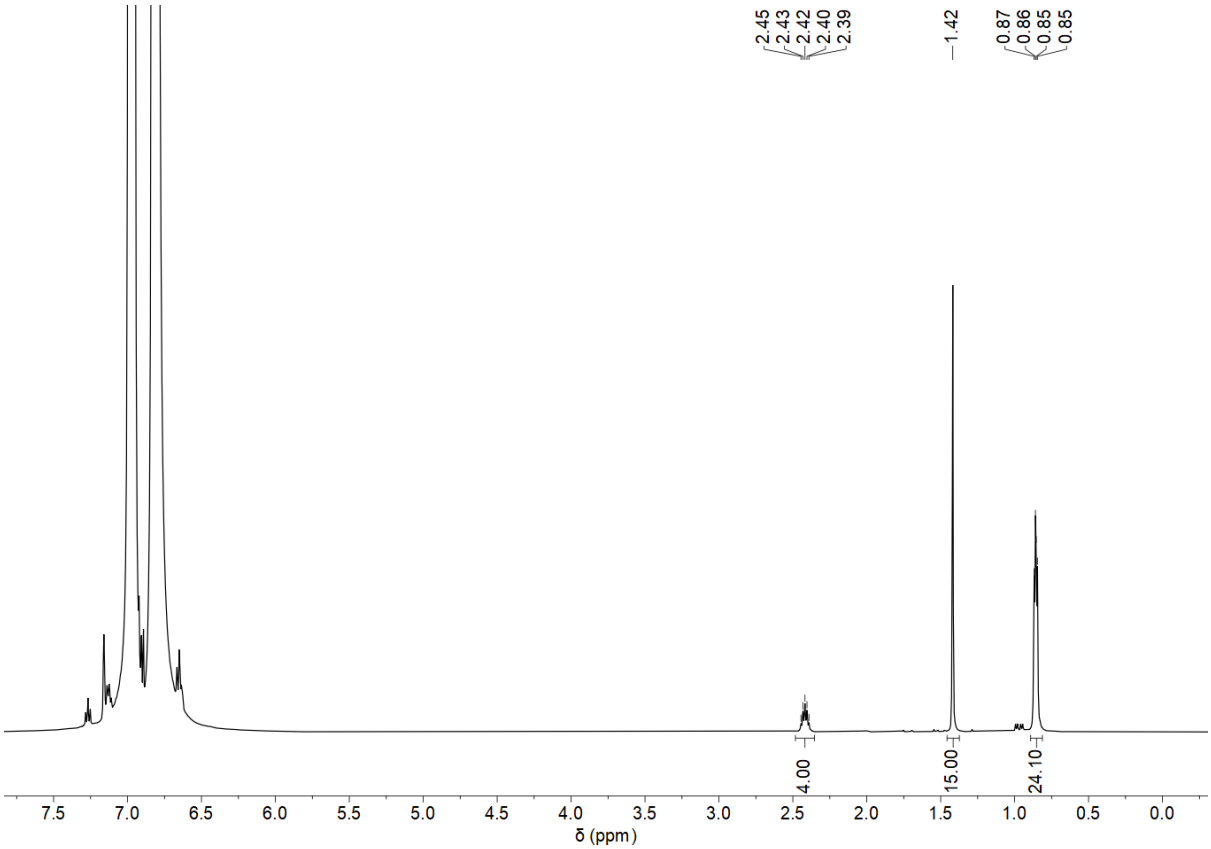


Figure S2-12 ^{1}H NMR spectrum of **4** in C_6D_6+fluorobenzene

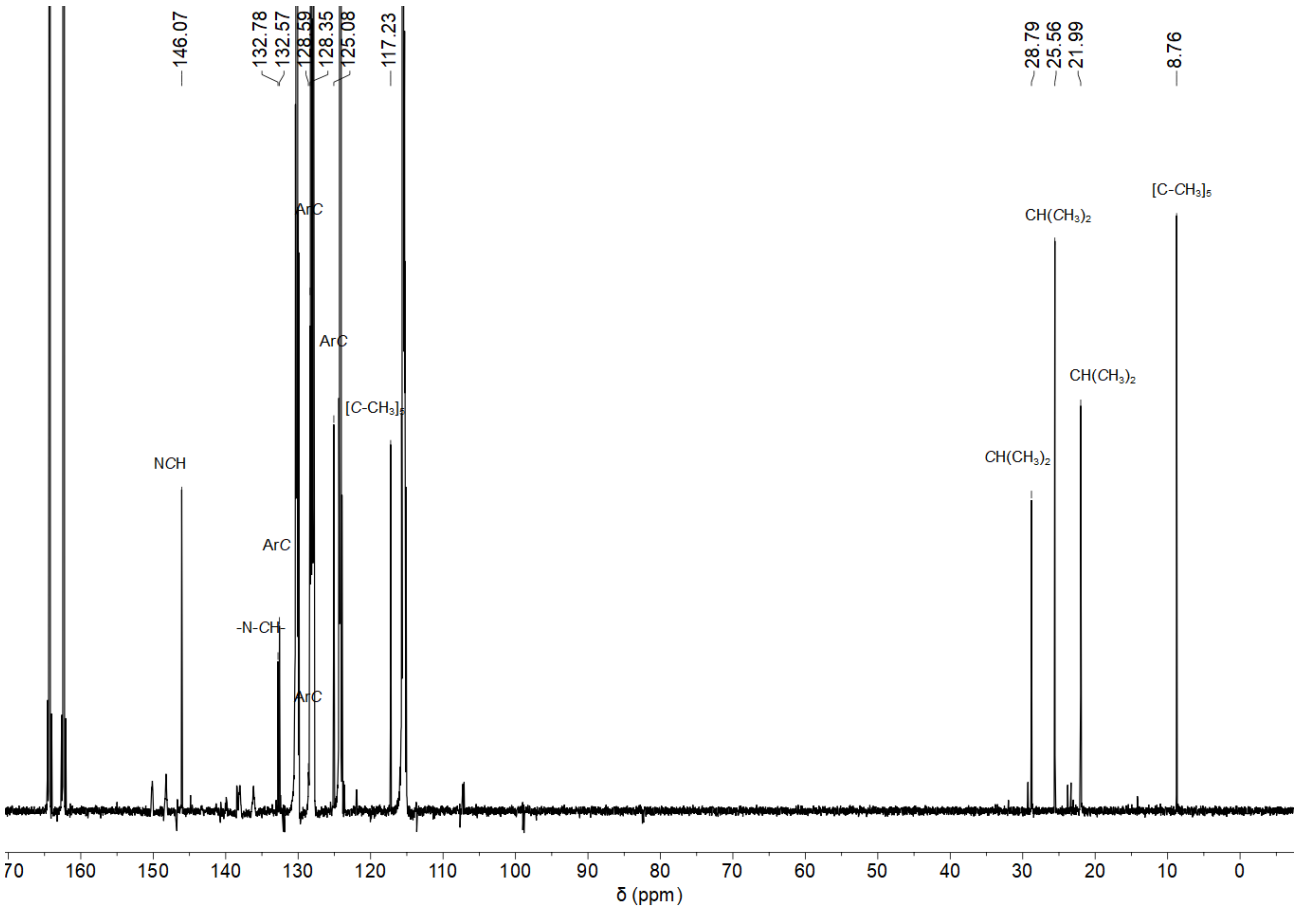


Figure S2-13 ^{13}C NMR spectrum of **4** in C_6D_6+fluorobenzene

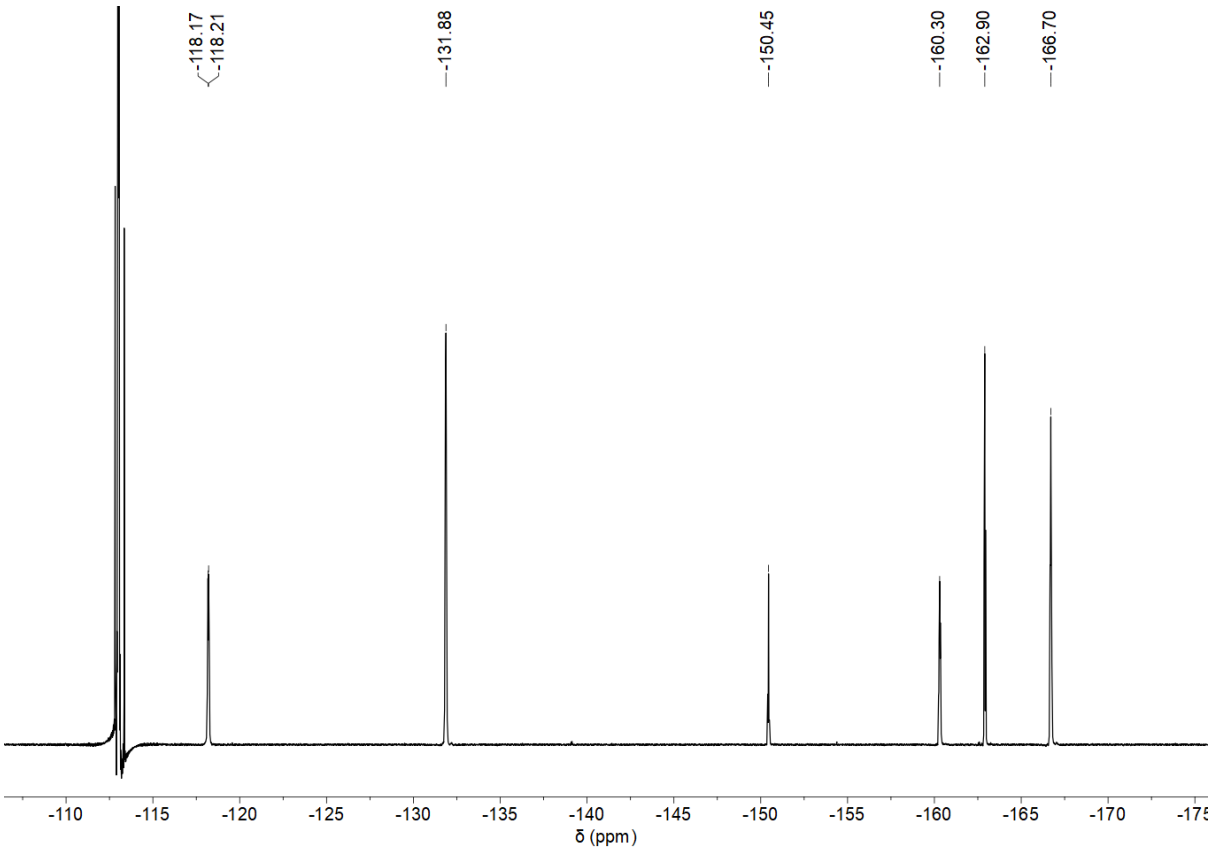


Figure S2-14 ^{19}F NMR spectrum of **4** in C_6D_6+fluorobenzene

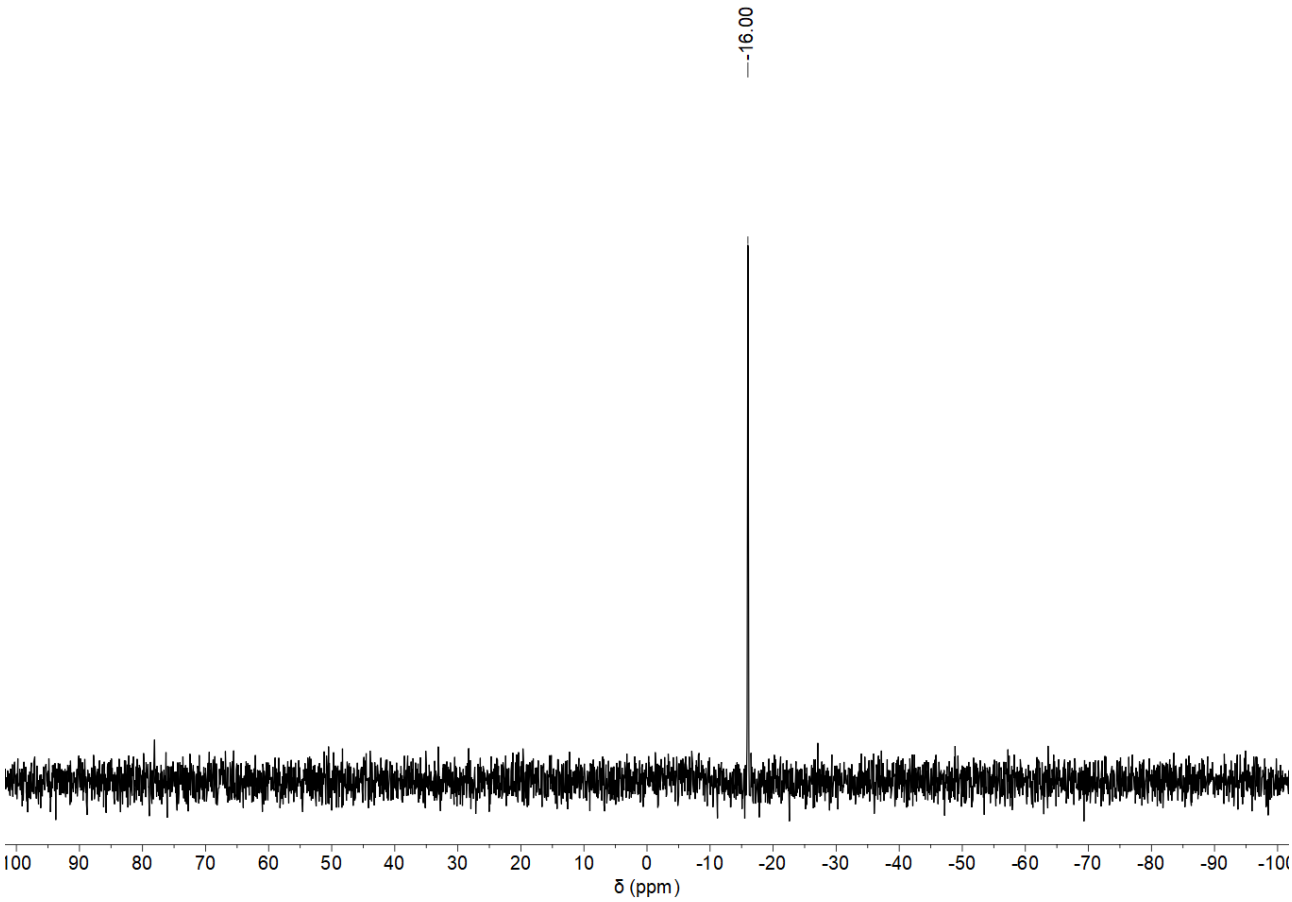


Figure S2-15 ^{11}B NMR spectrum of **4** in C_6D_6+fluorobenzene

Spectra of 5

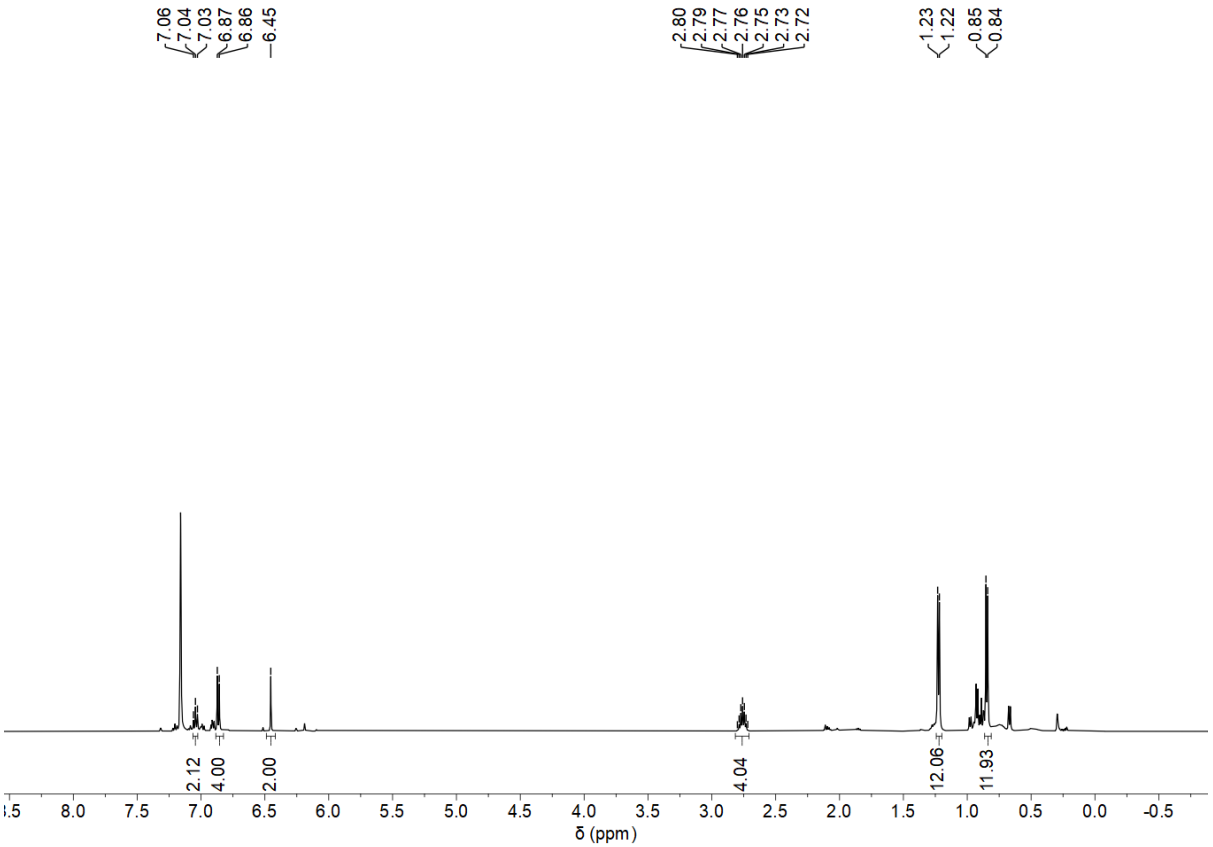


Figure S2-16 ^{1}H NMR spectrum of **5** in C_6D_6

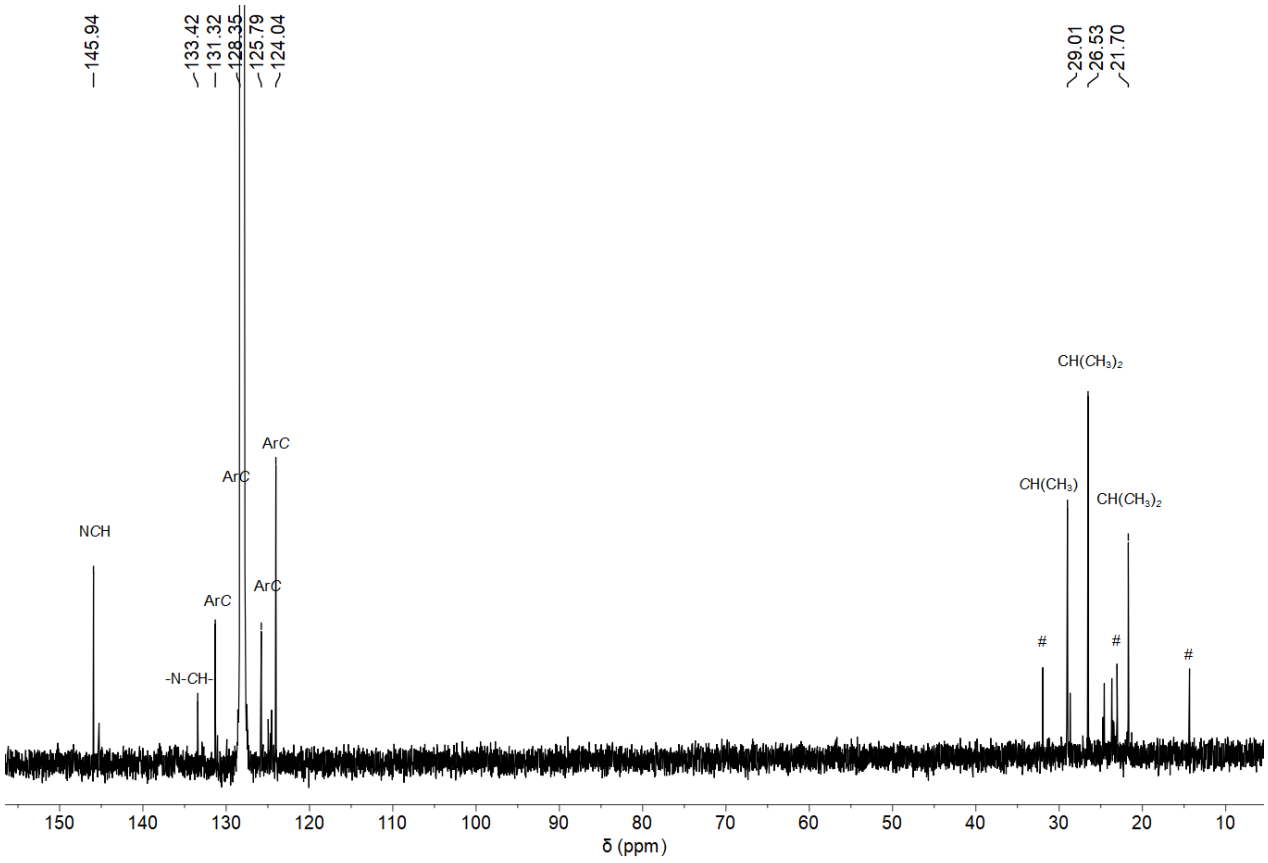


Figure S2-17 ^{13}C NMR spectrum of **5** in C_6D_6 (#n-hexane)

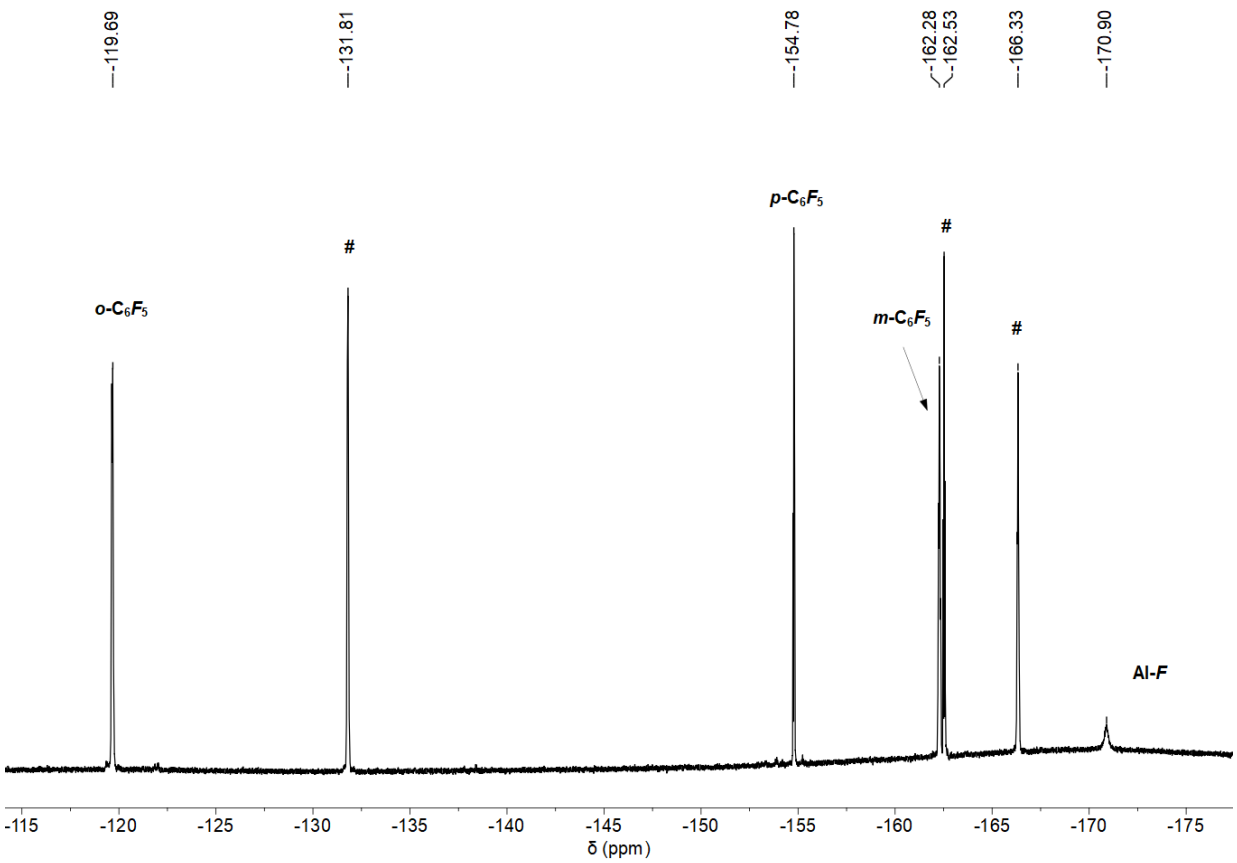
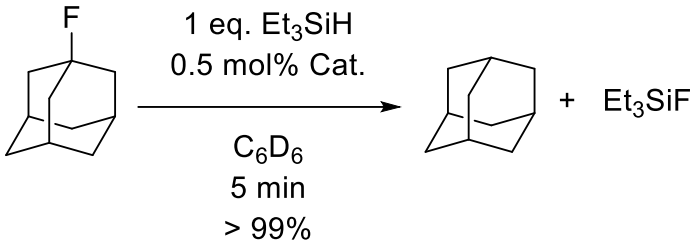


Figure S2-18 ^{19}F NMR spectrum of **5** in C_6D_6+1,2-dichlorobenzene ($^{\#}[B(C_6F_5)_4]^-$)

Lewis acid catalysis

a) Hydrodefluorination of 1-fluoroadamantane



To a mixture of 1-fluoroadamantane (21.0 mg, 138 mmol) and Et_3SiH (22.0 μL, 138 μmol) in 0.5 ml C_6D_6 were added **3** (1 mg, 0.69 mmol) at PTFE-sealed J-Young NMR tube. The tube was immediately removed from the glovebox and monitored the conversion by ^1H and ^{19}F NMR spectroscopy. To monitor the reaction conversion, mesitylene (10.0 μL, 71.9 mmol) were additionally added as an internal standard. The yield of hydrodefluorination was 99%. Product identification corresponds with literature values for adamantane and separately synthesized Et_3SiF.

^{1}H NMR (500 MHz, C_6D_6, ppm): Adamantane[S7] *(CAS: 281-23-2)*: δ 1.74 (br, 9H, R_2CH_2), 1.86 (br, 3H, R_3CH); Et_3SiF *(CAS: 358-43-0)*: δ 0.51-0.57(m, 4.8 H, $SiCH_2CH_3$), 0.92 (t, *J*=8.0 Hz, 6.8 H, CH_3).

^{19}F NMR (471 MHz, C_6D_6, ppm): δ -175.2 Et_3SiF.

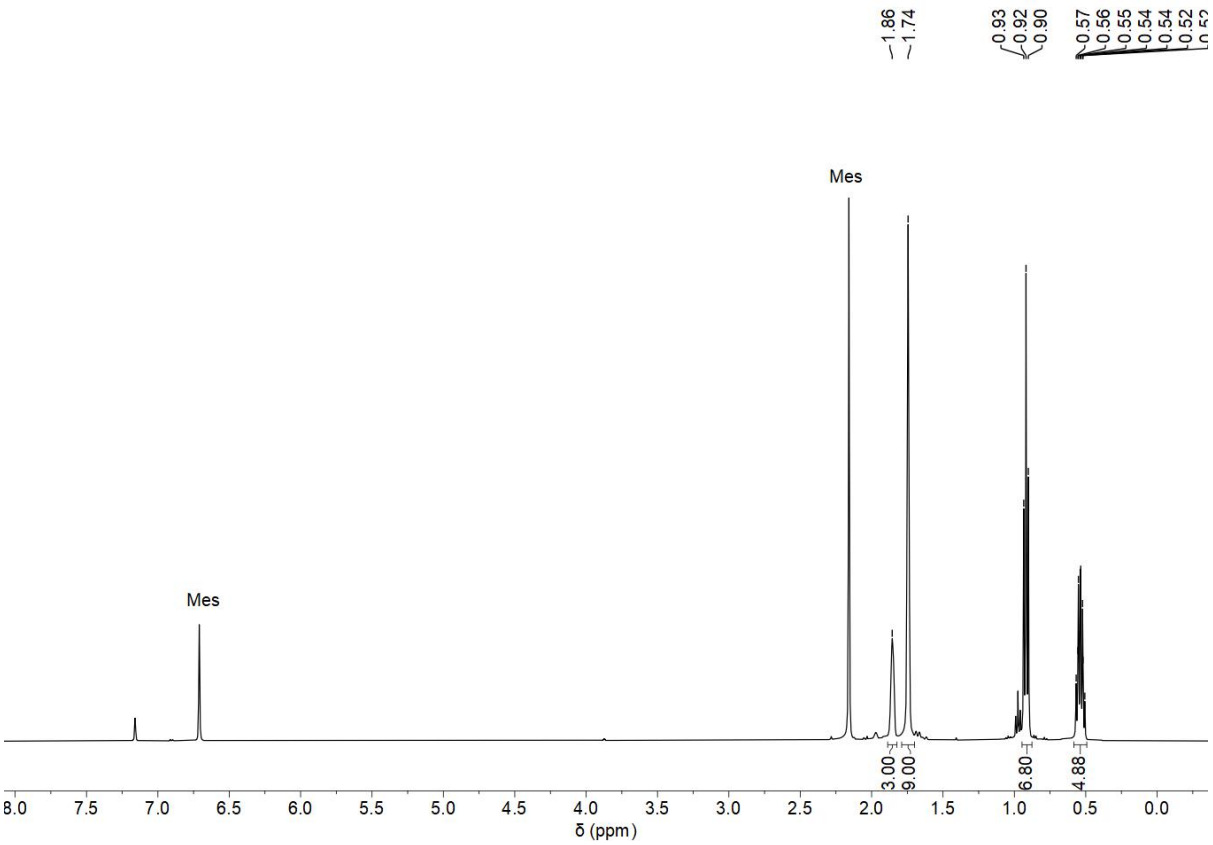


Figure S3-1. In-situ ^{1}H NMR spectrum of the hydrodefluorination of 1-fluoroadamantane in C_6D_6

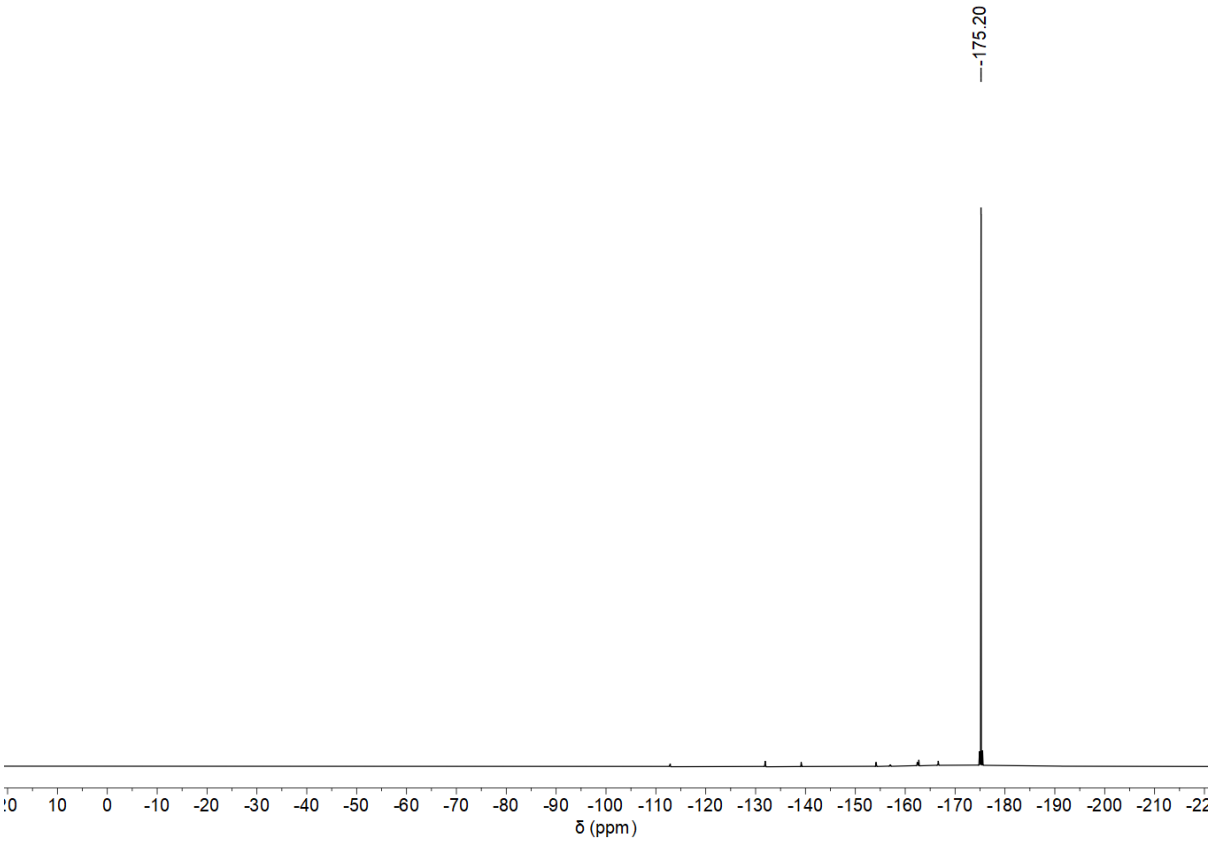
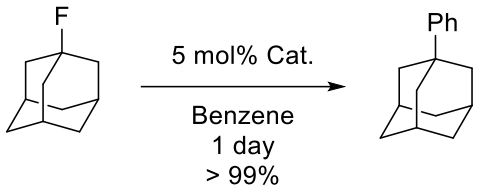


Figure S3-2. In-situ ^{19}F NMR spectrum of the hydrodefluorination of 1-fluoroadamantane in C_6D_6

b) Friedel-Crafts arylation



To a stirred benzene solution (3.0 mL) of 1-fluoroadamantane (154 mg, 1 mmol) were added **3** (75 mg, 0.05 mmol) dissolved in 5.0 mL benzene. The mixture was stirred and monitored by ^{19}F NMR. After 24 h, the volatiles were removed under vacuum and the desired product was eluented by n-hexane to afford the corresponding coupled product. The yield of 1-phenyladamantane was 99% (32.6 mg). Product identification corresponds with literature values.

1-phenyladamantane [S8] *(CAS: 780-68-7)*:

^{1}H NMR (500 MHz, C_6D_6, ppm): δ 1.42-1.47(m, 6H), 1.58 (d, J = 3.0 Hz, 6H), 1.72 (dt, J = 6.7, 3.4 Hz, 3H), 6.88-6.93 (m, 1H, Ph-*H*), 7.01-7.04 (m, 2H, Ph-*H*), 7.06-7.08 (m, 2H, Ph-*H*).

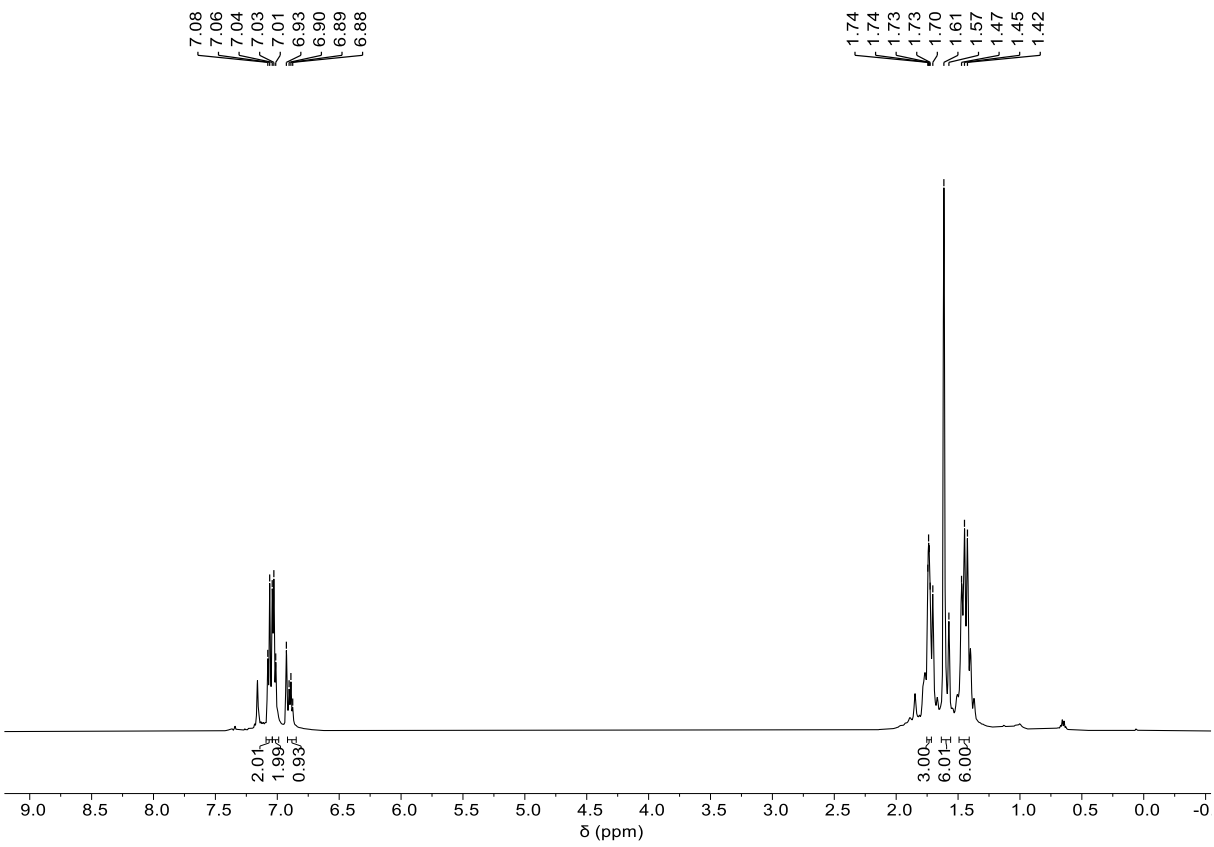
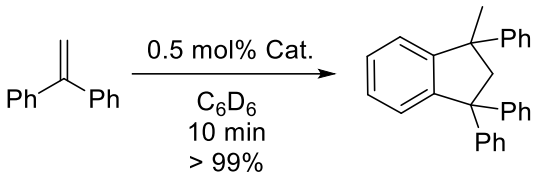


Figure S3-3. ^{1}H NMR spectrum of 1-phenyladamantane in C_6D_6

c) Friedel-Crafts-Dimerization of 1,1-diphenylethylene



To a solution of 1,1-DPE (36.0 mg, 0.2mmol) in C_6D_6 (1.0 mL) was added **3** (1.5 mg, 0.001 mmol), the mixture stirred for 1 min and then monitored by ^{1}H NMR. After completion of the reaction was confirmed, the volatiles were removed under vacuum and the desired product was eluented by n-hexane to afford a colorless oil. The yield of 1-methyl-1,3,3-triphenyl-2,3-dihydro-1H-indene was 99% (36 mg). Product identification corresponds with literature values.

1-Methyl-1,3,3-triphenyl-2,3-dihydro-1H-indene[S9] *(CAS: 84803-40-7)*:

^{1}H NMR (500 MHz, C_6D_6, ppm): δ 1.48 (s, 3H), 3.01 (d, *J*=13.6 Hz, 1H), 3.42(d, *J*=13.6 Hz, 1H), 7.21-6.89 (m, 20H).

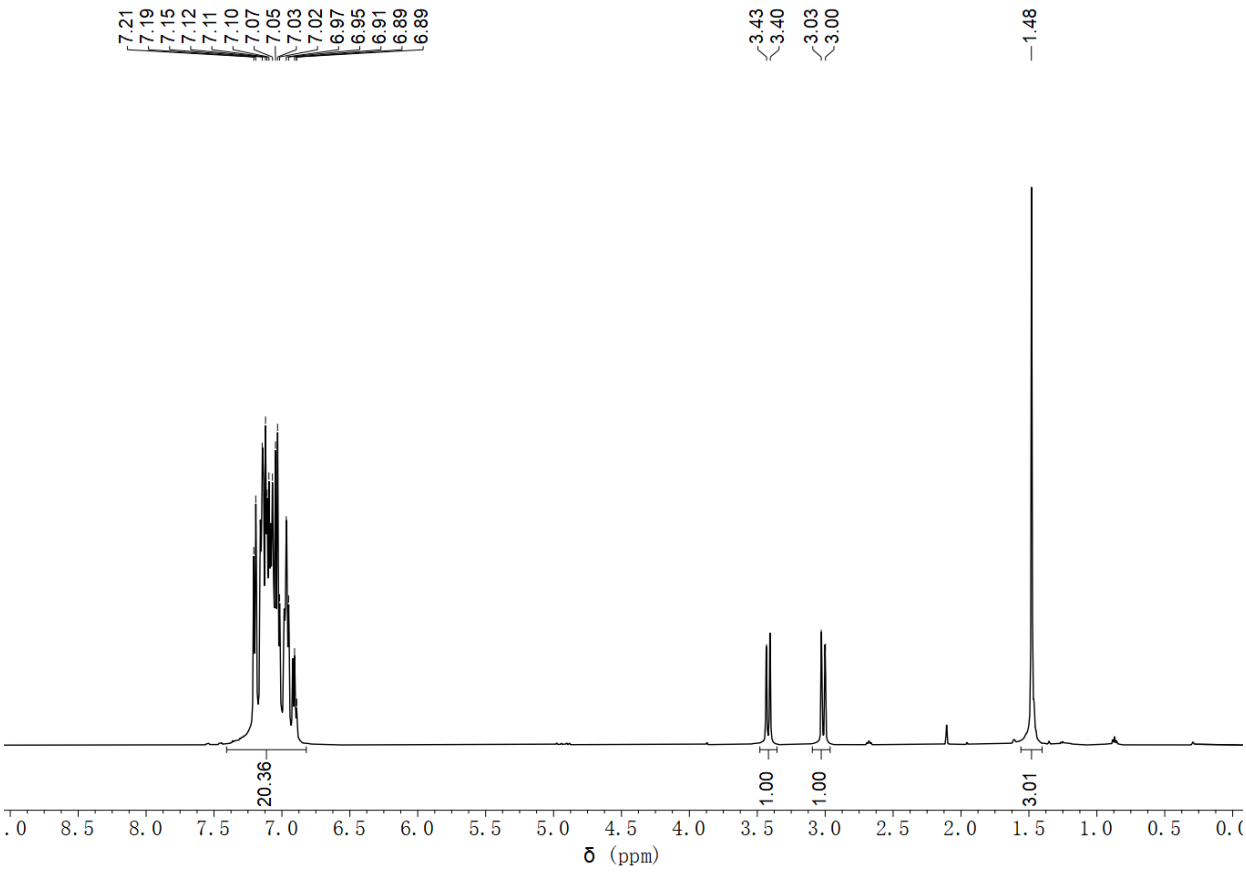
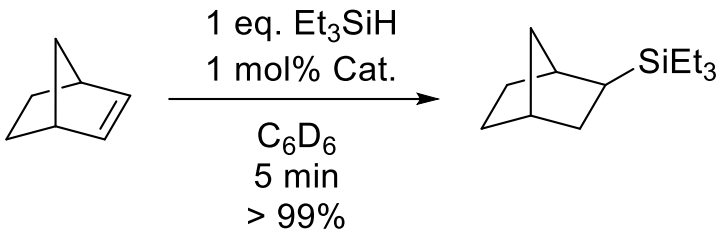


Figure S3-4. ^{1}H NMR spectrum of 1-methyl-1,3,3-triphenyl-2,3-dihydro-1H-indene in C_6D_6

d) Hydrosilylation of 2-norbornene



To a solution of norbornene (9.4 mg, 0.1 mmol) and triethylsilane (0.1 mmol, 1 eq.) in C_6D_6 (0.6 mL) was added the catalyst (**3**, 1.5 mg, 0.001 mmol), the solution mixed for 1 min and then probed by ^{1}H NMR to determine the reaction progress. After completion of the reaction was confirmed, the volatiles were removed under vacuum and the product was eluented by n-hexane to afford a colorless oil. The yield of (Bicyclo [2.2.1] heptan-2-yl)triethylsilane was 99% (20.8 mg). Product identification corresponds with literature values.

(Bicyclo [2.2.1] heptan-2-yl)triethylsilane[S10] *(CAS: 164859-22-7)*:

^{1}H NMR (500 MHz, C_6D_6, ppm): δ 2.23 (s, 1H), 2.17 (s, 1H), 1.55-1.52 (m, 2H), 1.45-1.42 (m, 1H), 1.38-1.33 (m, 1H), 1.23-1.19 (m, 3H), 1.13-1.11 (m, 1H), 0.99 (t, *J*=8.0 Hz, 9H), 0.65-0.62 (m, 1H), 0.53 (qd, *J*=7.9, 1.2 Hz, 6H).

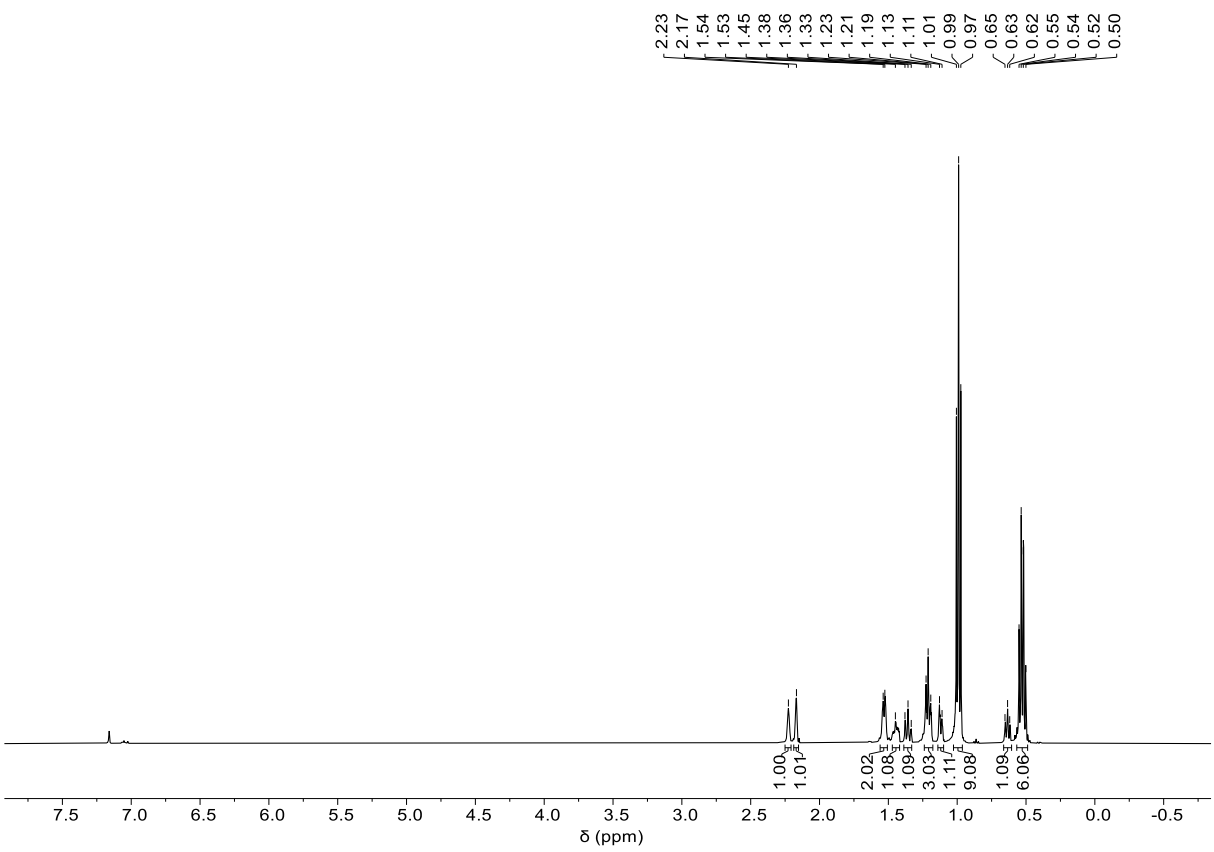


Figure S3-5. ^{1}H NMR spectrum of (bicyclo[2.2.1]heptan-2-yl)triethylsilane in C_6D_6

X-ray Crystallographic Data

Table S1. Crystal data and structure refinement details for compounds **1**, **2** and **3**

Compounds	**1**	**2**	**3**
CCDC	2294592	2294593	2294596
Empirical formula	$C_{39}H_{37}AlF_{10}N_2$	$C_{77}H_{52}AlBF_{30}N_2$	$C_{75.45}H_{48.2}AlBF_{31}N_2$
Formula weight	750.68	1612.99	1609.55
Temperature, K	150.00	150	150.0
Crystal system	orthorhombic	triclinic	monoclinic
Space group	*Pca*2$_1$	*P*-1	*P*2$_1$/c
a, Å	14.3469(3)	12.8701(5)	18.2366(7)
b, Å	12.6120(3)	14.0245(6)	12.6216(4)
c, Å	20.0825(4)	21.8859(9)	30.5952(12)
α, deg	90	75.193(2)	90
β, deg	90	78.870(2)	94.208(2)
γ, deg	90	70.815(2)	90
V, Å^3	3633.79(14)	3581.2(3)	7023.3(4)
Z	4	2	4
D_{calcd}, g/cm^3	1.372	1.496	1.522
μ/mm^{-1}	1.219	1.368	1.416
F(000)	1552.0	1632	3248.0
θ range, °	7.008-136.752	4.206-133.188	4.858-133.192
Index ranges	-17 ≤ h ≤ 17	-15 ≤ h ≤ 15	-21 ≤ h ≤ 21
	-15 ≤ k ≤ 11	-16 ≤ k ≤16	-14 ≤ k ≤ 15
	-23 ≤ l ≤ 24	-26 ≤ l ≤ 26	-36 ≤ l ≤ 36
Reflections collected	29274	148386	159556
Independent reflections	6530	12648	12386
	R_{int} = 0.0782	R_{int} = 0.0636	R_{int} = 0.1309
	R_{sigma} = 0.0524	R_{sigma} = 0.0252	R_{sigma} = 0.0432
Data/restraints/parameters	6530/1/481	12648/494/1266	12386/120/1091
Goodness-of-fit on F^2	1.018	1.049	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0343	R_1 = 0.0642	R_1 = 0.0510
	wR_2 = 0.0736	wR_2 = 0.1643	wR_2 = 0.1437
Final R indexes [all data]	R_1 = 0.0444	R_1 = 0.0719	R_1 = 0.0693
	wR_2 = 0.0779	wR_2 = 0.1694	wR_2 = 0.1556
Largest diff. peak/hole, e/Å^{-3}	0.16/-0.17	1.03/-0.42	0.44/-0.45

Table S2. Crystal data and structure refinement details for compounds **4**, **5**

	4	**5**
CCDC	2294597	2294599
Empirical formula	$C_{87}H_{67}Al_2BF_{30}N_2$	$C_{39}H_{36}AlF_{11}N_2$
Formula weight	1775.19	768.68
Temperature, K	200	260
Crystal system	monoclinic	orthorhombic
Space group	*P*21/n	*P*ca2$_1$
a, Å	13.1747(9)	14.4808(11)
b, Å	18.3068(13)	12.6637(9)
c, Å	33.223(3)	20.2440(14)
α, deg	90	90
β, deg	94.272(4)	90
γ, deg	90	90
V, Å^3	7990.8(10)	3712.4(5)
Z	4	4
D_{calcd}, g/cm^3	1.476	1.375
μ/mm^{-1}	1.383	1.247
F(000)	3616	1584
θ range, °	5.334-133.192	6.98 - 138.142
Index ranges	$-15 \le h \le 14$	$-17 \le h \le 17$
	$-20 \le k \le 21$	$-15 \le k \le 15$
	$-39 \le l \le 39$	$-24 \le l \le 24$
Reflections collected	79000	45397
Independent reflections	14061	6772
	R_{int} = 0.1152	R_{int} = 0.0873
	R_{sigma} = 0.0660	R_{sigma} = 0.0552
Data/restraints/parameters	14061/1146/1196	6772/1/486
Goodness-of-fit on F^2	1.037	1.092
Final R indexes [I>=2σ (I)]	R_1 =0.0718	R_1 = 0.0564
	wR_2 = 0.1938	wR_2 = 0.1304
Final R indexes [all data]	R_1 = 0.0965	R_1 = 0.0680
	wR_2 = 0.2135	wR_2 = 0.1391
Largest diff. peak/hole, e/Å^{-3}	0.86/-0.51	0.23/-0.22

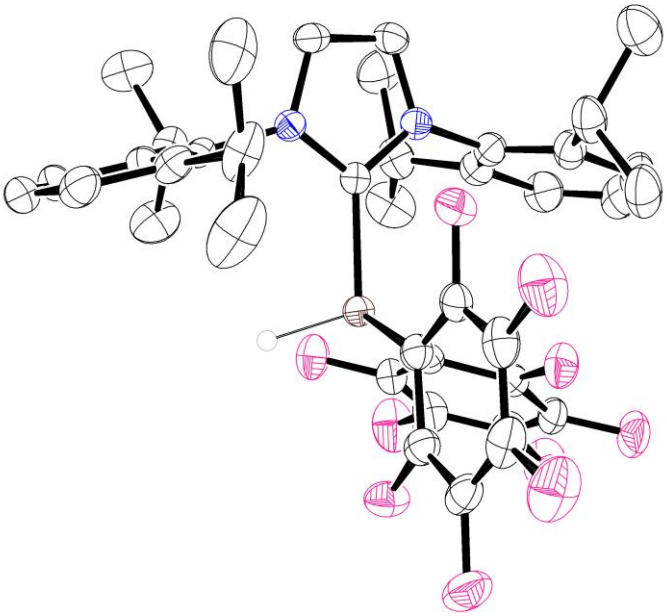


Figure S4-1. Solid-state structures of **1**. Hydrogen atoms except that on Al are omitted for clarity. Thermal ellipsoids are set at the 50% probability level.

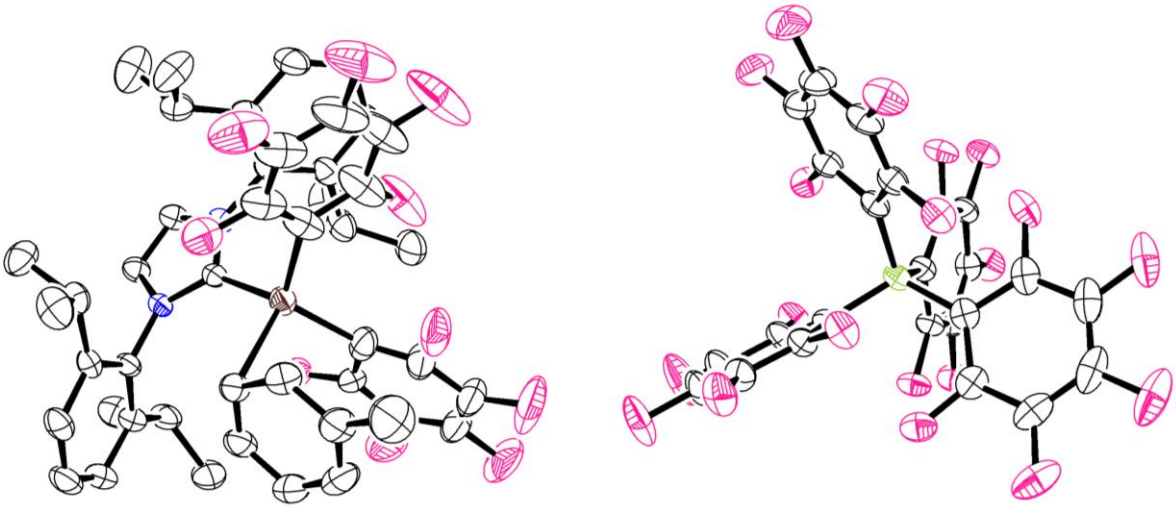


Figure S4-2. Solid-state structures of **2**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 50% probability level.

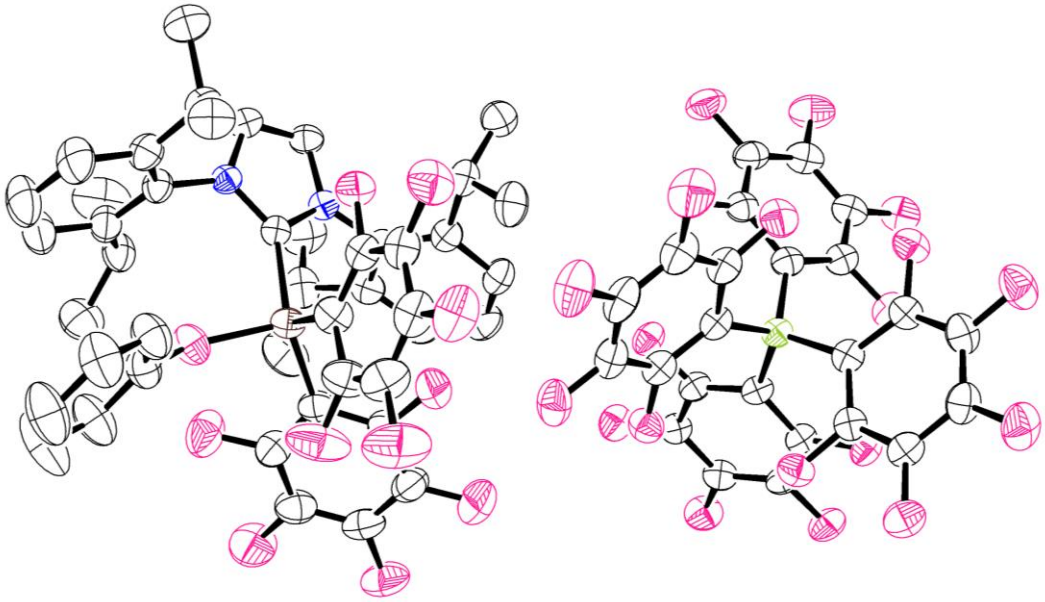


Figure S4-3. Solid-state structures of **3**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 50% probability level.

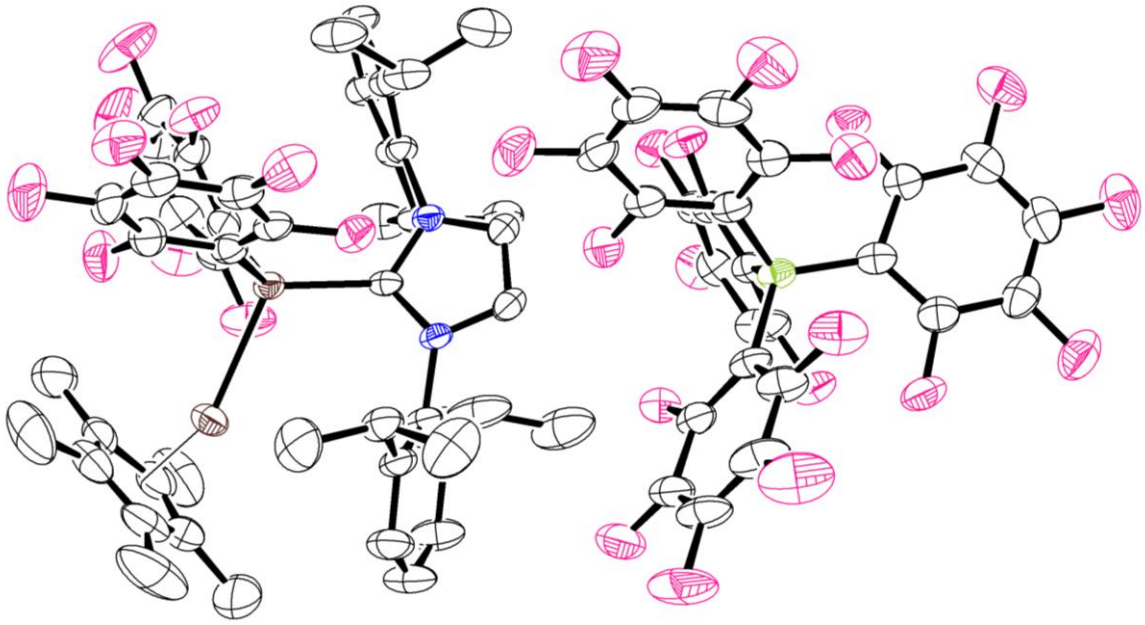


Figure S4-4. Solid-state structures of **4**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 50% probability level.

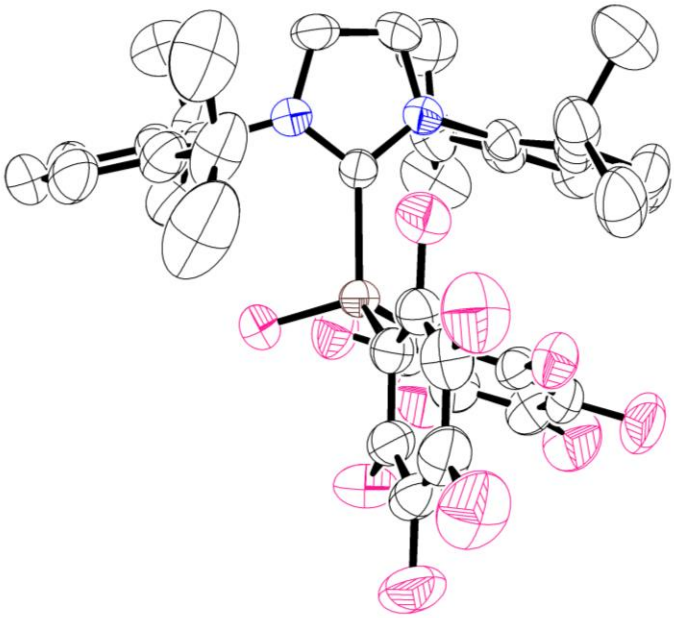
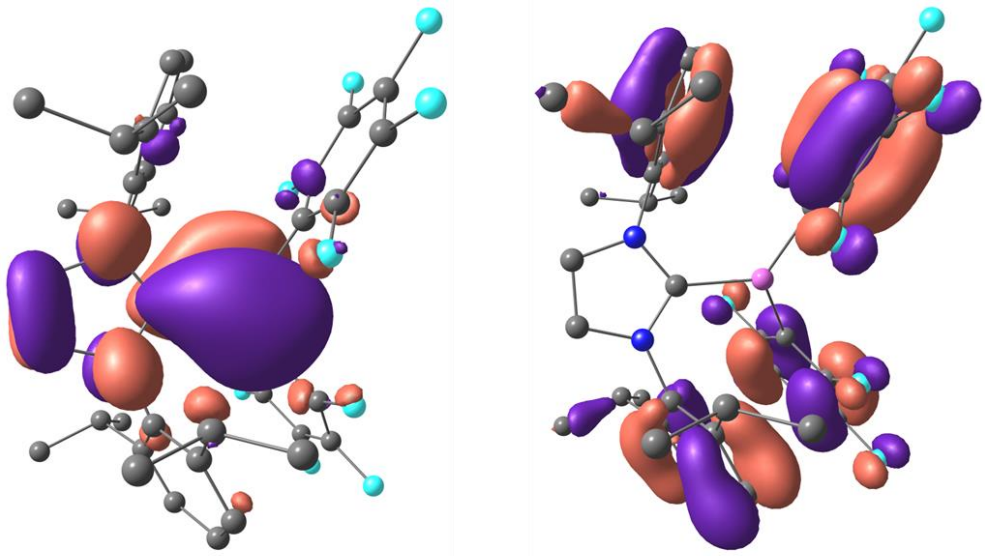


Figure S4-5. Solid-state structures of **5**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are set at the 50% probability level.

Computational Details

Density functional theory (DFT) calculations were carried out using the Gaussian 16 package[S12]. Geometry optimizations were performed with the hybrid B3LYP functional[S13] and The def2-SVP basis set[S14] was employed for all the atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum) and provide the thermal corrections of Gibbs free energy. The single-point energy calculations were performed at the B3LYP/def2-TZVP level of theory for solution-phase (fluorobenzene). Optimized structures were visualized by the Chemcraft[15] program.



LUMO (-5.44 eV)

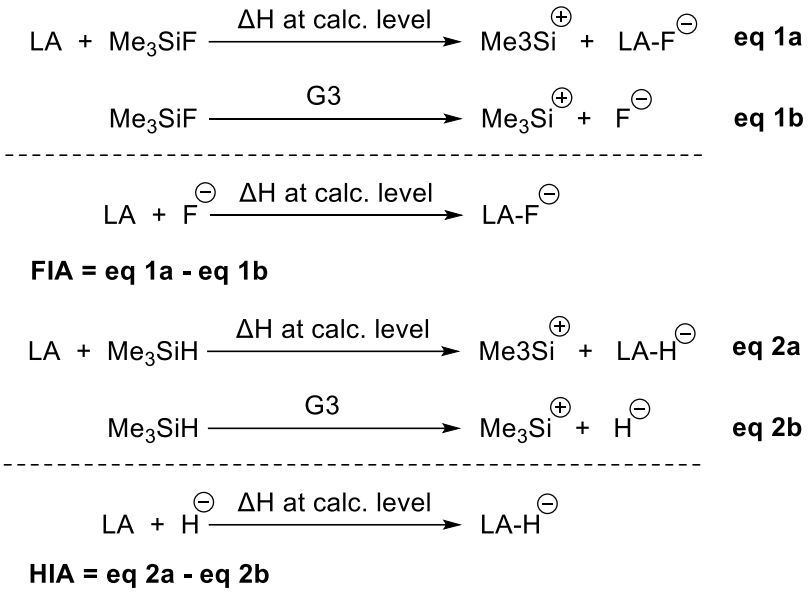
HOMO (-9.79 eV)

Gap: 4.34 eV (419.57 kJ/mol)

Figure S5-1. Selected molecular orbitals for **I** at B3LYP-D3/def2-TZVP level. Isovalue = 0.03.

FIA and HIA calculation

For gas phase FIA and HIA calculation, geometries and final electronic energies were obtained at the BP86-D3/def2-SVP level of theory. The FIA reaction enthalpies were calculated according to the scheme proposed by Krossing[S16] using the given G3 anchor points and isodesmic reactions according to: The TMS-system anchor enthalpy of $Me_3Si^+ + F^- \rightarrow Me_3SiF$ at the G3 (958 kJ/mol) and $Me_3Si^+ + H^- \rightarrow Me_3SiH$ at the G3 (959 kJ/mol). For solvent corrected (fluorobenzene) FIA (FIA_{solv}) and HIA (HIA_{solv}), the PCM method was used on the BP86-D3/def2-SVP-level. The final solvation corrected FIA_{solv} is obtained by eq. 3 and eq. 4:



$$FIA_{solv} = FIA - [\Delta G_{solv}(LA\text{-}F^-) - \Delta G_{solv}(LA) - \Delta G_{solv}(F^-)] \quad \textbf{eq 3}$$

$$HIA_{solv} = HIA - [\Delta G_{solv}(LA\text{-}H^-) - \Delta G_{solv}(LA) - \Delta G_{solv}(H^-)] \quad \textbf{eq 4}$$

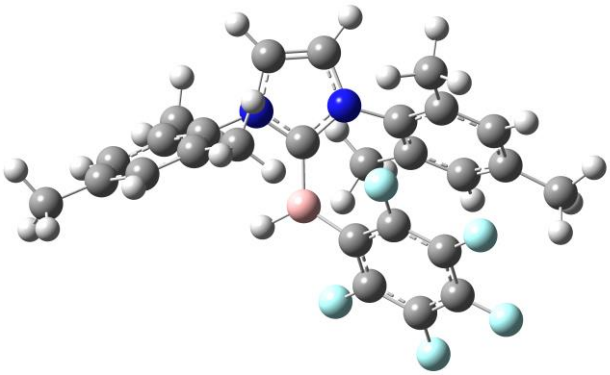
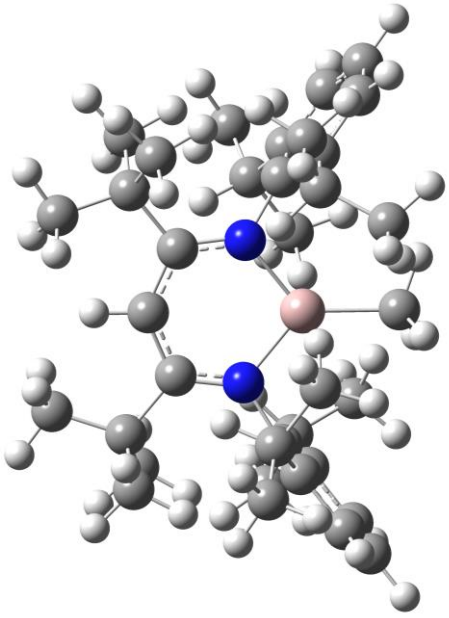
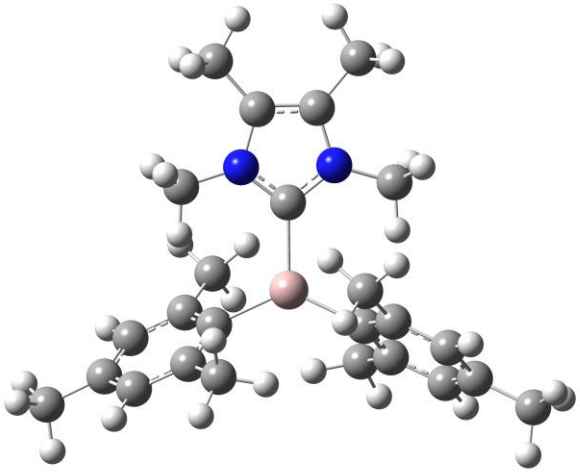
Table S3. Computed energies of FIAs and HIAs

	G (a.u.)	G_{solv} (a.u.)	ΔG_{solv} (kJ/mol)	FIA (kJ/mol)	FIA_{solv} (kJ/mol)	HIA (kJ/mol)	HIA_{solv} (kJ/mol)
SbF_5	-739.254323	-739.259417	-13.374297	**483.23**	**383.48**		
SbF_6-	-839.181431	-839.249054	-177.544187				
$B(C_6F_5)_3$	-2206.621965	-2206.625571	-9.467553	**458.29**	**261.34**	**488.09**	**263.11**
$B(C_6F_5)_3$-F	-2306.543723	-2306.588818	-118.396922				
$B(C_6F_5)_3$-H	-2207.316797	-2207.359579	-112.324141				
$Al(C_6F_5)_3$	-2424.18735	-2424.192192	-12.712671	**547.04**	**336.34**	**491.6**	**259.38**
$Al(C_6F_5)_3$-F	-2524.143788	-2524.18488	-107.887046				
$Al(C_6F_5)_3$-H	-2424.883787	-2424.92505	-108.336006				
$HAl(C_6F_5)_2$	-1697.502899	-1697.507665	-12.513133	**508.79**	**320.33**	**459.55**	**251.43**
$HAl(C_6F_5)_2$-F	-1797.445693	-1797.495179	-129.925493				
$HAl(C_6F_5)_2$-H	-1698.187145	-1698.237508	-132.228056				
J[17]	-1323.771359	-1323.810764	-103.457827	**758.77**	**379.37**	**692.63**	**287.57**
J-F	-1423.803313	-1423.814713	-29.9307				
J-H	-1324.539304	-1324.549299	-26.2418725				
F[18]	-1755.668391	-1755.707645	-103.061377	**764.78**	**372.04**	**693**	**276.02**
F-F	-1855.706326	-1855.712494	-16.194084				
F-H	-1756.439994	-1756.445293	-13.9125245				
D[19]	-1675.800245	-1675.843343	-113.153799	**767.2**	**375.97**	**802.5**	**380.34**
D-F	-1775.836654	-1775.847233	-27.7751645				
D-H	-1676.612247	-1676.619419	-18.830086				
I	-2855.619333	-2855.662861	-114.282764	**813.63**	**422.14**	**758.19**	**340.13**
I-F	-2955.672785	-2955.683704	-28.6678345				
I-H	-2856.412984	-2856.422149	-24.0627075				
F-	-99.698735	-99.815235	-305.87075				
H-	-0.498737	-0.623604	-327.838309				

G values are calculated at BP86-D3/def2-SVP level;

G_{solv} values are calculated at PCMBP86-D3/def2-SVP level.

Table S4. The Optimized structures of **D**, **F** and **J**

D	
F	
J	

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Cartesian Coordinates of the Optimized Geometries

I (B3LYP-D3/def2-TZVP)

SCF Done: E(RB3LYP) = -2859.23956883 A.U.

Al	0.00005900	0.62644700	0.00019500
F	1.79781500	0.81983500	-2.51152500
N	-0.98088300	-2.16544200	-0.44704400
N	0.98091400	-2.16567500	0.44652700
F	1.70884300	2.24492300	1.96743400
F	4.23600800	1.98659800	-2.83744300
F	-1.79797800	0.81906000	2.51185000
C	0.00004800	-1.35276000	-0.00013700
F	-1.70871600	2.24513300	-1.96679400
C	0.61637200	-3.48214700	0.28672300
H	1.25145900	-4.29263700	0.59004000
C	-0.61660900	-3.48200200	-0.28740700
H	-1.25188000	-4.29233000	-0.59078500
C	-2.20744700	-1.65595900	-1.01967800
C	2.20755300	-1.65651600	1.01930900
C	-2.15391600	-1.12990600	-2.31929000
F	5.41981800	3.23393200	-0.73743100
F	4.17169600	3.35671100	1.67067200
C	3.35998600	-1.65346800	0.22238300
C	2.15399200	-1.13069500	2.31900700
C	-3.35980900	-1.65296300	-0.22267800
C	-0.92167200	-1.27563800	-3.19963300
H	-0.03196100	-1.22196700	-2.56789000
C	-3.31749900	-0.53505800	-2.80214600
H	-3.32446500	-0.10292700	-3.79137900
C	-4.46589800	-0.48124500	-2.02741000
H	-5.35383000	-0.00322400	-2.41967600
F	-4.23635600	1.98541600	2.83775700
C	3.40975300	-2.33981700	-1.13129300
H	2.39229700	-2.39018500	-1.52571700
C	0.92164300	-1.27634400	3.19919900
H	0.03200800	-1.22280400	2.56733500

C	-4.49118500	-1.04454600	-0.76053200
H	-5.40192400	-1.00701000	-0.18056800
C	3.31757900	-0.53601300	2.80205400
H	3.32448800	-0.10403700	3.79135800
C	-3.40951400	-2.33965500	1.13082000
H	-2.39206400	-2.38994100	1.52526300
C	-1.70175800	1.50846200	0.26558600
C	1.70176600	1.50870200	-0.26509500
C	-3.92465100	-3.77920300	0.96073800
H	-4.95781600	-3.77147800	0.60989900
H	-3.89419500	-4.30975800	1.91322400
H	-3.34019100	-4.34569300	0.23580600
C	2.37268300	1.46761200	-1.47380000
C	4.49135100	-1.04519400	0.76041600
H	5.40211800	-1.00756700	0.18050200
C	-0.92162800	-2.66355900	-3.86225900
H	-0.95205100	-3.46743000	-3.12631600
H	-0.02489300	-2.79374400	-4.46951500
H	-1.79117200	-2.77253900	-4.51231900
C	-4.26129300	-1.60797900	2.17020800
H	-3.93827200	-0.58086300	2.31609800
H	-4.18513300	-2.11979400	3.12993200
H	-5.31618600	-1.59824900	1.89510800
C	-0.78198600	-0.18072800	-4.25825100
H	-1.55157900	-0.26438600	-5.02643300
H	0.18276000	-0.27680100	-4.75588400
H	-0.84049700	0.81659500	-3.82502500
C	4.46602700	-0.48213700	2.02740500
H	5.35396000	-0.00422800	2.41980700
C	0.78182800	-0.18125400	4.25760900
H	1.55137700	-0.26472900	5.02585800
H	-0.18294900	-0.27729100	4.75518900
H	0.84031400	0.81599400	3.82420300
C	-2.37280600	1.46700200	1.47420700
C	4.26136500	-1.60771700	-2.17051500

H	3.93830500	-0.58055100	-2.31596200
H	4.18510400	-2.11916200	-3.13042700
H	5.31629200	-1.59806300	-1.89554200
F	-5.42010100	3.23307300	0.73790100
C	3.92523600	-3.77929500	-0.96164300
H	4.95844700	-3.77140700	-0.61094300
H	3.89478300	-4.30961200	-1.91426200
H	3.34102800	-4.34612200	-0.23678200
C	2.32991100	2.17481100	0.77299300
C	3.61407400	2.04849600	-1.66307400
F	-4.17173700	3.35655600	-1.67004400
C	-2.32988800	2.17470900	-0.77242400
C	0.92158100	-2.66415300	3.86205900
H	0.95210700	-3.46814400	3.12625200
H	0.02478500	-2.79426300	4.46924000
H	1.79105900	-2.77299600	4.51223100
C	4.22102200	2.69115900	-0.58842900
C	3.57922300	2.75625400	0.64361000
C	-3.61429900	2.04766900	1.66347200
C	-4.22121600	2.69049500	0.58890600
C	-3.57929500	2.75595000	-0.64305200

SbF_5 (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -739.231044542 A.U.

Sb	0.00000200	0.00013600	0.00000000
F	0.00000200	0.00340300	1.92298800
F	0.00753400	1.91467900	0.00000000
F	0.00000200	0.00340300	-1.92298800
F	1.65161100	-0.96762500	0.00000000
F	-1.65916100	-0.95463100	0.00000000

SbF_5 (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -739.235527147 A.U.

Sb	-0.00000800	0.00074600	0.00000000
F	-0.00000800	0.00170600	1.92516500
F	0.00812200	1.91543600	0.00000000
F	-0.00000800	0.00170600	-1.92516500
F	1.65111300	-0.96842500	0.00000000

F	-1.65917400	-0.95465100	0.00000000

SbF_6^- (BP86-D3/Def2-SVP)

BP86-D3/Def2-SVP

SCF Done: E(RB-P86) = -839.163326436 A.U.

Sb	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	1.95131100
F	0.00000000	0.00000000	-1.95131100
F	0.00000000	1.95131100	0.00000000
F	-1.95131100	0.00000000	0.00000000
F	0.00000000	-1.95131100	0.00000000
F	1.95131100	0.00000000	0.00000000

SbF_6^- (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -839.229432939 A.U.

Sb	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	1.94979900
F	0.00000000	0.00000000	-1.94979900
F	0.00000000	1.94979900	0.00000000
F	-1.94979900	0.00000000	0.00000000
F	0.00000000	-1.94979900	0.00000000
F	1.94979900	0.00000000	0.00000000

$B(C_6F_5)_3$ (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -2206.70915384 A.U.

B	-0.00016400	0.00084300	0.00000800
C	1.31541200	0.85374600	0.00000100
C	2.45984600	0.46155500	-0.73047600
C	1.42556600	2.05828500	0.73087000
C	3.64318400	1.21537100	-0.75114100
C	2.59736100	2.82994400	0.75150600
C	3.70931300	2.40426600	0.00010200
C	0.08096500	-1.56491700	0.00018800
C	-0.83000900	-2.36047100	-0.73081600
C	1.06953000	-2.26192000	0.73095300
C	-0.76797900	-3.76213900	-0.75144800
C	1.15273500	-3.66250700	0.75169300
C	0.22865500	-4.41324200	0.00021700
C	-1.39684300	0.71318600	0.00020100

C	-2.49454900	0.20514100	0.73095000
C	-1.63082000	1.89961000	-0.73108900
C	-3.74943500	0.83270400	0.75140400
C	-2.87605000	2.54609300	-0.75196900
C	-3.93805600	2.00811100	-0.00031900
F	-1.63559100	-4.48104200	-1.47026300
F	0.29768100	-5.74378800	0.00016900
F	2.09035600	-4.28781800	1.47009900
F	1.96384600	-1.58809900	1.47367300
F	-1.78860400	-1.78284400	-1.47438000
F	2.43852400	-0.65814100	-1.47296100
F	0.39558900	2.49617100	1.47438600
F	2.67088200	3.95441500	1.47013400
F	4.82760600	3.12850700	0.00022000
F	4.69962200	0.82235400	-1.46928000
F	-2.35765000	-0.90616900	1.47374000
F	-0.65135000	2.44136100	-1.47446700
F	-3.06530400	3.65676200	-1.47090200
F	-5.12515300	2.61301300	-0.00055500
F	-4.75958000	0.33297500	1.46983100

$B(C_6F_5)_3$ (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -2206.71236231 A.U.

B	0.00041400	-0.00044500	0.00038000
C	1.54652600	-0.26046400	0.00062900
C	2.44092200	0.55176600	0.73321400
C	2.12665200	-1.32023600	-0.73192200
C	3.82579100	0.32977800	0.75348800
C	3.50809500	-1.56257900	-0.75233300
C	4.35918400	-0.73258300	0.00054000
C	-0.54723500	1.46868000	0.00022400
C	-1.69679800	1.83784600	0.73397700
C	0.07975800	2.50022100	-0.73391900
C	-2.19679900	3.14823400	0.75390700
C	-0.40106600	3.81777100	-0.75488900
C	-1.54441900	4.14059500	-0.00085500
C	-0.99828900	-1.20905200	-0.00007800

C	-2.20642100	-1.18023200	-0.73217800
C	-0.74291300	-2.39026400	0.73196100
C	-3.10794500	-2.25465700	-0.75267500
C	-1.62848300	-3.47787800	0.75208100
C	-2.81540000	-3.40733600	-0.00047300
F	-3.27752800	3.46382700	1.47637000
F	-2.01061300	5.38952000	-0.00148100
F	0.20877900	4.76371500	-1.47793900
F	1.16627600	2.23716000	-1.48054400
F	-2.34552600	0.92767700	1.48092200
F	1.97702900	1.56967200	1.47872600
F	1.35581700	-2.13100400	-1.47727900
F	4.02254500	-2.56491200	-1.47357800
F	5.67385300	-0.95337700	0.00064200
F	4.63933000	1.10902200	1.47490500
F	-2.52255400	-0.10678200	-1.47707700
F	0.37064300	-2.49874800	1.47715900
F	-1.36098400	-4.57263600	1.47282500
F	-3.66470200	-4.43484800	-0.00075100
F	-4.23336800	-2.19777900	-1.47357800

B(C_6F_5)$_3$-F (BP86-D3/Def2-SVP)

BP86-D3/Def2-SVP

SCF Done: E(RB-P86) = -2306.63094768 A.U.

B	-0.09818500	-0.05987500	-0.93680500
C	0.39594200	1.42673700	-0.36800000
C	-0.18350800	2.16971800	0.67219100
C	1.55101900	1.99503800	-0.93542500
C	0.31014800	3.41571200	1.10285900
C	2.08110200	3.23749000	-0.54120300
C	1.45381600	3.95209200	0.49172400
C	-1.64324200	-0.44943800	-0.48245700
C	-2.05746400	-1.65502400	0.10245400
C	-2.68138300	0.44365300	-0.80398900
C	-3.40498300	-1.95472000	0.38860200
C	-4.03786900	0.19103400	-0.54206300
C	-4.40188100	-1.02512300	0.06009400

C	1.04008800	-1.12251400	-0.36859000
C	1.85159900	-1.92721900	-1.18482000
C	1.30680500	-1.20474600	1.00807100
C	2.87204600	-2.75402300	-0.67064400
C	2.30718500	-2.01533400	1.56742700
C	3.10325900	-2.79561000	0.71222100
F	-3.74895200	-3.12909000	0.95634300
F	-5.69660600	-1.29487400	0.31773000
F	-4.99247600	1.08941700	-0.85942500
F	-2.40003000	1.63153000	-1.38188900
F	-1.17261100	-2.62551300	0.42864100
F	-1.27336000	1.72005800	1.33373400
F	2.22951300	1.34427200	-1.90336000
F	3.18872500	3.74113300	-1.12397900
F	1.94420600	5.14221300	0.89090500
F	-0.29230900	4.09556600	2.10020100
F	1.69330300	-1.96605500	-2.52181000
F	0.55539600	-0.49198600	1.88076800
F	2.51369500	-2.05893200	2.89974400
F	4.07371600	-3.58299700	1.21746400
F	3.62936300	-3.51002900	-1.49288000
F	-0.10547800	-0.02326300	-2.36070800

$B(C_6F_5)_3$-F (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -2306.67652092 A.U.

B	-0.10342800	-0.05892300	-0.93777700
C	0.40254600	1.42332100	-0.37786400
C	-0.16758600	2.17155200	0.66396000
C	1.56687100	1.97899200	-0.93800200
C	0.34403000	3.40697800	1.10236800
C	2.11645500	3.20992400	-0.53691900
C	1.49791300	3.92917200	0.49800300
C	-1.64957000	-0.43673100	-0.48818400
C	-2.07369700	-1.63841900	0.09834700
C	-2.68243800	0.46335200	-0.80639800
C	-3.42226500	-1.92659400	0.38887700
C	-4.03971500	0.22392600	-0.54006200

C	-4.41268600	-0.98897100	0.06337400
C	1.02733800	-1.12718600	-0.37173000
C	1.84101200	-1.93470100	-1.18176600
C	1.28844600	-1.21249100	1.00597800
C	2.85524600	-2.76670900	-0.66562700
C	2.28155300	-2.02821700	1.56938200
C	3.07932100	-2.81144200	0.71822300
F	-3.77095800	-3.09685600	0.95706400
F	-5.70564400	-1.24682800	0.32433400
F	-4.98377200	1.13093100	-0.85554800
F	-2.39195500	1.65031900	-1.38792400
F	-1.19528200	-2.61687600	0.42252400
F	-1.26565000	1.73437000	1.32293900
F	2.23875200	1.32143600	-1.91020800
F	3.23149000	3.69588900	-1.11562900
F	2.00451000	5.10627600	0.90441700
F	-0.25152200	4.08780500	2.10071100
F	1.68975900	-1.96994400	-2.52326500
F	0.53581800	-0.49641800	1.87709100
F	2.47845600	-2.07241300	2.90122700
F	4.04110800	-3.60198100	1.22668900
F	3.61129600	-3.52169000	-1.48660900
F	-0.11079700	-0.02845600	-2.37146800

$B(C_6F_5)_3$-H (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -2207.41087896 A.U.

B	-0.05536000	-0.06917000	-0.87572900
C	1.20972700	-0.97477200	-0.36630600
C	1.63944400	-0.98391000	0.97104500
C	1.97987700	-1.74795300	-1.24992300
C	2.75959000	-1.70077500	1.42445400
C	3.11187300	-2.48205200	-0.84541500
C	3.50503800	-2.45403500	0.50173000
C	0.19459400	1.47332600	-0.37493200
C	-0.47342200	2.12520300	0.67473400
C	1.18716800	2.23870400	-1.01414700
C	-0.20875100	3.45420100	1.05556800

C	1.49218200	3.56714000	-0.66723000
C	0.78636600	4.17922100	0.38148900
C	-1.53022000	-0.65762900	-0.48694500
C	-2.67587400	0.05178100	-0.89654900
C	-1.79776500	-1.86892500	0.17239600
C	-3.99211800	-0.38182100	-0.67087700
C	-3.09929700	-2.34884300	0.42159700
C	-4.20601600	-1.59836900	-0.00096000
F	-0.88501000	4.03607900	2.06805200
F	1.06062400	5.45141400	0.73516300
F	2.45147600	4.25801100	-1.31886200
F	1.91041600	1.70505800	-2.02365300
F	-1.42869900	1.48971000	1.38953600
F	0.94585800	-0.29758400	1.90749100
F	1.65769000	-1.83159500	-2.55839800
F	3.82404200	-3.21068900	-1.73099900
F	4.58515800	-3.15068600	0.90934700
F	3.12796300	-1.68218100	2.72239900
F	-2.53875400	1.22920100	-1.54876600
F	-0.79525300	-2.66620000	0.61221400
F	-3.29398100	-3.52086000	1.06187300
F	-5.45974800	-2.04010900	0.22725500
F	-5.04984900	0.34677100	-1.08515800
H	-0.02498300	-0.04416700	-2.10716200

$B(C_6F_5)_3$-H (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -2207.45467288 A.U.

B	-0.05572900	-0.07317500	-0.88765900
C	1.20720200	-0.97901800	-0.37402500
C	1.62258700	-0.99854900	0.96761000
C	1.99389300	-1.73928600	-1.25347500
C	2.74161300	-1.71164700	1.42778800
C	3.12610200	-2.46946600	-0.84415900
C	3.50396700	-2.45114400	0.50746100
C	0.19498900	1.46762400	-0.38098500
C	-0.47581400	2.11824200	0.66734600
C	1.19662600	2.23220600	-1.00617200

C	-0.20534500	3.44223300	1.05967000
C	1.50875200	3.55574600	-0.64898300
C	0.79950500	4.16574800	0.39859800
C	-1.53326000	-0.65924100	-0.50343800
C	-2.67623700	0.05003800	-0.91910800
C	-1.80749200	-1.86186400	0.16843500
C	-3.99447100	-0.37208100	-0.68662000
C	-3.11080000	-2.33181800	0.42522500
C	-4.21427200	-1.57997100	-0.00308400
F	-0.88589900	4.01851000	2.07031200
F	1.07888500	5.43058100	0.76293700
F	2.47680500	4.24117200	-1.28894300
F	1.92514600	1.69931500	-2.01556100
F	-1.44237300	1.48477700	1.37221900
F	0.91218000	-0.32567800	1.90420200
F	1.68719800	-1.81194300	-2.56907700
F	3.85076000	-3.18269800	-1.72895500
F	4.58178400	-3.14235500	0.92047100
F	3.09207500	-1.70077700	2.72904700
F	-2.53305900	1.22202000	-1.58403900
F	-0.80797300	-2.66035900	0.61723000
F	-3.30818500	-3.49428700	1.07804000
F	-5.46717000	-2.01061000	0.23260800
F	-5.04555100	0.35942900	-1.10637700
H	-0.01824300	-0.04451000	-2.12123400

$Al(C_6F_5)_3$ (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -2424.26512387 A.U.

C	1.75234200	0.86865500	0.00000600
C	1.96857600	2.08611100	0.66591500
C	2.85186400	0.30264600	-0.66567100
C	3.21675200	2.72976000	0.67938200
C	4.12029300	0.90538600	-0.67912900
C	4.29459600	2.12764900	0.00012100
C	-1.62855700	1.08339100	-0.00021600
C	-2.79167100	0.66041400	0.66368300
C	-1.68815600	2.31925400	-0.66471900

C	-3.97357000	1.41892900	0.67668000
C	-2.84479100	3.11575500	-0.67862400
C	-3.99096200	2.65419000	-0.00119300
C	-0.12384400	-1.95114600	0.00020900
C	-1.16469200	-2.62085100	-0.66353900
C	0.82403900	-2.74670500	0.66432600
C	-1.27649100	-4.02075600	-0.67648900
C	0.75785500	-4.14949800	0.67819600
C	-0.30360800	-4.78236800	0.00110400
F	-5.06746900	0.99788500	1.32022000
F	-5.10152900	3.39260800	-0.00164500
F	-2.87936700	4.28706500	-1.32273600
F	-0.60768600	2.76897100	-1.33761300
F	-2.78896600	-0.50981800	1.33671500
F	0.95437100	2.66805400	1.34057900
F	2.70023500	-0.85700900	-1.33996900
F	5.15145600	0.35003100	-1.32436000
F	5.48971900	2.71952100	0.00014200
F	3.39998800	3.88645200	1.32478100
F	-2.09437500	-1.91016800	-1.33660300
F	1.83630700	-2.15894100	1.33683100
F	1.66947600	-4.88610400	1.32193900
F	-0.38812900	-6.11333900	0.00154800
F	-2.27393900	-4.63656300	-1.31986000
Al	-0.00005100	0.00056100	0.00000000

$Al(C_6F_5)_3$ (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -2424.27000079 A.U.

C	-1.20418300	1.54301700	-0.00019300
C	-0.86906800	2.73736200	-0.65807100
C	-2.44418700	1.50761200	0.65754000
C	-1.71546400	3.85760100	-0.67156800
C	-3.32621100	2.60000900	0.67011900
C	-2.95109000	3.77980900	-0.00080800
C	1.93907100	0.27138400	0.00058700
C	2.80615800	-0.61586400	-0.65689200
C	2.52777500	1.36315900	0.65841900

C	4.19944800	-0.44264200	-0.66997000
C	3.91477800	1.58097000	0.67177400
C	4.74937000	0.66647100	0.00099800
C	-0.73394900	-1.81505700	-0.00019400
C	-0.08122700	-2.87236700	0.65365300
C	-1.93841700	-2.12064700	-0.65386300
C	-0.58701100	-4.18214200	0.66668700
C	-2.48619800	-3.41337300	-0.66672100
C	-1.79881800	-4.44580000	-0.00017000
F	5.00473000	-1.30072800	-1.30870400
F	6.07141600	0.85235400	0.00112800
F	4.45198500	2.62799100	1.31046200
F	1.74960200	2.24357200	1.32430900
F	2.30115700	-1.67640000	-1.32339100
F	0.30211400	2.83005000	-1.32432200
F	-2.81792500	0.39396000	1.32405100
F	-4.50174300	2.54216300	1.30850700
F	-3.77286400	4.83198700	-0.00119800
F	-1.37458000	4.98381700	-1.31048100
F	1.07278100	-2.64071800	1.31597900
F	-2.60632300	-1.15169000	-1.31647400
F	-3.63455400	-3.67977800	-1.30157900
F	-2.29963600	-5.68337300	-0.00035000
F	0.05277000	-5.17244800	1.30130400
Al	0.00038200	-0.00029400	-0.00008500

$Al(C_6F_5)_3$-F (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -2524.22100771 A.U.

C	0.99022500	-1.63865800	-0.33759900
C	0.55850800	-2.89189100	-0.78995700
C	2.08597300	-1.65031500	0.53199500
C	1.16941800	-4.10349800	-0.42417500
C	2.73920200	-2.83197900	0.93264900
C	2.27360900	-4.06482300	0.44563400
C	-1.91566300	-0.03804500	-0.33720600
C	-2.78543300	0.96209600	-0.78972900
C	-2.47310300	-0.98084500	0.53307500

C	-4.14003500	1.03882500	-0.42336300
C	-3.82285900	-0.95566900	0.93438500
C	-4.65814400	0.06347100	0.44702600
C	0.92391500	1.67786800	-0.33816800
C	0.38632100	2.63419900	0.52979600
C	2.22617000	1.92812300	-0.78880300
C	1.08448000	3.78978300	0.93079100
C	2.97143200	3.06189800	-0.42257000
C	2.38598900	4.00054500	0.44547400
F	-4.94642700	2.01819000	-0.88016900
F	-5.95212900	0.10911500	0.81661600
F	-4.32655200	-1.88236500	1.77505600
F	-1.71803000	-1.97746400	1.05603500
F	-2.32453800	1.92937300	-1.61874900
F	-0.51025800	-2.97628300	-1.61823300
F	2.57177300	-0.49824600	1.05522100
F	3.79396100	-2.80509900	1.77288800
F	2.88093200	-5.20844600	0.81494400
F	0.72381300	-5.29142700	-0.88067400
F	-0.85560400	2.48160600	1.05069500
F	2.83334300	1.04298300	-1.61537300
F	4.22406600	3.26747200	-0.87727900
F	3.07395900	5.09750800	0.81490800
F	0.53399300	4.69144900	1.76934700
Al	-0.00089700	0.00041400	-0.99940000
F	-0.00100700	0.00031400	-2.71115900

$Al(C_6F_5)_3$-F (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -2524.26635452 A.U.

C	-1.71967100	0.85805100	0.33883500
C	-2.93154600	0.31607800	0.78420500
C	-1.82599700	1.95349800	-0.52526000
C	-4.19106200	0.81669700	0.41634000
C	-3.05902700	2.50008800	-0.92824500
C	-4.24754100	1.92396900	-0.44875600
C	0.11442700	-1.91013400	0.34275900
C	1.19042100	-2.68536300	0.79333500

C	-0.77685300	-2.55363100	-0.52236800
C	1.39105600	-4.02664800	0.42843600
C	-0.62949400	-3.89544300	-0.92152200
C	0.46378600	-4.63319700	-0.43733400
C	1.59622200	1.05620200	0.33529500
C	2.58094200	0.60642900	-0.55123000
C	1.75359200	2.36677300	0.80354000
C	3.67443700	1.39639600	-0.95360700
C	2.82123800	3.20235400	0.43681900
C	3.79146400	2.70319300	-0.45070600
F	2.44184700	-4.73581100	0.88215200
F	0.62595800	-5.91496600	-0.80467800
F	-1.50908300	-4.48070900	-1.75655100
F	-1.83911100	-1.89063700	-1.04392600
F	2.11594300	-2.13368700	1.61969300
F	-2.92122400	-0.75937200	1.61306800
F	-0.71774300	2.54243500	-1.03945300
F	-3.12094500	3.55482800	-1.76347800
F	-5.43666400	2.42659000	-0.81968800
F	-5.33333100	0.26378700	0.86614700
F	2.51512100	-0.63693800	-1.08988100
F	0.83202400	2.89310600	1.65035100
F	2.93262000	4.45850900	0.90866700
F	4.82498400	3.47720300	-0.82108500
F	4.60167800	0.92766800	-1.81040900
Al	-0.00449900	0.00318600	0.97919600
F	-0.00317200	0.00651400	2.70098600

$Al(C_6F_5)_3$-H (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -2424.96609468 A.U.

C	1.91039600	0.08845900	0.45115500
C	2.73666800	1.11809200	0.91838500
C	2.49973300	-0.79139800	-0.46344800
C	4.07722200	1.28090900	0.52932400
C	3.83729100	-0.67957300	-0.89037200
C	4.62764200	0.36686800	-0.38641300
C	-1.03128300	1.60995500	0.45067400

C	-2.33540000	1.81194800	0.91936100
C	-0.56470600	2.55885600	-0.46577500
C	-3.14667600	2.89139700	0.53003300
C	-1.33040300	3.66110300	-0.89309800
C	-2.63106600	3.82364500	-0.38760100
C	-0.87860300	-1.69832700	0.45088900
C	-1.93581600	-1.76850300	-0.46310000
C	-0.39989200	-2.92887400	0.91759000
C	-2.50815400	-2.98267000	-0.88982300
C	-0.92957900	-4.17111600	0.52872600
C	-1.99693500	-4.19049300	-0.38636000
F	-4.39864100	3.04916600	1.00690000
F	-3.38343300	4.86890100	-0.78237600
F	-0.84551400	4.55638700	-1.77831400
F	0.67275600	2.45236400	-1.00884200
F	-2.87974500	0.92982400	1.79478700
F	2.24422400	2.03169600	1.79225700
F	1.78942000	-1.81105400	-1.00501600
F	4.37097400	-1.54848900	-1.77379600
F	5.90917500	0.49571300	-0.78079800
F	4.83914700	2.28746400	1.00474300
F	-2.46404600	-0.64343300	-1.00415000
F	0.63827700	-2.95947400	1.79056400
F	-0.43867200	-5.33437600	1.00364000
F	-2.52648800	-5.36461700	-0.78064000
F	-3.52805300	-3.01015600	-1.77261200
Al	0.00021500	-0.00005800	1.15780200
H	0.00014700	-0.00016400	2.77057000

$Al(C_6F_5)_3$-H (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -2425.00991475 A.U.

C	-0.36217000	1.87967400	0.44499300
C	-1.50324000	2.54226200	0.91329400
C	0.42186700	2.59891100	-0.46369200
C	-1.86423800	3.84446400	0.53034400
C	0.11333000	3.90644600	-0.88451200
C	-1.04052700	4.52961500	-0.38038700

C	-1.44493200	-1.25416900	0.44427200
C	-1.45226900	-2.57247500	0.91627300
C	-2.45600000	-0.93506100	-0.46908000
C	-2.40170300	-3.53456700	0.53418500
C	-3.43575000	-1.85457800	-0.88906400
C	-3.40353100	-3.16372900	-0.38017100
C	1.80905600	-0.62575000	0.44457500
C	2.03794600	-1.65988900	-0.46993900
C	2.95465900	0.02531300	0.91771100
C	3.32389600	-2.04748800	-0.89187300
C	4.26236600	-0.31425300	0.53355200
C	4.44188700	-1.36555800	-0.38287700
F	-2.36973300	-4.79245800	1.01449400
F	-4.32616300	-4.06048200	-0.76811400
F	-4.39378000	-1.50714000	-1.77013700
F	-2.53203800	0.30455700	-1.01584400
F	-0.49353200	-2.97781100	1.79043500
F	-2.33453500	1.91231100	1.78467400
F	1.53858800	2.04958600	-1.00441400
F	0.89566800	4.56500900	-1.76144400
F	-1.35762900	5.77645000	-0.76861000
F	-2.97305500	4.44221600	1.00702400
F	1.00227700	-2.34523000	-1.01683100
F	2.82679600	1.05565800	1.79472100
F	5.33577100	0.34207400	1.01422400
F	5.67951700	-1.71496000	-0.77289100
F	3.50128000	-3.04946500	-1.77471200
Al	0.00033700	0.00012000	1.12855900
H	-0.00313000	0.00061800	2.74991400

$HAl(C_6F_5)_2$ (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1697.55299243 A.U.

Al	-0.00048100	1.81403600	0.00303800
F	-2.87646000	2.39398000	1.12487300
F	2.90380600	-2.41205100	1.51429900
F	0.60825000	-0.94210800	1.40593700
F	-5.17610400	0.92605500	0.98819000

F	5.17888100	-1.47301100	0.32113300
F	2.87238600	2.39386100	-1.12723500
F	-0.60514800	-0.94399000	-1.39956700
F	-2.89985600	-2.41440600	-1.51208400
F	-5.17816100	-1.47480000	-0.32556900
F	5.17293200	0.92656000	-0.99496000
C	-1.66657500	0.77398100	-0.13222800
C	-2.86003400	1.21918500	0.46008100
C	2.88305600	-1.23850700	0.87285400
C	1.66637600	0.77471200	0.13452600
C	4.05661600	-0.75444500	0.26093200
C	-4.05488300	0.48133400	0.40999500
C	-1.71271300	-0.46502200	-0.79415100
C	1.71440800	-0.46360200	0.79747800
C	-4.05623400	-0.75591500	-0.26321800
C	-2.88101100	-1.24025800	-0.87169300
C	2.85812500	1.21966200	-0.46125000
C	4.05328300	0.48215600	-0.41347700
H	-0.00097800	3.39704600	0.00626600

$HAl(C_6F_5)_2$ (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1697.55726915 A.U.

Al	-0.00038000	1.80022100	0.00250900
F	-2.88248400	2.41285200	1.09624700
F	2.92638800	-2.43118500	1.47274900
F	0.62160000	-0.98172800	1.36736200
F	-5.19001500	0.96279200	0.96445900
F	5.20456200	-1.45649700	0.31165700
F	2.87932100	2.41286100	-1.09795900
F	-0.61913200	-0.98314100	-1.36219900
F	-2.92329600	-2.43294000	-1.47114500
F	-5.20401700	-1.45787200	-0.31541200
F	5.18750000	0.96321600	-0.96994800
C	-1.67162300	0.76345900	-0.12392800
C	-2.86640100	1.22622100	0.45082000
C	2.90129600	-1.24745600	0.84639500
C	1.67147600	0.76408000	0.12593600

C	4.07532600	-0.74608400	0.25205100
C	-4.06682400	0.49823100	0.40161700
C	-1.72530300	-0.48304500	-0.77016000
C	1.72664000	-0.48194700	0.77287800
C	-4.07504000	-0.74722400	-0.25397400
C	-2.89969800	-1.24878700	-0.84554000
C	2.86490900	1.22666600	-0.45163900
C	4.06555300	0.49890200	-0.40441900
H	-0.00076400	3.38381300	0.00487400

$HAl(C_6F_5)_2$-F (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1797.49456293 A.U.

F	-2.81301000	2.12903600	1.06123300
F	2.45333600	-1.46459100	2.65594500
F	0.46439600	0.22356600	1.88203300
F	-4.80384300	0.30650600	1.32068400
F	4.66976700	-1.78917600	1.06888200
F	2.90872500	1.26127000	-2.08741500
F	-0.53558700	-0.80230600	-1.94066400
F	-2.54168100	-2.62571400	-1.67054200
F	-4.68187700	-2.07333700	-0.03783200
F	4.88696000	-0.42188200	-1.29989000
C	-1.58234400	0.74022200	-0.44977800
C	-2.69436300	0.97386800	0.36713800
C	2.54577800	-0.78799200	1.49113100
C	1.59328300	0.80892700	-0.14057200
C	3.68268100	-0.95648700	0.68173000
C	-3.74454900	0.04806200	0.52312200
C	-1.57285000	-0.48798500	-1.12066000
C	1.53564800	0.09186500	1.06074400
C	-3.68669800	-1.17299300	-0.16988300
C	-2.59097300	-1.45154300	-1.00517300
C	2.74536300	0.61201300	-0.90976700
C	3.78892700	-0.25473500	-0.53099600
H	0.09165100	2.52118900	-2.21528700
Al	0.01703200	2.00221200	-0.68686400
F	-0.05524200	3.30892900	0.42115500

$HAl(C_6F_5)_2$-F (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1797.54585250 A.U.

F	-2.80142500	2.19703000	0.89475500
F	2.51147000	-1.08647100	2.82717300
F	0.51843600	0.51629100	1.89188200
F	-4.78153500	0.39663100	1.32212500
F	4.66803600	-1.66223100	1.22990600
F	2.83847600	0.95777300	-2.25680200
F	-0.54788500	-0.95936100	-1.88779100
F	-2.54187300	-2.76167800	-1.44510900
F	-4.66543900	-2.08566700	0.16111500
F	4.82260100	-0.63475100	-1.30794300
C	-1.58604200	0.69185900	-0.51330400
C	-2.69006200	0.98698000	0.29391700
C	2.57630700	-0.57795500	1.58138600
C	1.59279200	0.79975900	-0.22154600
C	3.68293400	-0.87448800	0.76609600
C	-3.73439600	0.07499500	0.53723400
C	-1.57959400	-0.58698800	-1.08234100
C	1.56524900	0.25231200	1.06672200
C	-3.67901500	-1.19841700	-0.05494300
C	-2.59106800	-1.54110400	-0.87698900
C	2.71426800	0.47884500	-0.99391700
C	3.75805900	-0.34590800	-0.53416400
H	0.08239400	2.31710300	-2.42971700
Al	0.01045200	1.91040000	-0.86142400
F	-0.06473600	3.33225200	0.10616900

$HAl(C_6F_5)_2$-H (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1698.24177470 A.U.

Al	-0.00013600	2.26282500	-0.09227400
F	-2.81666800	1.91280900	1.62838200
F	2.55468900	-1.80460100	2.37618300
F	0.55368400	0.00695500	2.03875600
F	-4.80428700	0.07956000	1.42683200
F	4.68617500	-1.83204900	0.64329400
F	2.81555900	1.77322000	-1.77965200

F	-0.55284300	-0.16003700	-2.03143500
F	-2.55351800	-1.99340300	-2.22026500
F	-4.68593100	-1.87894300	-0.49206600
F	4.80335500	-0.03736900	-1.42971300
C	-1.59076900	0.95673500	-0.19206200
C	-2.70033600	0.97134000	0.66120900
C	2.60081600	-0.91749000	1.35848300
C	1.59067000	0.96944900	0.11364000
C	3.69282400	-0.93546500	0.47365700
C	-3.74877100	0.03385100	0.58412500
C	-1.58262600	-0.06253600	-1.15231800
C	1.58307600	0.03224200	1.15414600
C	-3.69270400	-0.97139200	-0.39594800
C	-2.60022300	-1.02589900	-1.27869200
C	2.69978600	0.91412500	-0.73855600
C	3.74830400	-0.01389500	-0.58550900
H	0.06887000	3.08521400	-1.48841200
H	-0.06932000	3.19639400	1.23207400

$HAl(C_6F_5)_2$-H (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1698.29223129 A.U.

Al	0.00819200	-0.16311200	-2.24889900
F	-2.69572500	1.71664500	-1.83875300
F	2.58491700	2.49451900	1.64705900
F	0.59546000	2.08843500	-0.16357400
F	-4.67948900	1.56569700	0.00170200
F	4.65780900	0.70194900	1.83159200
F	2.75619300	-1.91443200	-1.61781000
F	-0.64996600	-2.15376400	0.07009600
F	-2.64379500	-2.28599000	1.91701900
F	-4.66616100	-0.42811900	1.88615700
F	4.72891400	-1.49813900	0.19341400
C	-1.58684100	-0.21689600	-0.96650000
C	-2.63985400	0.70469900	-0.93686000
C	2.61303800	1.41707500	0.83832500
C	1.59106200	0.07422100	-0.97313200
C	3.67505300	0.50085900	0.93662300

C	-3.68296600	0.65824100	0.00721200
C	-1.62959800	-1.21197500	0.01794700
C	1.60292600	1.17659300	-0.10962100
C	-3.67971700	-0.36065700	0.97529100
C	-2.64347300	-1.31074400	0.98708000
C	2.66848900	-0.80860700	-0.83668400
C	3.70810000	-0.62375500	0.09424100
H	0.07942700	-1.57211800	-3.05929800
H	-0.05665400	1.11705500	-3.25067100

J (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1324.21400979 A.U.

Al	0.00030900	-0.26130800	0.00000900
C	1.76508400	-1.07994200	0.01642000
C	2.17184400	-1.89409500	-1.08117700
C	2.65846500	-0.88567000	1.10498200
C	3.44908900	-2.47751600	-1.07813400
C	3.93430500	-1.48208600	1.07703900
C	4.34834600	-2.28204400	-0.00579200
H	3.76027300	-3.10232100	-1.93209400
H	4.62334700	-1.32974800	1.92477500
C	-1.76377000	-1.08143700	-0.01653900
C	-2.65718400	-0.88835600	-1.10532300
C	-2.17017500	-1.89500700	1.08157100
C	-3.93267100	-1.48541900	-1.07707300
C	-3.44714100	-2.47914200	1.07882600
C	-4.34636700	-2.28492600	0.00628100
H	-4.62174600	-1.33396300	-1.92494400
H	-3.75811000	-3.10345400	1.93322400
C	-0.00079600	1.76508700	-0.00004800
N	-1.02799700	2.60050400	0.35098200
N	1.02546400	2.60160200	-0.35119700
C	-0.65858800	3.93644000	0.22620800
C	-2.34824200	2.17574400	0.81776400
C	0.65456300	3.93714200	-0.22664400
C	2.34614800	2.17819400	-0.81796300
H	-2.40585700	1.07175400	0.79317700

H	2.40519200	1.07429300	-0.79254000
C	1.57274500	5.06665500	-0.54915600
H	2.48416300	5.05016200	0.08476800
H	1.90311000	5.03817600	-1.60881400
H	1.06601500	6.03496800	-0.38232900
C	-1.57797800	5.06498100	0.54868000
H	-2.49011200	5.04658300	-0.08414400
H	-1.90705800	5.03708300	1.60876400
H	-1.07279600	6.03383800	0.38032300
C	-2.23510500	-0.08508300	-2.31738900
H	-1.37993500	0.59442000	-2.09368000
H	-1.90886900	-0.74861800	-3.14756000
H	-3.05761600	0.54470400	-2.71407700
C	-1.23540600	-2.09172200	2.25767300
H	-0.19237800	-2.28387500	1.91923900
H	-1.21629400	-1.19582700	2.91887300
H	-1.53492200	-2.94858100	2.89244700
C	-5.70370900	-2.94354600	0.01792500
H	-6.20539400	-2.82127800	0.99978600
H	-6.36840900	-2.53282700	-0.76679700
H	-5.61056000	-4.03680500	-0.16000800
C	2.23624900	-0.08179300	2.31660600
H	1.37897000	0.59520000	2.09338600
H	1.91311000	-0.74497700	3.14825900
H	3.05779500	0.55067800	2.71105500
C	1.23683900	-2.09244300	-2.25682100
H	0.19480400	-2.28878700	-1.91778300
H	1.21396000	-1.19561800	-2.91664900
H	1.53893700	-2.94725300	-2.89312000
C	5.70624900	-2.93950400	-0.01758300
H	6.21083000	-2.81000700	-0.99707800
H	6.36821300	-2.53344800	0.77184300
H	5.61357900	-4.03404000	0.15238300
H	2.51826400	2.53975200	-1.85059000
H	3.13112200	2.59056000	-0.15493900

H	-2.52107400	2.53793600	1.85004300
H	-3.13360200	2.58651100	0.15419700

J (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1324.26106902 A.U.

Al	0.00005300	-0.22728700	-0.00007800
C	1.75588000	-1.07776800	0.02061400
C	2.16119000	-1.90174100	-1.07048000
C	2.64412500	-0.88798200	1.11299900
C	3.43019200	-2.50406700	-1.05502100
C	3.91313300	-1.50334400	1.09806700
C	4.32397300	-2.31432800	0.02344300
H	3.73901000	-3.13690700	-1.90425700
H	4.59818500	-1.35219100	1.94944500
C	-1.75558500	-1.07814900	-0.02077900
C	-2.64401800	-0.88842800	-1.11303500
C	-2.16065800	-1.90215600	1.07036600
C	-3.91296000	-1.50389500	-1.09791300
C	-3.42960500	-2.50462500	1.05507700
C	-4.32355200	-2.31497500	-0.02325200
H	-4.59818100	-1.35272100	-1.94914900
H	-3.73825000	-3.13748000	1.90436500
C	-0.00019100	1.78345100	-0.00005000
N	-1.00713000	2.61683300	0.40554200
N	1.00655900	2.61709500	-0.40556300
C	-0.64436300	3.95095700	0.26146300
C	-2.29802600	2.19020900	0.94446300
C	0.64348100	3.95112400	-0.26140000
C	2.29756300	2.19080900	-0.94449100
H	-2.35383800	1.08697300	0.92412000
H	2.35365100	1.08758400	-0.92416600
C	1.54316200	5.07880800	-0.63469000
H	2.48974300	5.05536700	-0.05542800
H	1.81040100	5.04743300	-1.71163300
H	1.04821800	6.04697800	-0.43664800
C	-1.54428900	5.07841400	0.63484700
H	-2.49095000	5.05471400	0.05572600

H	-1.81135700	5.04701300	1.71183200
H	-1.04962500	6.04670600	0.43669800
C	-2.23205000	-0.06605000	-2.31534000
H	-1.35937500	0.59105800	-2.09828400
H	-1.93974700	-0.71732400	-3.16728800
H	-3.05167900	0.58949500	-2.67418700
C	-1.23515300	-2.08903200	2.25480100
H	-0.18977000	-2.28324100	1.92626600
H	-1.21796200	-1.18342200	2.90210200
H	-1.54225700	-2.93799700	2.89663300
C	-5.67792400	-2.98261100	-0.01862600
H	-6.22956100	-2.76835300	0.92066900
H	-6.30218900	-2.65045200	-0.87106900
H	-5.57562600	-4.08729900	-0.08247100
C	2.23192300	-0.06570500	2.31529500
H	1.35872300	0.59075700	2.09838900
H	1.94035000	-0.71701900	3.16745900
H	3.05119100	0.59050900	2.67375600
C	1.23579900	-2.08880600	-2.25497200
H	0.19052400	-2.28366500	-1.92648300
H	1.21811400	-1.18303100	-2.90203000
H	1.54337200	-2.93743200	-2.89702700
C	5.67856500	-2.98151400	0.01877100
H	6.23200100	-2.76300800	-0.91851100
H	6.30103800	-2.65262400	0.87378200
H	5.57660700	-4.08648900	0.07764600
H	2.41176500	2.55100800	-1.98493200
H	3.11790400	2.60058500	-0.32491600
H	-2.41231700	2.55036000	1.98491000
H	-3.11847600	2.59978100	0.32489800

J-F (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1424.25153290 A.U.

Al	0.04078200	-0.25869300	0.85592500
C	-1.63524700	-1.11825200	0.16640000
C	-2.08007000	-2.28998600	0.85303900
C	-2.41287500	-0.67759500	-0.94002800

C	-3.26036100	-2.95145300	0.46397000
C	-3.59410600	-1.35827400	-1.30937800
C	-4.04369300	-2.49327300	-0.61331800
H	-3.57443100	-3.85824200	1.01049600
H	-4.17556200	-0.99854800	-2.17674200
C	1.83094400	-0.96679600	0.30632900
C	3.00224800	-0.45071700	0.94141100
C	2.01610200	-1.92743200	-0.73303900
C	4.28522100	-0.88804700	0.55472500
C	3.31290400	-2.34350100	-1.10095900
C	4.46361000	-1.84024400	-0.46603600
H	5.17285600	-0.47327200	1.06427900
H	3.42890100	-3.08686400	-1.90914500
C	-0.03606400	1.73683400	0.31022600
N	0.62470500	2.43408100	-0.65820700
N	-0.96863700	2.60998700	0.78808400
C	0.10456700	3.72346100	-0.80749300
C	1.70339900	1.89141000	-1.47653700
C	-0.91877700	3.83479400	0.11730300
C	-1.95052200	2.25581200	1.81212700
H	1.92907400	0.86558700	-1.12614400
H	-1.54086900	1.40976300	2.39763300
C	-1.83404300	4.97122900	0.42862800
H	-2.90068700	4.68524000	0.31122000
H	-1.70163300	5.33834500	1.46916000
H	-1.63731400	5.82114600	-0.25202100
C	0.64267900	4.70161900	-1.79696500
H	1.70982100	4.94304000	-1.60293700
H	0.57584000	4.31672400	-2.83686000
H	0.07229900	5.64867500	-1.75278000
C	2.89151500	0.61207700	2.01756700
H	2.56358000	1.58557000	1.58647700
H	2.13154900	0.34500400	2.77887600
H	3.86233700	0.78728000	2.52299100
C	0.83660700	-2.52140500	-1.47790500

H	0.14971600	-3.06597400	-0.79846500
H	0.21368900	-1.74072500	-1.96210300
H	1.16972600	-3.22652300	-2.26593300
C	5.84184700	-2.33148200	-0.84480900
H	6.61717700	-1.55948000	-0.66173900
H	6.12567900	-3.22566000	-0.24634100
H	5.89229800	-2.62754200	-1.91275800
C	-1.99702600	0.51262700	-1.78684900
H	-2.19307100	1.48300500	-1.28106200
H	-0.91321900	0.48780000	-2.02288400
H	-2.54691300	0.53304200	-2.74964400
C	-1.25908900	-2.86245300	1.99239100
H	-0.21440400	-3.06790600	1.66610100
H	-1.17847300	-2.14571000	2.83517700
H	-1.68417600	-3.81318300	2.37129000
C	-5.31795900	-3.20634700	-1.00408100
H	-6.10794000	-3.07415700	-0.23241700
H	-5.72204500	-2.82569100	-1.96381600
H	-5.15664800	-4.30006800	-1.11075500
H	-2.12311700	3.12026200	2.48059400
H	-2.90836500	1.95314600	1.34160600
H	1.40031800	1.86070700	-2.54267300
H	2.61486500	2.51339400	-1.37699900
F	-0.11381900	-0.06992100	2.58575800

J-F (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1424.26327442 A.U.

Al	0.02581200	-0.19988000	0.83979600
C	-1.63121900	-1.13290400	0.19138800
C	-1.97132400	-2.35941100	0.84166400
C	-2.47760200	-0.70333100	-0.86975500
C	-3.11434000	-3.09067000	0.46102800
C	-3.61926300	-1.45368000	-1.23122700
C	-3.96392800	-2.64766200	-0.57219000
H	-3.34513500	-4.03898500	0.97803200
H	-4.25477000	-1.10001600	-2.06236400
C	1.81492000	-0.92807000	0.28797900

C	2.99195400	-0.42864400	0.92721200
C	1.99455200	-1.89168300	-0.75018500
C	4.27073500	-0.89367200	0.55682700
C	3.28717400	-2.33738800	-1.10217700
C	4.44183500	-1.85747900	-0.45551500
H	5.16128600	-0.48815200	1.06877900
H	3.39693300	-3.08150000	-1.91065500
C	-0.06387900	1.78527000	0.29606400
N	0.56200400	2.45655300	-0.71364900
N	-0.95606600	2.68382200	0.80538900
C	0.06052700	3.75337200	-0.85618500
C	1.59646600	1.89192100	-1.57367000
C	-0.91436100	3.89816900	0.11603000
C	-1.89317300	2.37955900	1.88460700
H	1.83023800	0.87070200	-1.21936900
H	-1.51642200	1.49222000	2.42620000
C	-1.79000800	5.05620600	0.45752500
H	-2.86583700	4.78831000	0.39994900
H	-1.59539200	5.43197100	1.48470300
H	-1.61123500	5.89167600	-0.24483700
C	0.56797300	4.70627000	-1.88508500
H	1.64703200	4.92878100	-1.74394000
H	0.44501700	4.30463000	-2.91302700
H	0.01655300	5.66334700	-1.82782800
C	2.89394200	0.65055600	1.98826700
H	2.52680300	1.60571000	1.54980100
H	2.16649000	0.37976100	2.77945700
H	3.87638900	0.85634900	2.45814200
C	0.81516000	-2.45179500	-1.52154200
H	0.12530300	-3.02312000	-0.86733000
H	0.19773900	-1.64725800	-1.97237800
H	1.14914800	-3.12376800	-2.33771100
C	5.81470500	-2.37579000	-0.81808800
H	6.59724500	-1.60445900	-0.66569000
H	6.09265200	-3.24811400	-0.18563300

H	5.85926600	-2.71375000	-1.87352700
C	-2.17843700	0.54981400	-1.67298700
H	-2.35810800	1.47655500	-1.08796700
H	-1.11961400	0.58285700	-2.00248700
H	-2.81263000	0.60803400	-2.58045400
C	-1.07884100	-2.91763200	1.93434400
H	-0.02742600	-3.01239900	1.58060900
H	-1.04312200	-2.24190400	2.81339700
H	-1.41327200	-3.91941800	2.27009300
C	-5.20268000	-3.42783400	-0.94967500
H	-6.01732000	-3.27359400	-0.20785500
H	-5.59501700	-3.11884400	-1.93956200
H	-5.00392900	-4.51950700	-0.98186000
H	-1.95349700	3.23598500	2.58208800
H	-2.90276500	2.17280900	1.47516800
H	1.24420900	1.85084500	-2.62357500
H	2.51449300	2.50952200	-1.52604900
F	-0.09930600	-0.05782500	2.58224700

J-H (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1324.99228466 A.U.

Al	0.12717600	-0.30494900	1.00557700
C	-1.50062100	-1.24042900	0.25737100
C	-2.05491700	-2.32690200	1.00220800
C	-2.17350400	-0.86644800	-0.94024600
C	-3.23812500	-2.96444000	0.58185100
C	-3.36027600	-1.52117800	-1.33926300
C	-3.91874400	-2.56710500	-0.58571100
H	-3.63719600	-3.80531400	1.17644500
H	-3.85646500	-1.21538400	-2.27761800
C	1.97152100	-0.84976000	0.40893500
C	3.10183500	-0.21887200	1.01445200
C	2.22961800	-1.82532300	-0.60050400
C	4.41401400	-0.54202300	0.61178700
C	3.55331900	-2.12725400	-0.98374000
C	4.66324200	-1.49692600	-0.39082400
H	5.26739900	-0.03490700	1.09576600

H	3.72419800	-2.88232100	-1.77120100
C	-0.17741000	1.66406200	0.43559500
N	0.46194800	2.49360900	-0.43950500
N	-1.28206200	2.36555000	0.82611600
C	-0.23539200	3.69406200	-0.61412800
C	1.67711200	2.14729800	-1.16703800
C	-1.35506200	3.61017300	0.19341900
C	-2.30372300	1.81806500	1.71352100
H	1.98636400	1.12649100	-0.87093000
H	-1.82747000	1.04750000	2.35151000
C	-2.46740900	4.57777900	0.42338800
H	-3.45589000	4.13596700	0.17570600
H	-2.51153600	4.91862900	1.48031800
H	-2.33296400	5.47515600	-0.20990700
C	0.24260400	4.78091400	-1.51733300
H	1.23847800	5.16658000	-1.21046000
H	0.33374100	4.43504300	-2.56916600
H	-0.46423000	5.63211600	-1.50493600
C	2.91490400	0.83238000	2.09062500
H	2.38317700	1.73023100	1.70322800
H	2.28841100	0.45034200	2.92360800
H	3.88489500	1.17314500	2.50510500
C	1.10016200	-2.56335400	-1.29132900
H	0.44989600	-3.09354000	-0.56605700
H	0.42761100	-1.87266800	-1.84061000
H	1.48682700	-3.30791100	-2.01620300
C	6.07397300	-1.86278800	-0.79179800
H	6.78596100	-1.03777100	-0.58505000
H	6.43276700	-2.75275800	-0.22830900
H	6.14072800	-2.11575100	-1.87013900
C	-1.63860700	0.22230900	-1.85404700
H	-1.95829400	1.23942700	-1.53581700
H	-0.53019800	0.22501400	-1.87942200
H	-1.99878800	0.08497300	-2.89422900
C	-1.36280600	-2.83558000	2.25193700

H	-0.28211900	-3.02461400	2.07011800
H	-1.40648800	-2.09275800	3.07648600
H	-1.81381600	-3.78182400	2.61302900
C	-5.18911000	-3.26356500	-1.01754900
H	-5.98936200	-3.15991200	-0.25292500
H	-5.57766000	-2.85110300	-1.97047000
H	-5.02626100	-4.35341500	-1.16173500
H	-2.72025200	2.62094800	2.35034300
H	-3.11471100	1.34054700	1.12693000
H	1.48867900	2.17118400	-2.25927800
H	2.49339600	2.85696900	-0.92543100
H	-0.02091700	-0.14865900	2.62305100

J-H (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1325.00294447 A.U.

Al	0.03054900	-0.19864400	0.96399200
C	-1.62154100	-1.14604400	0.29119100
C	-1.98822900	-2.35360900	0.96192300
C	-2.44371400	-0.73403500	-0.79698400
C	-3.13285900	-3.08149300	0.57722100
C	-3.58703500	-1.48014000	-1.16157600
C	-3.95893500	-2.65373000	-0.48061200
H	-3.38231000	-4.01628700	1.11012500
H	-4.20083600	-1.14143500	-2.01513100
C	1.82773600	-0.91277800	0.37591900
C	3.00799500	-0.40554200	1.00373800
C	2.00497500	-1.89568100	-0.64472700
C	4.28611800	-0.87660900	0.63701000
C	3.29678700	-2.34716400	-0.99318900
C	4.45425200	-1.85686900	-0.35944400
H	5.17814700	-0.46236500	1.13945200
H	3.40355800	-3.10473600	-1.78962700
C	-0.09691900	1.77655200	0.38149900
N	0.56395700	2.47684900	-0.58610100
N	-1.02267900	2.65595000	0.86710200
C	0.05440500	3.77201500	-0.72348600
C	1.63211600	1.93903800	-1.42113100

C	-0.96404100	3.88613800	0.20597800
C	-2.00903300	2.31945600	1.88796400
H	1.84689200	0.90473900	-1.09374000
H	-1.67075100	1.40223600	2.40664700
C	-1.86958000	5.02595200	0.53064600
H	-2.93817200	4.74802700	0.41357900
H	-1.73073600	5.37947500	1.57463000
H	-1.66656200	5.88006500	-0.14217800
C	0.59406600	4.75050500	-1.71117800
H	1.66457300	4.97885100	-1.52214900
H	0.51656500	4.36970700	-2.75149800
H	0.03186300	5.70149400	-1.65688200
C	2.91671300	0.68580000	2.05186000
H	2.50696300	1.62641300	1.62093300
H	2.22570800	0.40319700	2.87345000
H	3.90780100	0.92219500	2.48821600
C	0.82430800	-2.47075900	-1.40214300
H	0.13926000	-3.03439500	-0.73606800
H	0.20203000	-1.67363800	-1.85878100
H	1.15640000	-3.15340400	-2.21035600
C	5.82580900	-2.38128100	-0.71887300
H	6.61085800	-1.61194800	-0.56926300
H	6.10085100	-3.25243100	-0.08343300
H	5.87012100	-2.72336500	-1.77309500
C	-2.11188500	0.49053100	-1.63036400
H	-2.32433200	1.43776400	-1.09045700
H	-1.03763100	0.51770100	-1.90566400
H	-2.70140200	0.51092200	-2.56923500
C	-1.12777000	-2.89875700	2.08620000
H	-0.05599600	-2.94841800	1.79121400
H	-1.16821800	-2.24700000	2.98511100
H	-1.44191600	-3.91860300	2.38649700
C	-5.20085100	-3.42695400	-0.86243700
H	-6.04216300	-3.20674200	-0.16828300
H	-5.54384300	-3.17099100	-1.88539400

H	-5.02992800	-4.52278700	-0.81893300
H	-2.09362100	3.14334200	2.62155900
H	-3.00102100	2.13722300	1.42726500
H	1.32269100	1.93621200	-2.48526400
H	2.54962300	2.55041200	-1.31499800
H	-0.06788100	-0.05591200	2.59280300

F (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1756.41448785 A.U.

Al	0.00210400	0.00447000	-0.90910000
N	1.44804100	-0.05833300	0.25997900
N	-1.45011600	0.06046700	0.25343200
C	-1.29579500	0.08722300	1.60958000
C	-2.68042200	-0.16371300	-0.48938400
C	1.29180500	-0.05292100	1.61590000
C	2.67265700	0.14966100	-0.49757500
C	2.49685300	-0.15718500	2.59618600
C	-0.00281300	0.02620600	2.18297400
C	-2.50455300	0.20440500	2.58372800
C	-2.05000400	0.42957800	4.04535400
C	-3.38008100	1.41444800	2.18545600
C	-3.37644500	-1.07794500	2.57210700
C	2.03689200	-0.34863600	4.06067400
C	3.36317400	-1.38037900	2.22203500
C	3.38383900	1.11405700	2.56048200
H	-0.00474000	0.03992000	3.26942600
C	-0.00660000	0.01148800	-2.84749300
H	-1.03541700	-0.15473100	-3.22661100
H	0.36653000	0.97580300	-3.24673700
H	0.64954600	-0.78053200	-3.25834900
C	3.05066400	1.50362700	-0.74456100
C	4.13496300	1.74077700	-1.60934100
C	4.80981900	0.68013300	-2.23121200
C	3.32558600	-0.93886800	-1.14052900
C	4.40432600	-0.63860200	-1.99917700
C	2.27802600	2.67222800	-0.12459900
H	4.45561600	2.77386800	-1.80593700

H	5.65466100	0.88625000	-2.90578500
C	2.90841000	-2.40018300	-0.96003600
H	4.93557500	-1.46281400	-2.49901000
C	-3.34206300	0.91349200	-1.13970700
C	-4.44553000	0.60347800	-1.96236500
C	-4.86462200	-0.71777100	-2.15475300
C	-3.06469400	-1.51981500	-0.70608500
C	-4.17344200	-1.76968400	-1.53565100
C	-2.88601100	2.36787300	-1.02099700
H	-4.98413800	1.42044600	-2.46603500
H	-5.73017800	-0.93296100	-2.79959200
C	-2.26101000	-2.67598900	-0.10584400
H	-4.50003500	-2.80543700	-1.70698200
H	2.93543900	-0.47744100	4.69559500
H	1.48778600	0.52917700	4.45638200
H	1.40829600	-1.25238600	4.19078800
H	4.13698100	-1.52992300	3.00139900
H	2.76013000	-2.30855600	2.16103500
H	3.88590900	-1.22829600	1.26318800
H	4.18145400	1.00723100	3.32333700
H	3.87827600	1.25598100	1.58256400
H	2.80376800	2.02494100	2.81017900
H	-2.95130200	0.56560000	4.67480000
H	-1.49632600	-0.43601400	4.46105600
H	-1.42795800	1.34017000	4.15833000
H	-4.17271300	-0.96926600	3.33610700
H	-3.87182400	-1.24279400	1.59845800
H	-2.78306600	-1.97681600	2.83412600
H	-4.15587300	1.57150900	2.96135600
H	-2.78262300	2.34535900	2.11140100
H	-3.90072800	1.24528300	1.22810100
C	3.15204000	3.90911200	0.13907400
C	1.05495200	3.05850800	-0.97550000
H	1.88533900	2.33584200	0.85493200
H	0.52853000	3.93497400	-0.54634400

H	1.33098300	3.28784300	-2.02436500
H	0.28535300	2.24948900	-1.01739300
H	2.58448000	4.66105400	0.72361200
H	4.06418900	3.64717300	0.71158800
H	3.47107800	4.40268200	-0.80188700
C	4.08664100	-3.30231200	-0.53491300
H	2.13945600	-2.43293100	-0.15867400
C	2.28346000	-2.97340900	-2.24923500
H	3.72053700	-4.32101200	-0.29357400
H	4.82499900	-3.40745500	-1.35614200
H	4.62512700	-2.91371000	0.34995500
H	1.97341100	-4.02725300	-2.09591900
H	1.39368500	-2.40502100	-2.57813500
H	3.01309700	-2.95642900	-3.08488000
C	-3.10633600	-3.92444000	0.19217100
C	-1.06945600	-3.04304500	-1.00841600
H	-1.83634900	-2.33068800	0.85759000
C	-4.03052100	3.32769500	-0.63820400
H	-2.11719700	2.41290400	-0.22003400
C	-2.23746200	2.84511900	-2.33777600
H	-1.85831300	3.88231000	-2.23356100
H	-1.39464200	2.20110000	-2.65060900
H	-2.97659200	2.83826200	-3.16533500
H	-3.63101800	4.34682900	-0.45987600
H	-4.77642200	3.40934500	-1.45529400
H	-4.56742100	3.00620200	0.27456000
H	-0.48743400	-3.88823500	-0.58877200
H	-1.39119300	-3.30472100	-2.03642900
H	-0.33694200	-2.20504000	-1.11638400
H	-2.50549500	-4.66923500	0.75206100
H	-3.99721900	-3.67458800	0.80231900
H	-3.45737200	-4.42157300	-0.73538100

F (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1756.45493820 A.U.

Al	-0.00390700	0.01412200	-0.90890900
N	-1.44977600	0.05526700	0.26139800

N	1.45147100	-0.06145500	0.24897000
C	1.29640100	-0.11353100	1.60455100
C	2.68215000	0.17376300	-0.48776400
C	-1.29024400	0.02515300	1.61641100
C	-2.67454300	-0.14236500	-0.49660100
C	-2.49341200	0.11639900	2.59960400
C	0.00452200	-0.06630200	2.17990400
C	2.50575600	-0.24434900	2.57581100
C	2.05217700	-0.48743500	4.03476600
C	3.37963400	-1.45020400	2.16167200
C	3.37884300	1.03697200	2.58028900
C	-2.03022300	0.28911000	4.06530600
C	-3.35969000	1.34473600	2.24319800
C	-3.38019600	-1.15417400	2.54877100
H	0.00762000	-0.09954900	3.26581200
C	-0.01670200	0.02492300	-2.84740100
H	1.00081900	0.22464500	-3.23995100
H	-0.36836000	-0.94727400	-3.24682900
H	-0.70184700	0.80194500	-3.23907500
C	-3.05207600	-1.49267800	-0.76307300
C	-4.13605800	-1.71822900	-1.63152000
C	-4.81068200	-0.64886600	-2.23920400
C	-3.32804100	0.95483900	-1.12406000
C	-4.40586500	0.66704200	-1.98835200
C	-2.27664200	-2.66871300	-0.16228000
H	-4.45413800	-2.74889700	-1.84418800
H	-5.65416800	-0.84595700	-2.91843800
C	-2.91232300	2.41334700	-0.92080300
H	-4.93546500	1.49845100	-2.47803800
C	3.34663400	-0.89443000	-1.14975000
C	4.45298900	-0.57399500	-1.96473400
C	4.87256500	0.75018900	-2.13757200
C	3.06720800	1.53249600	-0.68491700
C	4.17896800	1.79405000	-1.50692700
C	2.88768100	-2.34920100	-1.05331400

H	4.99154300	-1.38436500	-2.47924800
H	5.73971000	0.97424900	-2.77752500
C	2.25927500	2.67859300	-0.07285700
H	4.50426700	2.83245500	-1.66423900
H	-2.92880800	0.40981500	4.70198800
H	-1.47929500	-0.59343400	4.44733900
H	-1.40083700	1.19091700	4.20354800
H	-4.12998000	1.48445900	3.02781600
H	-2.75499700	2.27220000	2.18951600
H	-3.88733700	1.20342200	1.28535500
H	-4.17656500	-1.05551100	3.31406200
H	-3.87584000	-1.28328100	1.56967100
H	-2.79888100	-2.06752200	2.78510600
H	2.95558300	-0.62702400	4.66059500
H	1.49474000	0.37166800	4.45837900
H	1.43265700	-1.40090200	4.13663300
H	4.17628100	0.91450300	3.34101900
H	3.87257900	1.21508500	1.60825100
H	2.78677200	1.93243800	2.85543900
H	4.15176600	-1.62008000	2.93850900
H	2.77954200	-2.37765200	2.06950500
H	3.90502900	-1.26620100	1.20961300
C	-3.14755600	-3.91203300	0.07967500
C	-1.05193800	-3.03710400	-1.01826200
H	-1.88592400	-2.34872700	0.82309400
H	-0.52381400	-3.91800000	-0.60142900
H	-1.32469700	-3.24755400	-2.07172300
H	-0.28417200	-2.22626800	-1.04137100
H	-2.57558300	-4.66979800	0.65224500
H	-4.06023700	-3.66101000	0.65656300
H	-3.46391600	-4.38973900	-0.87040500
C	-4.09361300	3.30549400	-0.48383600
H	-2.14543200	2.43708600	-0.11797100
C	-2.28735300	3.00879600	-2.19971100
H	-3.72803900	4.32118000	-0.22913400

H	-4.83209700	3.41781800	-1.30434500
H	-4.62866700	2.90231000	0.39678300
H	-1.98203600	4.06081700	-2.02634100
H	-1.39339100	2.45120500	-2.53508900
H	-3.01610500	3.00042100	-3.03641700
C	3.10053800	3.92505300	0.24270000
C	1.06957900	3.05303700	-0.97424000
H	1.83290900	2.32177900	0.88519300
C	4.03056600	-3.31740200	-0.68824600
H	2.12039000	-2.40762000	-0.25245000
C	2.23699600	-2.80224400	-2.37725300
H	1.85110000	-3.83813100	-2.28675300
H	1.39743500	-2.14894300	-2.67883400
H	2.97732800	-2.78498300	-3.20380500
H	3.62682500	-4.33866800	-0.53255200
H	4.77870900	-3.38138400	-1.50507500
H	4.56311700	-3.01478000	0.23367800
H	0.48283300	3.88902000	-0.54402700
H	1.39214400	3.32631200	-1.99872500
H	0.34054900	2.21356100	-1.09311400
H	2.49226400	4.66031300	0.80701600
H	3.98766000	3.66879000	0.85598400
H	3.45544200	4.43170400	-0.67827000

F-F (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1856.45442606 A.U.

Al	0.01140400	-0.97384400	-0.63485400
N	1.51466500	-0.12718800	0.23510900
N	-1.46060100	-0.04987600	0.22927500
C	-1.26211300	0.31124700	1.52148500
C	-2.72911000	-0.02881500	-0.47135200
C	1.33760100	0.16019300	1.54926400
C	2.74158000	0.03324900	-0.50323000
C	2.53131800	0.29798500	2.55315900
C	0.03777400	0.29754000	2.09528700
C	-2.42417900	0.72511200	2.48442000
C	-1.92748800	1.07077900	3.90929500

C	-3.15039600	1.98359600	1.96108500
C	-3.43189900	-0.43719100	2.63509200
C	2.05715000	0.32258600	4.02665700
C	3.46633700	-0.92272400	2.40581300
C	3.34498300	1.59396400	2.32667500
H	0.03858300	0.48454300	3.16346100
C	-0.07748100	-0.88149100	-2.59417300
H	-1.06663500	-0.49624500	-2.91984000
H	0.70310300	-0.22324500	-3.03194800
H	0.04008700	-1.87865700	-3.06760700
C	3.12522200	1.34586400	-0.91299200
C	4.28349000	1.50205300	-1.69730500
C	5.04551000	0.39635100	-2.09681300
C	3.49677800	-1.10208300	-0.92372800
C	4.64330600	-0.88812700	-1.71670200
C	2.25488900	2.56222100	-0.60880900
H	4.58749200	2.51196200	-2.01120700
H	5.94825900	0.53733700	-2.71153900
C	3.11706500	-2.53880500	-0.56693600
H	5.23574100	-1.75863300	-2.03857800
C	-3.13593800	1.13011000	-1.19890400
C	-4.39296400	1.12380900	-1.83779600
C	-5.22270400	-0.00131400	-1.81474400
C	-3.52697600	-1.21486700	-0.52499600
C	-4.77083900	-1.16605200	-1.18512300
C	-2.24321300	2.35277100	-1.40797200
H	-4.71908800	2.02638000	-2.37784100
H	-6.20487900	0.01937500	-2.31225900
C	-3.05150300	-2.56190300	0.01641200
H	-5.39467700	-2.07255400	-1.20845800
H	2.95164100	0.33947700	4.68175500
H	1.46100900	1.22480100	4.27065500
H	1.46515000	-0.57615500	4.29208400
H	4.23075800	-0.90257800	3.20972400
H	2.90365500	-1.87418700	2.48803500

H	3.99910700	-0.91178000	1.44008800
H	4.11562000	1.68070600	3.12100200
H	3.86665600	1.59183800	1.35316300
H	2.69790100	2.49222800	2.38388900
H	-2.80337700	1.36948600	4.52007500
H	-1.45453500	0.20680500	4.41783500
H	-1.21503400	1.92002400	3.91553400
H	-4.16807500	-0.18643000	3.42690100
H	-3.99295600	-0.61841800	1.70256400
H	-2.91922500	-1.37539400	2.92798500
H	-3.89720200	2.31645000	2.71164200
H	-2.43342600	2.81438200	1.80312600
H	-3.68699400	1.79287900	1.01611000
C	3.04653300	3.85397600	-0.34676200
C	1.26275600	2.76427000	-1.76542200
H	1.65584100	2.34002100	0.29667800
H	0.57411900	3.60807400	-1.55426800
H	1.79941200	2.98372700	-2.71239100
H	0.65652900	1.85448500	-1.92963700
H	2.36140500	4.65778100	-0.00621400
H	3.82667600	3.71742900	0.42850100
H	3.54534700	4.22547200	-1.26641900
C	4.28797500	-3.33973800	0.03666000
H	2.29913800	-2.50306600	0.17930900
C	2.57144100	-3.28025000	-1.80450200
H	3.93074200	-4.33434700	0.37528100
H	5.08974000	-3.51861500	-0.71064200
H	4.74775400	-2.82926300	0.90529400
H	2.20200000	-4.28688700	-1.52102600
H	1.73244500	-2.73270400	-2.27104300
H	3.36287100	-3.40290000	-2.57448400
C	-4.11861400	-3.33521200	0.81272800
C	-2.55770500	-3.42733300	-1.16473400
H	-2.18245000	-2.38617200	0.67945500
C	-2.90859100	3.69305200	-1.03611700

H	-1.33914800	2.22166200	-0.77780200
C	-1.81107200	2.40993600	-2.89052400
H	-1.16325400	3.28896200	-3.08211600
H	-1.26005500	1.50136600	-3.19688900
H	-2.70109700	2.50021600	-3.54764000
H	-2.17841200	4.52187500	-1.14675700
H	-3.76059300	3.92059000	-1.71075000
H	-3.28892800	3.71027000	0.00161200
H	-2.07602800	-4.35455800	-0.79472800
H	-3.40706300	-3.70528800	-1.82474300
H	-1.81488800	-2.88977400	-1.78424700
H	-3.67007200	-4.25058300	1.25094700
H	-4.54729900	-2.73660800	1.64012000
H	-4.95844700	-3.66596800	0.16583900
F	0.03275600	-2.53763600	0.08205100

F-F (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1856.45976043 A.U.

Al	-0.01101800	0.97198000	-0.63737300
N	-1.51654900	0.13909100	0.23524500
N	1.46237500	0.06015100	0.22905000
C	1.26331800	-0.28863000	1.52582700
C	2.72972900	0.02313300	-0.47417200
C	-1.33823800	-0.13708100	1.55317400
C	-2.74237800	-0.03412200	-0.50310700
C	-2.53004900	-0.27509900	2.55826400
C	-0.03711900	-0.26368200	2.09924700
C	2.42231400	-0.70165300	2.49178600
C	1.92402700	-1.02677900	3.92096800
C	3.13506600	-1.97294000	1.98055300
C	3.44189800	0.45207100	2.62890500
C	-2.05515700	-0.28208600	4.03178400
C	-3.47848400	0.93397400	2.40061600
C	-3.32955300	-1.58186500	2.34279300
H	-0.03750500	-0.43981400	3.16953800
C	0.07334900	0.88183700	-2.59757900
H	1.05262200	0.47196200	-2.92309700

H	-0.72256700	0.23850700	-3.03011300
H	-0.02339800	1.88137800	-3.07110500
C	-3.12104000	-1.35143800	-0.90292400
C	-4.27789800	-1.51793600	-1.68831800
C	-5.04353300	-0.41824800	-2.09887000
C	-3.50283900	1.09442700	-0.93311200
C	-4.64709700	0.87127000	-1.72743800
C	-2.24786400	-2.56354200	-0.59143400
H	-4.57732000	-2.53148600	-1.99493400
H	-5.94444600	-0.56761800	-2.71439800
C	-3.13204800	2.53507900	-0.58333300
H	-5.24300700	1.73670000	-2.05682500
C	3.12669200	-1.14498800	-1.19284900
C	4.38361800	-1.15403800	-1.83310600
C	5.22266600	-0.03517100	-1.82111400
C	3.53805400	1.20180100	-0.53850000
C	4.78056800	1.13886700	-1.20061500
C	2.22546500	-2.36270400	-1.39318000
H	4.70245200	-2.06370800	-2.36553500
H	6.20413300	-0.06805200	-2.31943100
C	3.07696700	2.55687800	-0.00467600
H	5.41213600	2.03980800	-1.23243300
H	-2.94992300	-0.29967400	4.68616900
H	-1.45264400	-1.17766900	4.28373400
H	-1.47006400	0.62353200	4.28903000
H	-4.24442000	0.90843700	3.20259000
H	-2.92777800	1.89266900	2.48110800
H	-4.00884000	0.91216300	1.43371500
H	-4.09649400	-1.67079900	3.14010500
H	-3.85418000	-1.59230600	1.37096000
H	-2.67226100	-2.47222500	2.40417500
H	2.79871100	-1.32524000	4.53322400
H	1.45889800	-0.15298800	4.41975800
H	1.20530100	-1.87044600	3.93773900
H	4.17581900	0.20051600	3.42217800

H	4.00408200	0.61826000	1.69427100
H	2.93972600	1.39820000	2.91451900
H	3.87979200	-2.30340600	2.73387100
H	2.41010300	-2.79867600	1.83361400
H	3.67175800	-1.79804200	1.03257500
C	-3.03590600	-3.85356300	-0.30988200
C	-1.26733300	-2.77739100	-1.75597000
H	-1.64116800	-2.33108500	0.30621300
H	-0.57517500	-3.61685400	-1.54077600
H	-1.81387200	-3.01105800	-2.69390200
H	-0.66463200	-1.86843600	-1.93812900
H	-2.34558100	-4.65165300	0.03308000
H	-3.80893900	-3.71017400	0.47113100
H	-3.54173000	-4.23429600	-1.22177100
C	-4.30915500	3.33347500	0.01162100
H	-2.31835000	2.50467800	0.16746100
C	-2.58533400	3.27154900	-1.82336800
H	-3.95863200	4.33214400	0.34547500
H	-5.10907000	3.50220700	-0.73977700
H	-4.76717200	2.82476400	0.88215600
H	-2.22936200	4.28559800	-1.54760800
H	-1.73861600	2.72751700	-2.28069500
H	-3.37373900	3.38061400	-2.59836200
C	4.15390200	3.32591200	0.78281000
C	2.58899700	3.41848800	-1.19096000
H	2.20985100	2.39084700	0.66323600
C	2.87772000	-3.70443800	-1.00340300
H	1.31863800	-2.21804300	-0.77018600
C	1.80360500	-2.43245400	-2.87839700
H	1.14992600	-3.30814600	-3.06413500
H	1.26173000	-1.52283900	-3.19882200
H	2.69757800	-2.53838400	-3.52772800
H	2.14171500	-4.52781800	-1.11456800
H	3.73494800	-3.94294800	-1.66746000
H	3.24562100	-3.71500600	0.03877000

H	2.13457100	4.36301500	-0.82883500
H	3.43810900	3.67122400	-1.86120000
H	1.82953100	2.88887400	-1.79751800
H	3.71518100	4.24785000	1.21736000
H	4.57884900	2.72767900	1.61220100
H	4.99382500	3.64403800	0.13003400
F	-0.02820300	2.54797800	0.06587600

F-H (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1757.19307400 A.U.

Al	-0.01149200	1.08258000	-0.65638500
N	-1.51786600	0.20805700	0.23034000
N	1.45987600	0.12490500	0.22510300
C	1.26080200	-0.15835800	1.53334400
C	2.72460900	0.07247100	-0.47375200
C	-1.34064000	-0.00435900	1.55630400
C	-2.73585600	0.00643800	-0.50604600
C	-2.53377700	-0.12718900	2.56395600
C	-0.03783600	-0.08157300	2.11141400
C	2.41562000	-0.55856000	2.51185100
C	1.91501600	-0.83858200	3.94949800
C	3.10931700	-1.85226400	2.03288700
C	3.45291100	0.58261100	2.61677400
C	-2.06518300	-0.07715100	4.03833300
C	-3.50302100	1.05861100	2.36377400
C	-3.31083200	-1.45273100	2.38779600
H	-0.03600900	-0.19885500	3.18961000
C	0.07155500	0.81984100	-2.61688200
H	1.06802400	0.42664700	-2.91076700
H	-0.69539700	0.10667400	-2.98891600
H	-0.06849200	1.76343500	-3.18568000
C	-3.11279200	-1.32040400	-0.87325600
C	-4.26416900	-1.50623500	-1.66178600
C	-5.02617400	-0.41784400	-2.10617100
C	-3.49272100	1.12303300	-0.97205900
C	-4.63163900	0.88081700	-1.76675800
C	-2.24254700	-2.52317400	-0.51979100

H	-4.56259900	-2.52737300	-1.94349800
H	-5.92274500	-0.58316600	-2.72383400
C	-3.11652300	2.57051400	-0.65459900
H	-5.22422600	1.73780300	-2.12307300
C	3.13517400	-1.10856900	-1.16243500
C	4.39149000	-1.11832600	-1.80300500
C	5.21704500	0.00997000	-1.82062800
C	3.51953700	1.25828300	-0.56958200
C	4.76204300	1.19410000	-1.22987400
C	2.24716500	-2.34118300	-1.32655700
H	4.72070500	-2.03765600	-2.31212900
H	6.19813900	-0.02405700	-2.31949400
C	3.03615800	2.61831200	-0.06724500
H	5.38246200	2.10162600	-1.28517600
H	-2.96129900	-0.09062700	4.69143300
H	-1.44528100	-0.95151600	4.32086600
H	-1.49854000	0.84755400	4.26765000
H	-4.27657100	1.04318300	3.15911900
H	-2.96994900	2.02888900	2.42156700
H	-4.02319800	0.99959300	1.39273100
H	-4.07907300	-1.53176200	3.18534000
H	-3.83210200	-1.50004300	1.41520100
H	-2.63914900	-2.33011400	2.47659200
H	2.78463300	-1.13740000	4.56930900
H	1.46626700	0.05536200	4.42741300
H	1.18001400	-1.66744000	3.98729300
H	4.19114800	0.33789600	3.40867900
H	4.00847400	0.72277100	1.67365100
H	2.96599600	1.54101400	2.88776800
H	3.84628100	-2.18007500	2.79538800
H	2.37165700	-2.66906700	1.89894100
H	3.65219300	-1.70519800	1.08373000
C	-3.03528300	-3.80090300	-0.19801600
C	-1.25509500	-2.77811500	-1.67002500
H	-1.63973200	-2.26011700	0.37216000

H	-0.56765800	-3.61353500	-1.42396300
H	-1.79570600	-3.03884200	-2.60428400
H	-0.64837900	-1.87737700	-1.87524500
H	-2.34995300	-4.59089700	0.17320100
H	-3.81144800	-3.63010400	0.57445900
H	-3.53934500	-4.21038800	-1.09852400
C	-4.29679400	3.39084200	-0.09681200
H	-2.31551400	2.54974200	0.11348800
C	-2.54232300	3.27569800	-1.89987300
H	-3.94472900	4.39264700	0.22578800
H	-5.07961200	3.55347900	-0.86737300
H	-4.77867900	2.90188200	0.77213400
H	-2.20674100	4.30228300	-1.64501200
H	-1.67512300	2.73095100	-2.31688600
H	-3.30873000	3.35013000	-2.70041400
C	4.10494700	3.42812100	0.68986600
C	2.51388100	3.44127800	-1.26540600
H	2.17999200	2.44970500	0.61777100
C	2.91521800	-3.66353800	-0.89893300
H	1.34043800	-2.18562100	-0.70571500
C	1.82115600	-2.46032100	-2.80717900
H	1.17499200	-3.34744300	-2.96408900
H	1.27042900	-1.56579500	-3.15281400
H	2.71374600	-2.57748400	-3.45664000
H	2.18907400	-4.49901600	-0.98312800
H	3.77287300	-3.91276000	-1.55867500
H	3.28830300	-3.64040700	0.14129800
H	2.05785000	4.39161500	-0.91901100
H	3.34376100	3.68125800	-1.96368700
H	1.74283700	2.89230200	-1.84043800
H	3.65201600	4.34862500	1.11265700
H	4.55640000	2.85598300	1.52371600
H	4.92804300	3.75291200	0.01913000
H	-0.01808800	2.56452400	-0.01949600

F-H (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1757.19755889 A.U.

Al	-0.01157900	1.07469100	-0.66328500
N	-1.51929500	0.21696300	0.22814600
N	1.46132800	0.13357200	0.22291200
C	1.26206700	-0.13258900	1.53595100
C	2.72568700	0.06706600	-0.47682800
C	-1.34112000	0.02161300	1.55799900
C	-2.73641400	0.00166600	-0.50694300
C	-2.53216800	-0.09592500	2.56769300
C	-0.03703300	-0.04345200	2.11243400
C	2.41404300	-0.52717400	2.51904200
C	1.91180200	-0.78390600	3.96050700
C	3.09673800	-1.83272000	2.05609500
C	3.46062500	0.60691200	2.60883500
C	-2.06266800	-0.02404800	4.04094600
C	-3.51204500	1.07868800	2.35372400
C	-3.29743300	-1.43052300	2.40808400
H	-0.03468500	-0.14643300	3.19235200
C	0.06869800	0.80675100	-2.62388100
H	1.06109000	0.40004700	-2.91333300
H	-0.70483800	0.09616100	-2.98746300
H	-0.06348300	1.74897500	-3.19698800
C	-3.10841200	-1.33055000	-0.86027000
C	-4.25732300	-1.52883500	-1.65043200
C	-5.02186200	-0.44779700	-2.10970600
C	-3.49753100	1.11031800	-0.98584600
C	-4.63334600	0.85642300	-1.78211700
C	-2.23683700	-2.52795000	-0.49286800
H	-4.55139900	-2.55405700	-1.92184900
H	-5.91584500	-0.62299700	-2.72852400
C	-3.13086900	2.56248200	-0.67905200
H	-5.22880800	1.70721100	-2.14852100
C	3.13077200	-1.12359500	-1.15240100
C	4.38684500	-1.14600300	-1.79437400
C	5.21729200	-0.02102700	-1.82652800
C	3.52662000	1.24789200	-0.58621700

C	4.76800600	1.17207800	-1.24812900
C	2.23886900	-2.35504300	-1.30288700
H	4.71222400	-2.07253200	-2.29282400
H	6.19764000	-0.06490900	-2.32619600
C	3.05188900	2.61497500	-0.09529100
H	5.39266700	2.07598500	-1.31447100
H	-2.95886600	-0.03460000	4.69366500
H	-1.43802900	-0.89141600	4.33390900
H	-1.50155200	0.90684600	4.25845700
H	-4.28570800	1.06300700	3.14861900
H	-2.98879000	2.05479600	2.40348200
H	-4.03120500	1.00538700	1.38309000
H	-4.06297900	-1.50604100	3.20822300
H	-3.82047700	-1.49365600	1.43738100
H	-2.61792000	-2.30079600	2.50560900
H	2.78041000	-1.07879800	4.58325500
H	1.46878600	0.11958900	4.42555100
H	1.17246300	-1.60816200	4.01035000
H	4.19725000	0.36385800	3.40239400
H	4.01650500	0.73202700	1.66381300
H	2.98256400	1.57223100	2.87083600
H	3.83080000	-2.15557100	2.82314800
H	2.35279800	-2.64541700	1.93279700
H	3.64091000	-1.70218500	1.10527100
C	-3.02775000	-3.80176400	-0.15114300
C	-1.25511000	-2.79871000	-1.64451100
H	-1.63051900	-2.25258600	0.39280200
H	-0.56541900	-3.62897500	-1.38871900
H	-1.80066100	-3.07563400	-2.57128200
H	-0.65040900	-1.90043000	-1.86667100
H	-2.33916900	-4.58527200	0.22730200
H	-3.79962500	-3.62105300	0.62331000
H	-3.53572900	-4.22250200	-1.04413100
C	-4.31825700	3.38092200	-0.13358300
H	-2.33475900	2.55091600	0.09409100

C	-2.55556500	3.26014600	-1.92819800
H	-3.97286500	4.38728900	0.18188100
H	-5.09843000	3.53143800	-0.90912200
H	-4.79932200	2.89606200	0.73810100
H	-2.23272100	4.29340800	-1.68315800
H	-1.68093200	2.71899900	-2.33506300
H	-3.31869100	3.31934600	-2.73307300
C	4.12711200	3.42734600	0.64998200
C	2.53012100	3.42844600	-1.30021400
H	2.19870000	2.45516100	0.59530100
C	2.90108200	-3.67449900	-0.85749100
H	1.33095700	-2.18921200	-0.68669000
C	1.81770400	-2.49078800	-2.78368900
H	1.16798800	-3.37677700	-2.93104900
H	1.27172300	-1.59809200	-3.14231300
H	2.71215200	-2.62098600	-3.42807900
H	2.17224100	-4.50791400	-0.93696800
H	3.76202200	-3.93226400	-1.50954900
H	3.26648700	-3.64049100	0.18511100
H	2.08670900	4.38844300	-0.96347500
H	3.35894700	3.65334000	-2.00464100
H	1.75159100	2.87912100	-1.86533400
H	3.67940600	4.35365200	1.06556200
H	4.57736100	2.86040800	1.48791900
H	4.94904700	3.74086800	-0.02727100
H	-0.01668600	2.56950500	-0.04369600

D (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1676.18090473 A.U.

N	-0.28474000	1.87929600	-0.43169200
N	-2.36720800	1.25057400	-0.20766900
F	0.79987100	0.21412200	2.02549800
C	-1.08534700	0.77823900	-0.25245900
F	0.73291300	-2.82479200	-1.63979700
C	-2.37702800	2.62375200	-0.34258200
H	-3.30554700	3.20230300	-0.30074400

C	-1.06157500	3.01910000	-0.50289000
H	-0.62148000	4.00689700	-0.67116300
C	1.15285600	1.81721500	-0.56961100
C	-3.52121500	0.40805500	0.01532100
C	1.68519300	1.12604200	-1.68355300
C	-4.31711100	0.05516500	-1.09812100
C	-3.77590700	-0.04337600	1.32988200
C	1.95846900	2.35913800	0.45903100
C	3.07405900	0.91042200	-1.70318900
H	3.51253900	0.36479100	-2.55410000
C	3.91483300	1.36663700	-0.66711200
F	3.40235300	-0.42408500	2.49865300
C	3.34202100	2.11578800	0.38027400
H	3.98997000	2.50245900	1.18257900
C	-4.89512700	-0.87643100	1.51154700
H	-5.12293000	-1.23998400	2.52624000
C	0.68659800	-1.24781700	0.14813500
C	-5.41857900	-0.78314200	-0.85437100
H	-6.05107400	-1.08366300	-1.70504300
C	-5.72826100	-1.25560900	0.43904600
C	1.40791200	-0.67809100	1.22288700
F	4.64517900	-2.28753900	0.93749900
F	3.30861100	-3.51130800	-1.10776600
C	1.35116400	-2.25134100	-0.59967400
C	2.73713700	-1.00742700	1.50259000
C	3.37544900	-1.97779300	0.70144300
C	2.68743600	-2.60571600	-0.35674400
H	-1.50680200	-1.46561600	-0.82025400
B	-0.69280300	-0.73367800	-0.30706700
C	0.81147400	0.60917500	-2.80213100
H	0.43943000	-0.42116500	-2.60301800
H	-0.07279200	1.25277900	-2.98028100
H	1.38571600	0.55013800	-3.74677300
C	1.38454600	3.14831200	1.61032700
H	0.37615500	2.79857400	1.90315800

H	2.03987100	3.07193600	2.49854500
H	1.30521900	4.22727900	1.35529400
C	5.38262800	1.02337400	-0.65452900
H	5.77752300	0.85706000	-1.67570500
H	5.98664600	1.81280900	-0.16589800
H	5.54654800	0.08542600	-0.08008800
C	-3.97531000	0.53248700	-2.48865900
H	-4.09885000	1.63132000	-2.59407800
H	-2.92234800	0.29677200	-2.75293600
H	-4.62760300	0.05286200	-3.24216000
C	-2.89579500	0.36013400	2.48982900
H	-1.87506100	-0.07154200	2.41637400
H	-2.77213500	1.46228600	2.54786300
H	-3.32906100	0.01907000	3.44854900
C	-6.93764000	-2.12691400	0.66810500
H	-7.85491400	-1.50422800	0.75190900
H	-7.09877100	-2.82926400	-0.17390500
H	-6.85023400	-2.71385500	1.60296500

D (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1676.22794797 A.U.

N	-0.29278600	-1.87203100	0.45563000
N	-2.37422900	-1.24607100	0.22576000
F	0.82725800	-0.23326300	-2.05000800
C	-1.09033500	-0.77288100	0.24866500
F	0.73685600	2.81766900	1.60442400
C	-2.38599000	-2.61217800	0.40116000
H	-3.31413000	-3.19181200	0.38611900
C	-1.06943900	-3.00606800	0.56500900
H	-0.63408800	-3.99029600	0.76280500
C	1.14405000	-1.80660900	0.59025300
C	-3.52879500	-0.40846800	-0.00771000
C	1.67616400	-1.10482400	1.69734200
C	-4.29125500	0.00250300	1.10927400
C	-3.81535700	-0.01762000	-1.33395200
C	1.94741500	-2.36070900	-0.43254400
C	3.06533300	-0.89022100	1.71483100

H	3.50289000	-0.33179100	2.55761300
C	3.90437700	-1.35904300	0.68295800
F	3.42540100	0.41315700	-2.52060500
C	3.33193300	-2.11842200	-0.35711500
H	3.97887300	-2.51348400	-1.15604900
C	-4.93123500	0.81986300	-1.52467700
H	-5.18252000	1.13852000	-2.54888100
C	0.70234700	1.23221000	-0.17680900
C	-5.39028000	0.84180800	0.85726100
H	-5.99687800	1.18684400	1.70994100
C	-5.72792500	1.25917200	-0.44838700
C	1.42769000	0.66119100	-1.24600400
F	4.66396100	2.28212300	-0.95679300
F	3.31553200	3.50410600	1.08447900
C	1.36262400	2.23570300	0.57005800
C	2.75743700	0.99511200	-1.52254800
C	3.39167000	1.96590900	-0.72242900
C	2.69845100	2.59170100	0.33138400
H	-1.52855600	1.49306400	0.69352300
B	-0.69689800	0.73437500	0.25289000
C	0.80034000	-0.57728800	2.80833700
H	0.38858700	0.43054500	2.57648400
H	-0.05969500	-1.24298600	3.01978700
H	1.38620800	-0.46152800	3.74008200
C	1.36672700	-3.16154800	-1.57162200
H	0.37415700	-2.78711400	-1.88774500
H	2.03941100	-3.13131300	-2.44936400
H	1.24429800	-4.22802500	-1.28495700
C	5.37275300	-1.01556400	0.66886300
H	5.77255500	-0.87599400	1.69236000
H	5.97199500	-1.79169500	0.15375300
H	5.53228000	-0.06144800	0.12081600
C	-3.92114000	-0.42564700	2.50793000
H	-4.09449600	-1.51173200	2.66321500
H	-2.84828400	-0.23636900	2.72250900

H	-4.52246400	0.11965000	3.25917900
C	-2.97007500	-0.48342700	-2.49555300
H	-1.94618400	-0.05428500	-2.46653300
H	-2.85371400	-1.58758900	-2.50086500
H	-3.42690900	-0.18373800	-3.45713200
C	-6.92678000	2.14619700	-0.67961900
H	-7.87005300	1.58001600	-0.52275700
H	-6.94092500	2.99686400	0.03212500
H	-6.94405500	2.55131500	-1.70981200

D-F (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1776.22168812 A.U.

N	-0.17375300	-1.09965500	1.34169500
N	-2.26321200	-0.63538300	1.00714000
F	1.78779500	-0.96463700	-2.44087300
C	-1.03007400	-0.54709800	0.42988500
F	-0.00837900	2.47940100	0.34325600
C	-2.18582500	-1.23181600	2.26291000
H	-3.07650600	-1.39370100	2.87710700
C	-0.86167000	-1.52382100	2.47552400
H	-0.34589500	-1.99864100	3.31525000
C	1.24966400	-1.25180200	1.15553500
C	-3.49746400	-0.19999000	0.39863900
C	2.11383400	-0.32811900	1.78712200
C	-3.98681300	1.08596300	0.71361500
C	-4.16458000	-1.08471300	-0.47426500
C	1.71347500	-2.29762600	0.33037000
C	3.48829500	-0.45245400	1.52816900
H	4.17929200	0.27890200	1.97829500
C	4.00091000	-1.45852700	0.68278400
F	4.22205100	0.14072800	-2.22057000
C	3.10264000	-2.37882700	0.11241600
H	3.48680000	-3.16980000	-0.55108700
C	-5.38095200	-0.64520900	-1.03057000
H	-5.92152500	-1.31828400	-1.71595000
C	0.76013500	0.72502600	-1.08610400

C	-5.20599400	1.47391600	0.13053500
H	-5.60681800	2.47506600	0.35936200
C	-5.91669600	0.62504100	-0.74269200
C	1.88258500	0.17386600	-1.72641700
F	4.60519400	2.39195900	-0.70421500
F	2.45705900	3.56377800	0.56932700
C	1.00741000	1.89396000	-0.35070100
C	3.16954700	0.73246500	-1.62664400
C	3.37021900	1.88576500	-0.85356300
C	2.27419600	2.48101800	-0.20744200
H	-1.58898000	0.94092400	-1.24919500
B	-0.73532400	0.06387900	-1.06882300
C	1.58176100	0.76263200	2.68420400
H	0.69078800	1.25729800	2.25068800
H	1.28360600	0.36445700	3.67849200
H	2.34998700	1.54153100	2.85156100
C	0.75276300	-3.24464800	-0.34147300
H	0.20157000	-2.72353700	-1.15315500
H	1.29155100	-4.10409800	-0.78385200
H	-0.00364300	-3.63600000	0.37075900
C	5.47451100	-1.49553400	0.35958400
H	6.09691800	-1.36973300	1.26931500
H	5.76349600	-2.44359500	-0.13464000
H	5.72800000	-0.66544000	-0.33315200
C	-3.19646900	2.01606100	1.59897300
H	-2.95817500	1.55640000	2.58129800
H	-2.22835800	2.27355200	1.12063000
H	-3.75123900	2.95532100	1.78574600
C	-3.56689000	-2.42343800	-0.82571200
H	-2.64237600	-2.27395200	-1.42408700
H	-3.28246100	-3.00018500	0.07959300
H	-4.27634100	-3.03412200	-1.41610400
C	-7.20466200	1.08675700	-1.38329900
H	-7.80955200	1.70252100	-0.68697800
H	-6.99637800	1.71539800	-2.27666100

H	-7.82452000	0.23188700	-1.71937400
F	-0.89560700	-1.01227200	-2.01135700

D-F (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1776.23159253 A.U.

N	-0.17461100	-1.11444700	1.32215100
N	-2.26520700	-0.65094900	0.99507100
F	1.78527700	-0.93973600	-2.44079200
C	-1.03280900	-0.55334400	0.41768000
F	0.00073100	2.50751900	0.34893500
C	-2.18539200	-1.26203000	2.24357200
H	-3.07347800	-1.43387800	2.85892300
C	-0.86072100	-1.55394200	2.45145400
H	-0.34542100	-2.03821700	3.28608400
C	1.24844800	-1.26296000	1.13487700
C	-3.49978700	-0.20820800	0.39383900
C	2.11319600	-0.34730100	1.77751100
C	-3.99077700	1.07333500	0.72806000
C	-4.16934700	-1.08233700	-0.48740400
C	1.71319900	-2.30497500	0.30541900
C	3.48903400	-0.47430000	1.52378500
H	4.18064700	0.24922000	1.98546900
C	4.00245600	-1.47766600	0.67503300
F	4.22494200	0.14951900	-2.20812100
C	3.10334300	-2.39074200	0.09288100
H	3.48851300	-3.18201600	-0.56991100
C	-5.38553500	-0.63448200	-1.04057000
H	-5.92822500	-1.29951700	-1.73195400
C	0.76429500	0.74605000	-1.07405200
C	-5.20844400	1.47074200	0.14798500
H	-5.60981800	2.46830300	0.39096100
C	-5.92000300	0.63305200	-0.73751600
C	1.88558800	0.19346100	-1.71424100
F	4.61577000	2.39845500	-0.68727400
F	2.47089200	3.57907000	0.58133300
C	1.01532800	1.91325400	-0.33653000
C	3.17535700	0.74289100	-1.60986900

C	3.37949800	1.89416000	-0.83538400
C	2.28510100	2.49299700	-0.19097500
H	-1.58165600	0.98238300	-1.22401500
B	-0.73516500	0.09135400	-1.06254700
C	1.58174200	0.73292900	2.68696800
H	0.68025000	1.22122200	2.26839200
H	1.29661900	0.32236100	3.67965900
H	2.34632400	1.51525000	2.85488200
C	0.75099800	-3.24966400	-0.36856300
H	0.18234500	-2.72179000	-1.16287000
H	1.29047900	-4.09721400	-0.83243900
H	0.00845500	-3.65806100	0.34838900
C	5.47956900	-1.52566500	0.36842300
H	6.09112300	-1.44378100	1.29046100
H	5.75998100	-2.45903300	-0.15747700
H	5.75789500	-0.67316000	-0.28649700
C	-3.20902900	1.98312500	1.64203700
H	-3.02570200	1.51650600	2.63279400
H	-2.21449700	2.21218900	1.20590500
H	-3.74452100	2.93747900	1.80613000
C	-3.58174000	-2.42534000	-0.84162600
H	-2.64671300	-2.28704200	-1.42496200
H	-3.31740400	-3.01032400	0.06421000
H	-4.29016600	-3.02283400	-1.44636100
C	-7.21401800	1.10254000	-1.35984800
H	-7.89193900	1.54395100	-0.60030800
H	-7.02371400	1.89238500	-2.11836300
H	-7.74930200	0.27479800	-1.86491600
F	-0.90459200	-0.94612300	-2.05160000

D-H (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -1677.00262771 A.U.

N	-0.21617100	-1.22982300	1.19848200
N	-2.30710300	-0.75887600	0.87584500
F	1.68733900	-0.80508400	-2.54801500
C	-1.06552300	-0.60407100	0.32159000

F	0.01377100	2.46561100	0.50375800
C	-2.23937300	-1.46644800	2.07598400
H	-3.13640600	-1.69055900	2.66049200
C	-0.91683300	-1.76134700	2.28130000
H	-0.40671300	-2.30376700	3.08248200
C	1.20778100	-1.35963700	1.01539000
C	-3.53152700	-0.26994400	0.29628400
C	2.06479100	-0.48227300	1.71888700
C	-4.01235900	0.99398100	0.70026400
C	-4.19687700	-1.07491900	-0.65122600
C	1.68605000	-2.33643000	0.11737600
C	3.44097000	-0.57559300	1.45568000
H	4.12464500	0.12543300	1.96188800
C	3.96464300	-1.50870400	0.53666900
F	4.15868000	0.23431600	-2.29324900
C	3.07580900	-2.39130100	-0.10357900
H	3.46794700	-3.12610700	-0.82468100
C	-5.40178500	-0.58392000	-1.18797400
H	-5.94002500	-1.19664900	-1.92966700
C	0.72689800	0.79708300	-1.05237200
C	-5.22054700	1.43833100	0.13396200
H	-5.61431900	2.42364000	0.43323200
C	-5.92900000	0.66639100	-0.80949800
C	1.82724400	0.27810400	-1.75418300
F	4.60748800	2.36817700	-0.63182900
F	2.50622800	3.48662800	0.75839700
C	1.00597800	1.90951500	-0.24345300
C	3.12668300	0.80123600	-1.64101500
C	3.36029900	1.89462800	-0.79292900
C	2.28710100	2.46238100	-0.08614200
H	-1.63557200	0.95808700	-1.25543600
B	-0.74857700	0.12317600	-1.07204300
C	1.52082500	0.53247000	2.69397900
H	0.62481800	1.04705700	2.29605500
H	1.22536900	0.05677100	3.65444000

H	2.28016900	1.30515500	2.92063500
C	0.73452900	-3.23652100	-0.62830700
H	0.21296300	-2.66359400	-1.42427000
H	1.27511000	-4.07488400	-1.10777300
H	-0.04619300	-3.65709400	0.03868700
C	5.43832000	-1.50396100	0.21173200
H	6.06025400	-1.44190900	1.12835800
H	5.73781000	-2.40737500	-0.35467700
H	5.68186700	-0.61967200	-0.41437500
C	-3.22123900	1.84426100	1.66169500
H	-2.99969400	1.30667300	2.60765700
H	-2.24416500	2.12351000	1.21422600
H	-3.76614600	2.77403700	1.91388300
C	-3.60750900	-2.39201900	-1.09047000
H	-2.65839100	-2.22242900	-1.64303500
H	-3.36508700	-3.04583000	-0.22646000
H	-4.30272500	-2.93981400	-1.75500800
C	-7.20443400	1.18943700	-1.42796800
H	-7.81134400	1.75749800	-0.69389500
H	-6.97947400	1.88146500	-2.26893400
H	-7.82917500	0.36931000	-1.83437600
H	-0.83675900	-0.74513700	-1.95113600

D-H (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -1677.01115414 A.U.

N	-0.21787800	-1.22933700	1.18822600
N	-2.30788100	-0.75216300	0.87380400
F	1.68757300	-0.78759600	-2.54929200
C	-1.06810700	-0.59786800	0.31793500
F	0.02294800	2.49064800	0.50126900
C	-2.23870700	-1.46534300	2.07076600
H	-3.13337000	-1.69225600	2.65790500
C	-0.91665700	-1.76454400	2.27097800
H	-0.40751800	-2.31215500	3.06932300
C	1.20513700	-1.36176800	1.00187300
C	-3.53338300	-0.26574100	0.29462100
C	2.06649000	-0.49055800	1.70797700

C	-4.02048800	0.99515000	0.70184900
C	-4.19758300	-1.07447600	-0.65102800
C	1.67913500	-2.34167800	0.10478700
C	3.44305300	-0.59108200	1.44648800
H	4.13031000	0.10290200	1.95753600
C	3.96262700	-1.52741000	0.52777100
F	4.16329200	0.23788000	-2.28608200
C	3.06927100	-2.40442200	-0.11518700
H	3.45875300	-3.14481700	-0.83218700
C	-5.40237100	-0.58505400	-1.19160800
H	-5.93973300	-1.20046800	-1.93161700
C	0.73183800	0.81244400	-1.04678500
C	-5.22831600	1.43820200	0.13224800
H	-5.62709100	2.42059000	0.43420000
C	-5.93252500	0.66546400	-0.81501600
C	1.83174300	0.29064900	-1.74700100
F	4.61846000	2.37073000	-0.62293100
F	2.51914900	3.49991500	0.76024200
C	1.01445400	1.92443100	-0.23817400
C	3.13346500	0.80609100	-1.63060300
C	3.36997000	1.89870900	-0.78306200
C	2.29787800	2.47098700	-0.07943500
H	-1.62775000	0.98826500	-1.24649300
B	-0.74702700	0.14144400	-1.07220800
C	1.52781100	0.51976800	2.69013700
H	0.62336500	1.02878400	2.30443000
H	1.24380200	0.03790400	3.65060900
H	2.28669100	1.29381200	2.91356900
C	0.72311700	-3.24581400	-0.63066500
H	0.16887700	-2.67313400	-1.40410400
H	1.26431000	-4.06871000	-1.13529500
H	-0.03263300	-3.68770600	0.05110500
C	5.43912100	-1.53955400	0.21450100
H	6.05327300	-1.53239700	1.13853800
H	5.72400700	-2.42296600	-0.38949700

H	5.71022800	-0.63250300	-0.36595300
C	-3.24408400	1.83802900	1.68213400
H	-3.06847700	1.30230800	2.63873700
H	-2.24554400	2.09365900	1.27004000
H	-3.77879900	2.78013800	1.90839900
C	-3.61546500	-2.40013800	-1.07501600
H	-2.64972900	-2.25064900	-1.60357500
H	-3.40528800	-3.05455500	-0.20314000
H	-4.30261500	-2.93851400	-1.75511400
C	-7.20874000	1.18516600	-1.43454000
H	-7.81945300	1.74707500	-0.69907200
H	-6.98426300	1.88350700	-2.27030400
H	-7.82676400	0.36381200	-1.84819700
H	-0.83404600	-0.71068100	-1.96755000

I (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -2856.18410406 A.U.

Al	-0.00004100	-0.62045500	0.00001300
F	1.93098400	-0.69600100	2.48844100
N	-0.99255300	2.18259400	0.44856800
N	0.99250400	2.18270100	-0.44814900
F	1.63268100	-2.28374400	-1.97015700
F	4.43257000	-1.79943200	2.71906300
F	-1.93068500	-0.69487600	-2.48814600
C	-0.00002600	1.36395400	0.00012300
F	-1.63319200	-2.28486000	1.96971700
C	0.62657600	3.50964900	-0.28940000
H	1.27443300	4.33555200	-0.59619800
C	-0.62671800	3.50958600	0.28992400
H	-1.27460200	4.33540900	0.59687700
C	-2.20221900	1.62654600	1.02393000
C	2.20225300	1.62677000	-1.02345500
C	-2.10066000	1.02729100	2.30742200
F	5.54906100	-3.08518900	0.57624600
F	4.16935800	-3.32284800	-1.77713400
C	3.37075000	1.59371800	-0.22260800
C	2.10096700	1.02800400	-2.30718100

C	-3.37089900	1.59384100	0.22335600
C	-0.84592700	1.17494000	3.17017400
H	0.04508900	1.08922600	2.50761000
C	-3.24002800	0.34401700	2.77563000
H	-3.21135900	-0.14645100	3.75792800
C	-4.40183900	0.25905500	1.99537000
H	-5.26913400	-0.30392800	2.37277500
F	-4.43224800	-1.79822300	-2.71977300
C	3.45734500	2.34676600	1.10131900
H	2.42904800	2.41017400	1.52151400
C	0.84646400	1.17606400	-3.17018600
H	-0.04470100	1.09065600	-2.50779400
C	-4.47206500	0.88681900	0.74332200
H	-5.39672300	0.81835700	0.15231300
C	3.24042900	0.34485500	-2.77537600
H	3.21196800	-0.14524300	-3.75786600
C	-3.45783400	2.34731100	-1.10031100
H	-2.42959200	2.41123800	-1.52055200
C	-1.72337000	-1.48129900	-0.25704800
C	1.72325400	-1.48138300	0.25700500
C	-3.96003400	3.78664300	-0.83864200
H	-5.00057500	3.76665100	-0.45395900
H	-3.95240800	4.38111700	-1.77484200
H	-3.34802100	4.32113300	-0.08491400
C	2.46176800	-1.37429700	1.44040000
C	4.47201300	0.88687500	-0.74258200
H	5.39653300	0.81816200	-0.15138600
C	-0.80439200	2.58397700	3.80337400
H	-0.83407500	3.38820900	3.04132900
H	0.12085800	2.71466700	4.40065800
H	-1.67269400	2.72871700	4.47877300
C	-4.34520300	1.66870900	-2.15541900
H	-4.02877600	0.63298300	-2.37100100
H	-4.29866600	2.23713600	-3.10583100
H	-5.41045300	1.64797400	-1.84700800

C	-0.70346600	0.08973600	4.24736000
H	-1.47348900	0.19632200	5.03899700
H	0.28451100	0.17651500	4.74041000
H	-0.78592000	-0.92879900	3.82204500
C	4.40205700	0.25958000	-1.99488900
H	5.26942400	-0.30328500	-2.37230400
C	0.70385900	0.09088100	-4.24737600
H	1.47404100	0.19720900	-5.03889200
H	-0.28401100	0.17793700	-4.74059300
H	0.78594300	-0.92766500	-3.82201500
C	-2.46171100	-1.37363800	-1.44050400
C	4.34491200	1.66815400	2.15625100
H	4.02885000	0.63225500	2.37153000
H	4.29815000	2.23628000	3.10683300
H	5.41017800	1.64788600	1.84786500
F	-5.54908100	-3.08506800	-0.57777300
C	3.95904900	3.78636700	0.84017800
H	4.99962600	3.76685400	0.45556600
H	3.95114800	4.38051400	1.77658200
H	3.34691800	4.32090900	0.08658400
C	2.31836100	-2.16826200	-0.80770900
C	3.74349800	-1.92545200	1.58198600
F	-4.16975500	-3.32391200	1.77569400
C	-2.31862900	-2.16875200	0.80721200
C	0.80554900	2.58510300	-3.80341800
H	0.83535300	3.38933000	-3.04137300
H	-0.11953300	2.71610500	-4.40089500
H	1.67403700	2.72955300	-4.47864100
C	4.32007800	-2.58733100	0.47817300
C	3.60660000	-2.71814000	-0.73048500
C	-3.74339500	-1.92475000	-1.58262200
C	-4.32014000	-2.58719900	-0.47923500
C	-3.60685200	-2.71861300	0.72946700

I (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -2856.23036386 A.U.

Al	-0.00032000	0.58832500	-0.00001200

F	1.97099100	0.63578000	-2.44213500
N	-0.99396400	-2.20959600	-0.44205700
N	0.99503600	-2.20835900	0.44515100
F	1.59751200	2.33374100	1.97264200
F	4.45284000	1.77863100	-2.67580100
F	-1.97202000	0.64139600	2.44245400
C	0.00014800	-1.39004000	0.00124700
F	-1.59816200	2.32860300	-1.97645400
C	0.62920500	-3.53520100	0.28878500
H	1.27293200	-4.36371700	0.59663500
C	-0.62694200	-3.53598400	-0.28472900
H	-1.27009900	-4.36526100	-0.59173200
C	-2.20124000	-1.64600400	-1.01300700
C	2.20184500	-1.64332800	1.01559900
C	-2.09562500	-1.03818000	-2.29235800
F	5.52128600	3.14336800	-0.55619900
F	4.10800500	3.42026800	1.77397100
C	3.37039800	-1.60600200	0.21542000
C	2.09534800	-1.03280500	2.29364900
C	-3.36921500	-1.60711500	-0.21204000
C	-0.84486500	-1.19723400	-3.15844800
H	0.04804100	-1.13273500	-2.49724600
C	-3.22604700	-0.33477300	-2.75258700
H	-3.19303600	0.16371600	-3.73063800
C	-4.38421200	-0.23888200	-1.96792000
H	-5.24298700	0.34298800	-2.33569700
F	-4.45434900	1.78356800	2.67260400
C	3.46719200	-2.37301100	-1.09939100
H	2.44210200	-2.45245200	-1.52276900
C	0.84424700	-1.19045000	3.15957500
H	-0.04857600	-1.12643700	2.49817800
C	-4.46137200	-0.87908100	-0.72259100
H	-5.38277800	-0.80082900	-0.12805600
C	3.22534200	-0.32823900	2.75310200
H	3.19165200	0.17226400	3.73009400

C	-3.46445300	-2.37122600	1.10456700
H	-2.43909700	-2.44759900	1.52792600
C	-1.72236200	1.46913200	0.23042500
C	1.72155800	1.46898400	-0.23219900
C	-3.97863500	-3.80361900	0.82875900
H	-5.01756100	-3.76855100	0.43988200
H	-3.97973800	-4.40272700	1.76210900
H	-3.36691400	-4.33839800	0.07588100
C	2.47617800	1.34566600	-1.40392700
C	4.46211800	-0.87673900	0.72518400
H	5.38394700	-0.79984500	0.13111600
C	-0.82556000	-2.60085100	-3.80395400
H	-0.86594000	-3.41049600	-3.04864200
H	0.09840200	-2.73748400	-4.40186400
H	-1.69716900	-2.72433900	-4.47963600
C	-4.35125200	-1.69577300	2.16210700
H	-4.03438200	-0.66052000	2.37910000
H	-4.30068600	-2.26789200	3.11029300
H	-5.41661900	-1.67445600	1.85365800
C	-0.68851300	-0.10424700	-4.22575200
H	-1.46447600	-0.18955400	-5.01421100
H	0.29657500	-0.20463600	-4.72225000
H	-0.75182100	0.91083100	-3.78837100
C	4.38404900	-0.23384900	1.96903800
H	5.24250300	0.34888300	2.33618500
C	0.68797300	-0.09626900	4.22566000
H	1.46364500	-0.18106000	5.01445800
H	-0.29731500	-0.19574000	4.72193300
H	0.75181800	0.91833900	3.78724600
C	-2.47718300	1.34843300	1.40231000
C	4.35263900	-1.69836300	-2.15858900
H	4.03332900	-0.66447000	-2.37841300
H	4.30352000	-2.27319000	-3.10522000
H	5.41791400	-1.67369900	-1.85009400
F	-5.52286600	3.14278700	0.54946500

C	3.98430300	-3.80361400	-0.81983700
H	5.02312800	-3.76533400	-0.43095800
H	3.98676000	-4.40517900	-1.75160100
H	3.37364000	-4.33763300	-0.06554300
C	2.29271200	2.19456800	0.81955700
C	3.74877800	1.91696500	-1.54601700
F	-4.10915700	3.41444200	-1.78111400
C	-2.29358800	2.19194000	-0.82319900
C	0.82432200	-2.59337600	3.80654800
H	0.86500200	-3.40379000	3.05208400
H	-0.09997600	-2.72923000	4.40411000
H	1.69556700	-2.71628700	4.48280700
C	4.29988500	2.61870600	-0.45599700
C	3.57033500	2.76832300	0.73883200
C	-3.75006300	1.91953900	1.54267000
C	-4.30122100	2.61841100	0.45083500
C	-3.57145600	2.76537500	-0.74418900

I-F (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -2956.24215214 A.U.

Al	-0.19033200	-0.00840900	-1.08848400
F	-0.78255900	-0.97776700	-2.36337600
F	1.64250600	2.55171300	-0.30733200
F	2.15691000	-1.83955800	-2.10218900
F	-0.18568800	2.36431000	-2.96585700
F	-2.33335800	1.26787500	1.14879300
F	4.31345500	2.90482200	-0.42061700
F	-1.38003300	4.81619200	-2.92013700
F	5.92965200	0.92682800	-1.42367100
F	-3.50734400	3.68616800	1.18562800
F	4.83171400	-1.43620900	-2.29003800
F	-3.04662500	5.48484800	-0.84792100
C	-0.54683300	-1.06638200	0.63302700
C	-0.61607300	-1.62949300	2.83523000
H	-0.28538100	-1.63258600	3.87728300
C	1.36932300	-0.30364900	2.02473000
C	2.38687200	1.53753700	-0.81149900

C	-2.49406200	-2.42888400	-0.14233500
C	-2.83070500	-3.94137400	-1.98721700
H	-2.44647300	-4.67596800	-2.70870800
C	-1.68489400	-2.23101700	2.21920200
H	-2.47480400	-2.88160300	2.60522100
C	2.52958500	-1.06229000	1.70493600
C	-1.01190700	2.66107300	-1.93626300
C	2.64627100	-0.63256800	-1.71903700
C	-0.48865800	-3.81326900	-0.98488200
H	0.10797300	-2.92585700	-0.69101400
C	-2.07536200	2.10397000	0.10047900
C	-3.84766300	-2.02324000	-0.17118300
C	-2.70217200	3.35865400	0.15967100
C	0.16942100	1.76031900	2.95847800
H	-0.70512200	1.21892000	2.55375800
C	-1.95003600	-3.37952200	-1.04611600
C	-4.18424700	-3.57544500	-2.02904900
H	-4.85100600	-4.03009600	-2.77829200
C	3.77210400	1.76261500	-0.87277500
C	-1.60739700	3.93384200	-1.93721400
C	4.60247000	0.75001000	-1.38074600
C	1.41897200	1.03079000	2.48651900
C	1.77893200	0.34211500	-1.21371600
C	-1.21947500	1.70841800	-0.92778000
C	-4.68470000	-2.62465800	-1.13359600
H	-5.74371700	-2.32804500	-1.18438900
C	-2.46418500	4.28007000	-0.87417600
C	-4.40834700	-0.95920400	0.76283300
H	-3.57415500	-0.57254200	1.37674600
C	4.03554200	-0.45653200	-1.82532300
C	3.84458000	0.93974900	2.20439700
H	4.82252900	1.44368000	2.23818700
C	-0.28615600	-4.89142800	0.09994600
H	-0.60071500	-4.53620800	1.10261600
H	0.78311400	-5.18235700	0.16456500

H	-0.87459900	-5.80293400	-0.13631300
C	2.68819500	1.64021900	2.56376000
H	2.76271800	2.68764800	2.89088600
C	2.44252100	-2.54689300	1.35614000
H	1.53596000	-2.68998900	0.73088900
C	0.07274100	3.21067300	2.45571200
H	0.84226900	3.86333700	2.91937200
H	-0.91955200	3.63287800	2.71483000
H	0.19632400	3.26340300	1.35853800
C	3.76719800	-0.40205000	1.79786100
H	4.68801600	-0.94134700	1.53475200
C	0.07031300	-4.26197800	-2.34107100
H	-0.37862400	-5.21789000	-2.68486100
H	1.16414100	-4.42118400	-2.26082100
H	-0.10597300	-3.48194000	-3.10665300
C	0.08244900	1.69983800	4.49869500
H	0.09479300	0.65468600	4.87143800
H	-0.85205500	2.18049200	4.85580600
H	0.94027300	2.22800600	4.96610700
C	2.27232900	-3.38670000	2.64309000
H	3.16107200	-3.26934200	3.29793400
H	2.16924700	-4.46249300	2.39214400
H	1.38034700	-3.09334600	3.22774200
C	-5.46594100	-1.54158800	1.71946600
H	-6.34030400	-1.94119300	1.16375500
H	-5.83737300	-0.75934700	2.41371500
H	-5.05379700	-2.37288500	2.32884600
C	3.64018800	-3.08810900	0.56271800
H	3.83645700	-2.51933800	-0.36179800
H	3.44597000	-4.13984300	0.26998600
H	4.56785400	-3.08868000	1.17256700
C	-4.96123000	0.23723600	-0.03713900
H	-4.22051300	0.59498700	-0.77974500
H	-5.20201300	1.08077300	0.64154500
H	-5.88677700	-0.03259000	-0.58793200

N	-1.61799000	-1.88070900	0.87345900
N	0.07810300	-0.94043500	1.84474000

I-F (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -2956.25265684 A.U.

Al	-0.19418000	0.00338000	-1.05354900
F	-0.76938500	-0.92004400	-2.37762100
F	1.61769200	2.57881100	-0.26554400
F	2.15828800	-1.77430500	-2.14640600
F	-0.23011100	2.36752800	-2.95707700
F	-2.33157300	1.27719500	1.18409400
F	4.28310100	2.96474100	-0.40661900
F	-1.45905000	4.80046000	-2.92373200
F	5.90920900	1.02150400	-1.46127200
F	-3.54348100	3.67737100	1.20608100
F	4.82709900	-1.33826300	-2.35645300
F	-3.12229300	5.46371700	-0.84548700
C	-0.53482400	-1.08589000	0.63956700
C	-0.57965300	-1.69764400	2.82911200
H	-0.24252000	-1.72522800	3.86890200
C	1.38304100	-0.32892700	2.02852400
C	2.36769900	1.57897700	-0.79043100
C	-2.46895500	-2.45120600	-0.15336900
C	-2.80051700	-3.94691700	-2.01467300
H	-2.41746900	-4.68039500	-2.73823700
C	-1.64766400	-2.29660900	2.20876300
H	-2.42404100	-2.96638300	2.58968500
C	2.55028000	-1.06672100	1.68547300
C	-1.05364300	2.65998900	-1.91952900
C	2.64032100	-0.57102300	-1.74011800
C	-0.46365200	-3.83593600	-0.99357500
H	0.13324600	-2.95352700	-0.68406800
C	-2.09309800	2.10552400	0.12959300
C	-3.82121200	-2.04114500	-0.18543100
C	-2.73818900	3.35165500	0.17955300
C	0.16792100	1.69995500	3.02035300
H	-0.70543700	1.14173700	2.63575800

C	-1.92313900	-3.39645500	-1.06267700
C	-4.15305900	-3.57447700	-2.06092300
H	-4.81779000	-4.02103600	-2.81677000
C	3.74927200	1.82037600	-0.86503700
C	-1.66722200	3.92322500	-1.92887400
C	4.58441800	0.82679700	-1.40064300
C	1.42016500	0.99660900	2.51656000
C	1.76869400	0.38330400	-1.20474500
C	-1.23932100	1.71314900	-0.90258000
C	-4.65540500	-2.62974700	-1.15906000
H	-5.71374300	-2.33126600	-1.21198700
C	-2.52118200	4.26666600	-0.86376900
C	-4.38299600	-0.99113500	0.76328200
H	-3.54684700	-0.60742400	1.37666400
C	4.02583900	-0.37773100	-1.85934600
C	3.84449700	0.94316600	2.20959800
H	4.81700900	1.45724400	2.24834000
C	-0.27244500	-4.92658600	0.08117900
H	-0.59946200	-4.58385300	1.08366000
H	0.79656200	-5.21576500	0.15426600
H	-0.85668800	-5.83541000	-0.17477700
C	2.68232500	1.62156000	2.59346800
H	2.74755800	2.66148100	2.94606500
C	2.47984000	-2.54734500	1.31768500
H	1.56506800	-2.69637900	0.70598100
C	0.03394400	3.14878400	2.52150900
H	0.80598100	3.81220000	2.96499400
H	-0.95734600	3.55559000	2.80783900
H	0.12721800	3.20434300	1.42124200
C	3.78048500	-0.39209300	1.77862400
H	4.70647300	-0.91524000	1.50133800
C	0.10585800	-4.27708000	-2.34818300
H	-0.34728600	-5.22594600	-2.70464100
H	1.19732400	-4.44698200	-2.25656500
H	-0.05615400	-3.49288300	-3.11288900

C	0.11954200	1.63569600	4.56201400
H	0.16321200	0.59044800	4.93078100
H	-0.81687800	2.09549400	4.94084600
H	0.97596000	2.18390300	5.00846600
C	2.34243700	-3.40577600	2.59627500
H	3.24159500	-3.28545300	3.23609600
H	2.24874800	-4.47904700	2.33174900
H	1.45770500	-3.13062600	3.20012200
C	-5.42993000	-1.59375700	1.71955800
H	-6.30402700	-1.99264900	1.16289200
H	-5.80230700	-0.82136400	2.42415300
H	-5.00521800	-2.42672700	2.31706700
C	3.67280900	-3.05934600	0.49796900
H	3.84700800	-2.47165600	-0.41946000
H	3.48776000	-4.10888300	0.19198300
H	4.60946300	-3.05509000	1.09353200
C	-4.95148300	0.20971300	-0.01866200
H	-4.21777900	0.58698100	-0.75892600
H	-5.19959200	1.04019300	0.67339300
H	-5.87662900	-0.06241400	-0.56872500
N	-1.59608300	-1.91530300	0.87082200
N	0.09857100	-0.97897800	1.84853500

I-H (BP86-D3/Def2-SVP)

SCF Done: E(RB-P86) = -2856.98725541 A.U.

Al	0.26489700	-0.12794700	-1.17631500
F	1.98973400	1.38993600	-3.29222700
F	1.31969300	1.55850200	1.42817900
F	-1.16410000	2.40345600	0.11287200
F	-2.19824600	-1.03373200	-3.02195600
F	3.70234400	3.49757100	-3.11305800
F	-3.70540500	3.33110300	-0.06746400
F	3.02178300	3.64884500	1.59309300
F	-5.50439700	2.08762500	-1.72460900
F	-4.73323600	-0.09042500	-3.20742100
F	4.21506800	4.64252200	-0.67293600
N	1.30156700	-1.86654500	1.06778400

N	-0.62851100	-1.10844500	1.69442400
C	-2.01271100	1.77264100	-0.73706300
C	0.25281700	-1.09130400	0.64847500
C	2.36896600	-2.30740900	0.19418100
C	-0.13150100	-1.86774200	2.75295300
H	-0.69791500	-2.00457500	3.67785000
C	-1.95161200	-0.51743600	1.68766600
C	3.62330200	-1.65476400	0.23798700
C	-2.51912200	0.06827800	-2.30094600
C	2.74528300	3.10695900	0.39390500
C	2.22867700	1.91731100	-2.07011900
C	-2.18093000	0.63387000	2.47736400
C	1.87623700	2.01337400	0.26753000
C	1.08765100	-2.35196400	2.35374400
H	1.80576500	-3.00876300	2.85190300
C	-1.57393600	0.65021300	-1.44845300
C	3.11304900	3.01109900	-2.01047000
C	4.36386200	-3.17172400	-1.53412600
H	5.15276900	-3.50693800	-2.22538700
C	2.08340500	-3.38472200	-0.68177500
C	3.11292800	-3.80325700	-1.54498700
H	2.92573800	-4.63238800	-2.24386000
C	0.74235800	-4.10959300	-0.66480700
H	0.02162100	-3.47432000	-0.11387800
C	1.58891000	1.38058600	-0.94438600
C	3.36910800	3.60796800	-0.76214600
C	-4.23879600	1.65075600	-1.66417300
C	-3.31651000	2.28544900	-0.81500500
C	-2.96388600	-1.13749500	0.90239000
C	4.61605200	-2.11333400	-0.65078900
H	5.60199100	-1.62623900	-0.65396600
C	-1.11016100	1.23016000	3.38459400
H	-0.13103800	0.83178400	3.05582500
C	3.91428600	-0.53874400	1.23305200
H	2.94734300	-0.06153100	1.48755900

C	-3.83804500	0.53889100	-2.42433900
C	0.86820500	-5.43570700	0.11287900
H	1.58178000	-6.12405600	-0.38713500
H	-0.11400900	-5.94884200	0.17591000
H	1.23347700	-5.26735600	1.14702900
C	-4.48207400	0.63141900	1.65535500
H	-5.47623900	1.10235300	1.61514200
C	-1.02890300	2.76477600	3.29393100
H	-0.96287400	3.10049700	2.24391500
H	-0.13168600	3.12913900	3.83425900
H	-1.91344100	3.25018300	3.75786100
C	-2.71404300	-2.43005400	0.12191600
H	-1.77158800	-2.29271000	-0.45351500
C	-3.47290000	1.19786500	2.43968400
H	-3.67945000	2.10739300	3.02233400
C	0.15570100	-4.32178200	-2.07006400
H	0.07277100	-3.35695100	-2.60863900
H	-0.85771900	-4.76811000	-1.99530800
H	0.77408400	-5.01384000	-2.67931100
C	-4.23109800	-0.52657100	0.90373200
H	-5.03821300	-0.95726500	0.29602800
C	-1.34425100	0.78767900	4.84533200
H	-2.31455800	1.17410000	5.22253500
H	-0.54192300	1.17802200	5.50551700
H	-1.36815200	-0.31610900	4.95309300
C	-3.81627900	-2.77449600	-0.89051900
H	-4.76488800	-3.04446100	-0.38031700
H	-3.50433200	-3.65234900	-1.49085000
H	-4.02652700	-1.95286400	-1.59773900
C	4.83761300	0.54815300	0.65744500
H	5.88079400	0.18504800	0.54397900
H	4.86713400	1.42263200	1.33798600
H	4.48435000	0.89503600	-0.33329700
C	4.50635900	-1.11615700	2.53696800
H	3.82742500	-1.85263100	3.01167900

H	4.69366700	-0.30577600	3.27179000
H	5.47033300	-1.62991400	2.33744200
C	-2.52017400	-3.63161900	1.07428400
H	-1.66628300	-3.50397900	1.76559500
H	-2.33800000	-4.55667800	0.48972000
H	-3.43367400	-3.78964700	1.68501200
H	0.70024500	-1.22772600	-2.24756400

I-H (BP86-D3/Def2-SVP, PCM, Fluorobenzene)

SCF Done: E(RB-P86) = -2856.99667175 A.U.

Al	-0.26472700	0.11010700	-1.15254400
F	-1.99437100	-1.42583900	-3.27583300
F	-1.30326800	-1.58344700	1.44368700
F	1.18043600	-2.40721600	0.15176400
F	2.18022400	0.98112800	-3.04966600
F	-3.70283700	-3.53188100	-3.08378500
F	3.72002900	-3.33489500	-0.03998600
F	-3.00218100	-3.67613100	1.61980700
F	5.50144500	-2.11659800	-1.73520700
F	4.71196700	0.03716700	-3.24523400
F	-4.20562100	-4.67308400	-0.63890000
N	-1.30327900	1.89045200	1.05213800
N	0.62986500	1.14486700	1.68448100
C	2.02074800	-1.78399500	-0.71185900
C	-0.25635200	1.10796300	0.64331400
C	-2.37468400	2.31084700	0.17374200
C	0.13831000	1.92587900	2.72951600
H	0.70890400	2.08708700	3.64791600
C	1.95200700	0.55277900	1.68110100
C	-3.62120300	1.64288900	0.22219800
C	2.50964500	-0.10606600	-2.30722600
C	-2.73273600	-3.13289400	0.41915600
C	-2.22550600	-1.94952600	-2.04693500
C	2.18451900	-0.58628500	2.48772500
C	-1.86446300	-2.03889300	0.28862500
C	-1.08304300	2.40199000	2.32693000
H	-1.79522600	3.07093700	2.81763800

C	1.57330500	-0.67268400	-1.43542200
C	-3.10890000	-3.04273400	-1.98239400
C	-4.37845200	3.13623600	-1.56382600
H	-5.17120800	3.45700000	-2.25749500
C	-2.10229100	3.38711700	-0.70782100
C	-3.13583800	3.78532800	-1.57700700
H	-2.96096600	4.61450200	-2.27908400
C	-0.77115600	4.13023400	-0.69232200
H	-0.04396000	3.51242200	-0.12976600
C	-1.58141200	-1.40893700	-0.92650600
C	-3.36052900	-3.63667700	-0.73277100
C	4.23716800	-1.67555200	-1.66365500
C	3.32431800	-2.29614800	-0.79493000
C	2.96194100	1.16238100	0.88454400
C	-4.61854300	2.08067600	-0.67255300
H	-5.59950500	1.58361600	-0.67217600
C	1.11878700	-1.16429800	3.41272700
H	0.13779300	-0.77010500	3.08346100
C	-3.89962400	0.53713200	1.23220100
H	-2.92823800	0.06765700	1.48502100
C	3.82731800	-0.57692800	-2.43690500
C	-0.91793700	5.46493700	0.06701400
H	-1.63464600	6.13814000	-0.44893600
H	0.05884000	5.98816000	0.12914800
H	-1.28844800	5.30518100	1.10033300
C	4.48357200	-0.59531800	1.65764300
H	5.47930300	-1.06360600	1.62488400
C	1.03717100	-2.70038700	3.35313000
H	0.94876800	-3.05738300	2.31155700
H	0.15251200	-3.05392500	3.92092800
H	1.93171800	-3.17554000	3.80799100
C	2.70958800	2.44667800	0.09162900
H	1.75786100	2.30933900	-0.46851600
C	3.47687600	-1.15069500	2.45400000
H	3.68825500	-2.04784900	3.05411700

C	-0.18264100	4.33475100	-2.09813300
H	-0.08598600	3.36620800	-2.62774200
H	0.82479800	4.79407800	-2.02474300
H	-0.80909900	5.01142200	-2.71607700
C	4.22984200	0.55209000	0.89010800
H	5.03661000	0.97646100	0.27736800
C	1.36244300	-0.69421000	4.86344600
H	2.33484000	-1.07522800	5.24078800
H	0.56351200	-1.07305600	5.53420300
H	1.38510300	0.41094000	4.94997300
C	3.80097500	2.77180000	-0.93886500
H	4.75671200	3.04375600	-0.44380100
H	3.48529900	3.64307100	-1.54677800
H	4.00036600	1.93755700	-1.63479700
C	-4.82493300	-0.55918900	0.67830300
H	-5.86945100	-0.19924000	0.56976400
H	-4.84692100	-1.42414500	1.37129900
H	-4.48134800	-0.91826200	-0.31176100
C	-4.48208000	1.12842000	2.53448200
H	-3.80179800	1.87266400	2.99399000
H	-4.65945900	0.32510300	3.27937400
H	-5.45022600	1.63441200	2.33568500
C	2.53496100	3.66104600	1.03173200
H	1.69272800	3.54436400	1.73879600
H	2.34660000	4.57878900	0.43798100
H	3.45901900	3.82260700	1.62519700
H	-0.70711900	1.16286200	-2.27364300