# Supplementary Data for :

## Electronic effects of triarylphosphines in the metal-free hydrogen activation: A kinetic and computational study

Lutz Greb,[a] Sebastian Tussing,[a] Birgitta Schirmer,[b] Pascual Oña-Burgos,[c] Karl Kaupmees,[d] Märt Lõkov,[d] Ivo Leito,[d] Stefan Grimme,[e] Jan Paradies*[a]

[a] *Karlsruhe Institute of Technology, Institute of Organic Chemistry, Fritz-Haber-Weg 6, 76131 Karlsruhe, Germany. Fax: +49 721 608 45637; Tel: +49 721 608 45344; E-mail: jan.paradies@kit.edu*
[b] *Westfälische Wilhelms-Universität Münster, Institute of Organic Chemistry, Corrensstrasse 40, 48149 Münster. E-mail: b.schirmer@uni-muenster.de*
[c] *Karlsruhe Institute of Technology, Institute of Inorganic Chemistry, Fritz-Haber-Weg 6, 76131 Karlsruhe, Germany. E-mail: pob081@ual.es*
[d] *University of Tartu, Institute of Chemistry Ravila 14a, Tartu 50411, Estonia. E-mail: ivo.leito@ut.ee*
[e] *Unsiversität Bonn, Mulliken Center for Theoretical Chemistry, Institute of Physical and Theoretical Chemistry, Beringstr. 4, D-53115 Bonn, Germany. E-mail: grimme@thch.uni-bonn.de*

## General Information

**Synthesis and techniques**

All preparations were done in oven dried (140 °C) glassware under an atmosphere of dry, $O_2$-free Ar employing both Schlenk line techniques and a MBraun inert atmosphere glove box. Experiments on NMR tube scale were carried out in Teflon cap sealed *J* Young NMR tubes. Toluene, hexane and pentane were purified with a Grubbs-type column system manufactured by MBraun and dispensed into thick-walled glass Schlenk bombs equipped with Young –type Teflon valve stop-cocks. THF and $Et_2O$ were distilled from Na-benzophenone ketal. Dichloromethane was distilled from $CaH_2$ (followed by 3 freeze-pump-thaw cycles). All solvents were stored over 4 Å molecular sieves in the glove box. Molecular sieves (4 Å) were dried at 140 °C under vacuum for 24 h prior to use. Deuterated solvents were vacuum transferred from sodium/benzophenone ($C_6D_6$ / $C_7D_8$) or $CaH_2$ ($CD_2Cl_2$), degassed by 3 freeze-pump-thaw cycles and stored over 4 Å molecular sieves for usage in a glove box. Solvents for chromatography were used as received from commercial sources and were analytical grade. Silica gel 60 (particle size 0.040 – 0.063 mm) was purchased from Sigma Aldrich. TLC's were run on silica gel coated aluminum plates with UV indicator (F254) obtained by Merck and analyzed by UV/VIS and stained using a cerium ammonium molybdate solution.

**Reagents and materials**

Reagents for substrate synthesis and substrates for the catalytic hydrogenation were used as received without further purification unless noted otherwise. Liquid substrates were stored over 4 Å molecular sieves in a glove box. Hydrogen 5.0 was purchased from AirLiquide and purified through a Johnson Matthey Model HIG 35XL™ gas purifier. Tris(pentafluorophenyl)borane (**1**), P(napht-1-yl)$_3$ and P($C_6F_5$)$Ph_2$ (**8**) was purchased from Sigma Aldrich and used as received. P(2-F-$C_6H_4$)$Ph_2$ (**2**), P(2-F-$C_6H_4$)$_2$Ph (**3**), P(2-F-$C_6H_4$)$_3$ (**4**), P(2,6-$F_2$-$C_6H_3$)$Ph_2$ (**5**), P(2,6-$F_2$-$C_6H_3$)$_2$Ph (**6**) and P(2,6-$F_2$-$C_6H_3$)$_3$ (**7**) were prepared using modified literature methods.[1]

**Characterization**

$^1$H, $^{13}$C, $^{11}$B, $^{19}$F and $^{31}$P-NMR spectra were recorded on a *Bruker* AC 300 (300 MHz), *Bruker* AM 400 (400 MHz) or a *Bruker* DRX 500 (500 MHz) spectrometer as solutions in non-spinning mode. Chemical shifts are expressed in parts per million (ppm, δ) downfield from tetramethylsilane (TMS) and are referenced to $CDCl_3$ (2.26 ppm) or $CD_2Cl_2$ (5.32 ppm) as internal standards. $^{31}$P, $^{11}$B and $^{19}$F NMR spectra are referenced to 85% $H_3PO_4$, $BF_3(OEt_2)$ and $CFCl_3$ respectively. All coupling constants are absolute values and *J* values are expressed in Hertz (Hz). The description of signals include: s = singlet, br. s = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, etc. The spectra were analyzed according to first order.

## Determination of p$K_a$ of the corresponding acids of $PR_{3-n}Ph_n$ (R = (2-F-$C_6H_4$) or (2,6-$F_2$-$C_6H_3$)), P($C_6F_5$)$Ph_2$ and P(napht-1-yl)$_3$ *via* non-aqueous titration.

The results of the p$K_a$ measurements in MeCN are presented in Table 1. Due to experimental difficulties – insolubility of P(naph)$_3$ in MeCN and very low basicity of (2,6-$F_2$-$C_6H_3$)$_3$P – 1,2-dichloroethane (DCE) was used to predict the p$K_a$ values of P(naph)$_3$ and (2,6-$F_2$-$C_6H_3$)$_3$P in acetonitrile (MeCN). For that, a small basicity scale was constructed in DCE, which incorporated compounds (2-F-$C_6H_4$)(Ph)$_2$P, (2-F-$C_6H_4$)$_2$(Ph)P and ($C_6F_5$)(Ph)$_2$P for which also the MeCN p$K_a$ values were measured. For the construction of basicity scale altogether 19 individual measurements were made (See Figure 1 and Table 1). The consistency standard deviation of the scale is s = 0.05 p$K_{ip}$ units. As is customary among organic chemists, the term "p$K_a$ of base X" is used in this paper with the actual meaning of p$K_a$ of the conjugate acid of base X.

**Table 1 p$K_a$ values of the studied phosphines, including all individual measurements in acetonitrile.**

| Base | Reference Base | p$K_a$ (reference)[a] | Δp$K_a$ | s(Δp$K_a$)[b] | p$K_a$ (Base) | Assigned p$K_a$ |
|---|---|---|---|---|---|---|
| (2-F-$C_6H_4$)(Ph)$_2$P | 2,6-$Cl_2$-Aniline | 5.06 | -1.04 | 0.01 | 6.10 | **6.11** |
| | 2-Cl-Pyridine | 6.79 | 0.68 | 0.01 | 6.11 | |
| (2-F-$C_6H_4$)$_2$(Ph)P | 2,6-$Cl_2$-Aniline | 5.06 | 0.50 | 0.01 | 4.56 | **4.55** |
| | 2-$NO_2$-Aniline | 4.80 | 0.25 | 0.02 | 4.55 | |
| (2,6-$F_2$-$C_6H_3$)(Ph)$_2$P | 2,6-$Cl_2$-Aniline | 5.06 | -0.11 | 0.01 | 5.17 | **5.16** |
| | 2-$NO_2$-Aniline | 4.80 | -0.36 | 0.04 | 5.16 | |
| (2-F-$C_6H_4$)$_3$P | 2,3,5,6-$Cl_4$-Aniline | 2.73 | -0.30 | 0.04 | 3.03 | **3.03** |
| | 5-Cl-2-$NO_2$-Aniline | 3.22 | 0.19 | 0.02 | 3.03 | |
| (2,6-$F_2$-$C_6H_3$)$_2$(Ph)P | 2,3,5,6-$Cl_4$-Aniline | 2.73 | 0.28 | 0.02 | 2.45 | **2.52** |
| | 5-Cl-2-$NO_2$-Aniline | 3.22 | 0.64 | 0.05 | 2.58 | |
| | 2,3,4,5,6-$Cl_5$-Aniline | 2.35 | -0.19 | 0.02 | 2.54 | |
| ($C_6F_5$)(Ph)$_2$P | 2,3,5,6-$Cl_4$-Aniline | 2.73 | 0.24 | 0.02 | 2.49 | **2.56** |
| | 5-Cl-2-$NO_2$-Aniline | 3.22 | 0.63 | 0.01 | 2.59 | |
| | 2,3,4,5,6-$Cl_5$-Aniline | 2.35 | -0.26 | 0.03 | 2.61 | |
| (2,6-$Cl_2$-$C_6H_3$)$_3$P | 2,3,4,5,6-$Cl_5$-Aniline | 2.35 | 0.61 | 0.03 | 1.74 | **1.72** |
| | 2,3,5,6-$Cl_4$-Aniline | 2.73 | 1.03 | 0.03 | 1.70 | |
| (2,6-$F_2$-$C_6H_3$)$_3$P | Estimated from correlation with DCE data | | | | | **0.7** |
| P(naph)$_3$ | Estimated from correlation with DCE data | | | | | **6.8** |

[a] experimental values from reference [2]; [b] experimental standard deviation of Δp$K_a$ allows evaluating the within-series agreement of Δp$K_a$ values.

Determination of p$K_a$ values in acetonitrile (and p$K_{ip}$ in case of 1,2-dichloroethane) is based on measurements of relative difference in basicities of two bases, the phosphine and a reference base. This method has been previously used in measurements of acidity and basicity of different compounds in acetonitrile,[3] tetrahydrofuran[4] and 1,2-dichloroethane.[5] In short, this method is bases on spectrophotometric titration of mixture of two compounds. Knowing the spectra of neutral and ionic form of both compounds allows the calculation of degree of protonation/deprotonation in the mixtures formed during titration, which in turn can be used to calculate the differences in p$K_a$ (or p$K_{ip}$) values of the studied compounds according to the following formula.

$$\Delta pK_a = pK_a(B_2) - pK_a(B_1) = \log \frac{[B_1^z]\cdot[HB_2^{z+1}]}{[HB_1^{z+1}]\cdot[B_2^z]} \qquad (1)$$

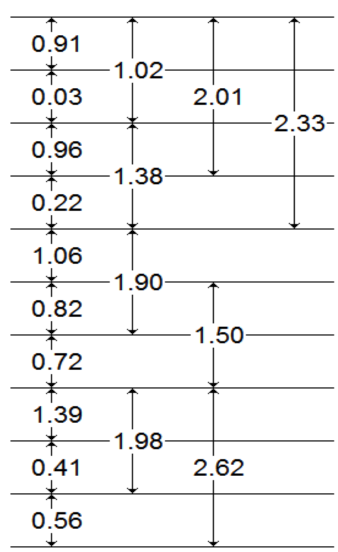
The mixture is titrated, the degree of dissociation of both species is changed and a number of $\Delta pK_a$ (or $\Delta pK_{ip}$)values are obtained, which can be averaged. If a compound is measured against different reference compounds and the results are averaged then an absolute $pK_a$ value can be assigned. In MeCN t-BuP(pyrr) as basic and triflic acid as acidic titrant was used. In DCE $CF_3SO(=NTf)NHTf$ had to be used as acidic titrant, because triflic acid was found to be too weak to protonate the investigated bases. A more detailed description of measurement and details about the apparatus can be found in references [5] and [2].

Assigning zero as absolute $pK_{ip}$ for $(2,6\text{-}F_2\text{-}C_6H_3)_3P$ in the constructed scale, the $pK_{ip}$ values for all the phosphines can be calculated. Knowing their $pK_a$ values in acetonitrile allows the construction of a correlation equation (See Graph 1) which can be used to predict the $pK_a$ values in acetonitrile for compounds $P(naph)_3$ and $(2,6\text{-}F_2\text{-}C_6H_3)_3P$. Alternatively, the directly measured $\Delta pK_{ip}$ values between two phosphines in DCE can be used to describe the changes in basicity.

**Figure 1 Constructed basicity scale in DCE together with the assigned $pK_{ip}$ values.**

| Compound | $pK_{ip}$ |
|---|---|
| $P(naph)_3$ | **6.86** |
| $P(2\text{-}F\text{-}C_6H_4)Ph_2$ | **5.91** |
| 2,6-MeO Pyridine | **5.90** |
| 4-Br Aniline | **4.81** |
| $P(2\text{-}F\text{-}C_6H_4)_2Ph$ | **4.55** |
| $4\text{-}CF_3$ Aniline | **3.47** |
| $4\text{-}F\text{-}3\text{-}NO_2$ Aniline | **2.66** |
| $P(C_6F_5)Ph_2$ | **1.96** |
| $2\text{-}NO_2$ Aniline | **0.49** |
| $P(2,6\text{-}F_2C_6H_3)_3$ | **0** |
| $NPh_3$ | **-0.61** |

Individual measurements

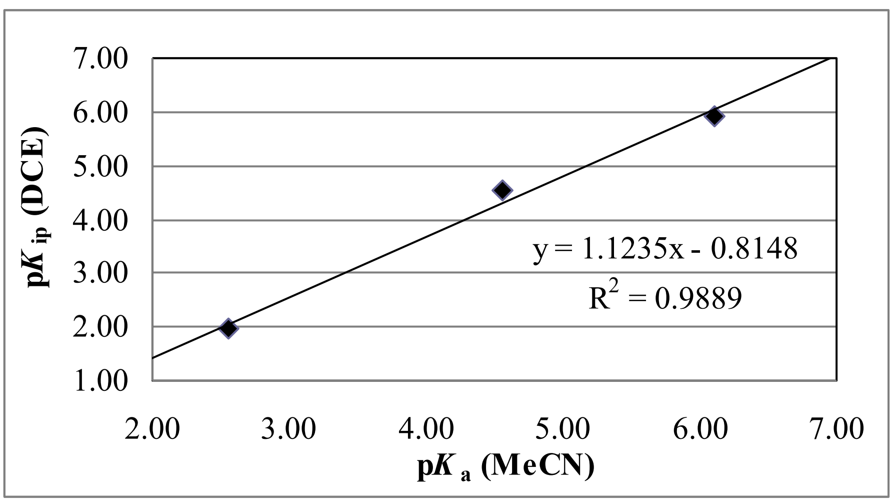


**Tabel 2 Individual $\Delta pK_{ip}$ measurements in DCE.**

| Base | Reference Base | $\Delta pK_{ip}$ | s($\Delta pK_{ip}$)[a] |
|---|---|---|---|
| (2-F-$C_6H_4$)$(Ph)_2$P | $P(naph)_3$ | 0.91 | 0.05 |
| | 2,6-MeO Pyridine | 0.03 | 0.04 |
| | 4-Br Aniline | -1.10 | 0.01 |
| (2-F-$C_6H_4)_2$(Ph)P | $P(naph)_3$ | 2.33 | 0.06 |
| | 2,6-MeO Pyridine | 1.38 | 0.02 |
| | 4-Br Aniline | 0.22 | 0.04 |
| | 4-$CF_3$ Aniline | -1.06 | 0.03 |
| | 4-F-3-$NO_2$ Aniline | -1.90 | 0.03 |
| $P(naph)_3$ | 2,6-MeO Pyridine | -1.02 | 0.02 |
| | 4-Br Aniline | -2.01 | 0.03 |
| 2,6-MeO Pyridine | 4-Br Aniline | -0.96 | 0.04 |
| $(C_6F_5)(Ph)_2$P | 4-$CF_3$ Aniline | 1.50 | 0.04 |
| | 4-F-3-$NO_2$ Aniline | 0.72 | 0.03 |
| | 2-$NO_2$ Aniline | -1.39 | 0.03 |
| | $NPh_3$ | -2.62 | 0.03 |
| | (2,6-$F_2$-$C_6H_3)_3$P | -1.98 | 0.02 |
| (2,6-$F_2$-$C_6H_3)_3$P | 2-$NO_2$ Aniline | 0.41 | 0.05 |
| | $NPh_3$ | -0.56 | 0.04 |
| 4-$CF_3$ Aniline | 4-F-3-$NO_2$ Aniline | -0.82 | 0.06 |

[a] experimental standard deviation of $\Delta pK_{ip}$ allows evaluating the within-series agreement of $\Delta pK_{ip}$ values,

**Graph 1 Correlation between $pK_a$ values in acetonitrile and $pK_{ip}$ values in DCE.**



## Synthesis of intermediate [$C_6H_5$-$C(CH_3)_2$-$P(C_6H_4F)_2Ph$][$HB(C_6F_5)_3$] (12)

In a glove box, $B(C_6F_5)_3$ (**1**) (0.17 mmol, 86.0 mg), $P(C_6H_4F)_2Ph$ (**3**) (0.17 mmol, 50.0 mg) and α-methylstyrene (**11**) (0.17 mmol) was dissolved in $CH_2Cl_2$ (5 ml) and transferred to a *J* Young glass bomb. The solution was freeze-pump-thawed, charged at 77 K with $H_2$ and stirred at room temperature for 5 h. The product was precipitated as yellow oil by addition of pentanes (10 ml), washed rapidly with pentanes (2 x 3 ml), dried in vacuum for 15 min and directly subjected to NMR spectroscopy. All attempts to crystalize the intermediate failed due to the conversion to the hydrogenation product and the free FLP.

**$^1$H-NMR** (400 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 7.97 – 7.85 (m, 3H, $H_o$ and $H_p$ / $P(C_6H_5)$), 7.72 – 7.63 (m, 2 H, $H_p$ / $C_6H_4F$), 7.58 – 7.27 (m, 11H, $C_6H_5$, $H_m$ / $P(C_6H_5)$ and $C_6H_4F$), 7.22 – 7.14 (m, 2H, $H_o$ / $C_6H_4F$), 3,63 (q, $^1J_{H\text{-}B}$ = 86 Hz, 1H, B*H*), 2.12 (d, $^3J_{H\text{-}P}$ = 20 Hz, 6H, C*H*$_3$). - **$^1$H{$^{31}$P}-NMR** (400 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 7.97 – 7.85 (m, 3H, $H_o$ and $H_p$ / $P(C_6H_5)$), 7.72 – 7.63 (m, 2 H, $H_p$ / $C_6H_4F$), 7.58 – 7.27 (m, 11H, $C_6H_5$, $H_m$ / $P(C_6H_5)$ and $C_6H_4F$), 7.22 – 7.14 (m, 2H, $H_o$ / $C_6H_4F$), 3,63 (q, $^1J_{H\text{-}B}$ = 89 Hz, 1H, B*H*), 2.12 (s, 6H, C*H*$_3$). – **$^{13}$C-NMR** (100 MHz, $CD_2Cl_2$): δ/ppm = 163.3 (d, $^1J_{C\text{-}F}$ = 253 Hz, *C*F), 148.1 (d, $^1J_{C\text{-}F}$ = 234 Hz, *o*-$C_6F_5$), 138.62 (dd, *J* = 9.7, 2.3 Hz, CH), 137.1 (d, J = 2 Hz, $C_{ipso}$ / $C_6H_5$), 136.4 (d, $^1J_{C\text{-}F}$ = 245 Hz, *m*- $C_6F_5$), 135.70 (d, *J* = 3.0 Hz, CH), 135.4 (d, $^1J_{C\text{-}F}$ = 233 Hz, *p*-$C_6F_5$), 134.9 (d, *J* = 5.6 Hz, CH), 134.2 (d, *J* = 8.9 Hz, CH), 130.2 (d, *J* = 12.3 Hz, CH), 129.7 (d, *J* = 3.8 Hz, CH), 128.9 (d, *J* = 3.0 Hz, CH), 128.4 (d, *J* = 5.3 Hz, CH), 126.4 (dd, *J* = 10.9, 3.0 Hz, CH), 118.15 (dd, *J* = 22.8, 5.8 Hz, CH), 115.2 (d, $^1J_{C\text{-}P}$ = 81 Hz, $C_{ipso}$ / $P(C_6H_5)$), 106.5 (dd, $^1J_{C\text{-}P}$ = 81, $^2J_{C\text{-}F}$ = 16 Hz, $C_{ipso}$ / $C_6H_4F$), 46.3 (d, $^1J_{C\text{-}P}$ = 36 Hz, $C_{quart}$), 26.1 (d, *J* = 6 Hz, *C*H$_3$) – **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 298 K): -89.8 (m, 2 F, P-*o*-$FC_6H_4$), -133.8 (m, 6 F, B-*o*-$C_6F_5$), -164.6 (m, 3 F, B-*p*-$C_6F_5$), -167.5 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P{$^1$H}-NMR** (162 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 31.6. – **$^{11}$B-NMR** (128 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -25.5 (d, $^1J_{B\text{-}H}$ = 92 Hz). – **$^{11}$B{$^1$H}-NMR** (128 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -25.5.

## Variable Temperature $H_2$-Activation with $PR_{3\text{-}n}Ph_n$ (R = (2-F-$C_6H_4$) (n=2,3) or (2,6-$F_2$-$C_6H_3$) (n=1-3)) and $B(C_6F_5)_3$

**General Procedure:** A solution of 0.01 mmol (1.0 equiv.) of the corresponding phosphine (**2-7**) and 0.01 mmol (5.1 mg, 1.0 equiv.) $B(C_6F_5)_3$ (**1**) in $CD_2Cl_2$ (0.45 ml) was transferred in a glove box in a sealable NMR tube with *J* Young Teflon tap. The solution was freeze-pump thawed for 2 cycles and charged with $H_2$ at 77 K (the NMR tube was immersed into the liquid $N_2$ in a controlled depth of 15 cm to create reproducible pressures). The solution was subjected to variable temperature NMR and every temperature was hold for 30 min before taking the spectra to ensure full equilibration (no change of the spectra as a function of time was observed). All preparations and measurements were repeated twice to ensure consistency. In all cases, the reversible formation of a phosphonium-borate was established by the inerrable detection of PH couplings, the characteristic $^{11}$B resonance of $H(BC_6F_5)_3^-$ and the complete recurrence to the parent FLP at room temperature. All combinations were measured in the absence of dihydrogen gas at both room- and low temperature and compared with the analog $H_2$ pressurized sample. In contrast to the samples charged with hydrogen, no significant change (apart from the temperature dependent shift and adduct formation) was observed. The determined temperatures for the reversible $H_2$

activation were defined as the highest measured temperatures, at which in the $^{11}$B NMR spectra the presence of the hydrido-borate species (-25 ppm) was detectable (NMR spectra at pages S50, S56, S63, S70). All combinations were homogeneous solutions at room temperature and precipitation was observed to some extent while lowering the temperature, but in all cases the precipitation started below the determined activation temperature. Hence, low solubility of the formed phosphonium-borates at lower temperature cannot be ruled out but does not interfere with the herein determined equilibriums and temperatures of the $H_2$ activation. Due to highly dynamic processes of the formed phosphonium borates in solution at low temperature no BH coupling could be detected in some cases (**4**, **6**).

**P(2-F-$C_6H_4$)$_2$Ph (3) and B($C_6F_5$)$_3$ (NMR spectra page S44-51)**

**FLP + $H_2$ at rt: $^1$H-NMR** (400 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 7.58 – 7.37 (m, 7 H, $H_{Ar}$), 7.25 – 7.12 (m, 4 H, $H_{Ar}$), 7.03 – 6.92 (m, 2 H, $H_{Ar}$). – **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 298 K): -103.9 (m, 2 F, P-*o*-$FC_6H_4$), -127.9 (m, 6 F, B-*o*-$C_6F_5$), -143.7 (m, 3 F, B-*p*-$C_6F_5$), -160.8 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P{$^1$H}-NMR** (162 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -29.1. – **$^{11}$B-NMR** (128 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 58.1.

**[HP(2-F-$C_6H_4$)$_2$Ph ][HB($C_6F_5$)$_3$]: $^1$H-NMR** (400 MHz, $CD_2Cl_2$, 213 K): δ/ppm = 8.80 (d, $^1J_{P\text{-}H}$ = 527 Hz, 1 H, P*H*), 8.10 – 7.00 (m, 13 H, $H_{Ar}$), 3.90 – 3.10 (br m, 1 H, B*H*). - **$^1$H{$^{31}$P}-NMR** (400 MHz, $CD_2Cl_2$, 213 K): δ/ppm = 8.80 (s, 1 H, P*H*), 8.14 – 7.05 (m, 13 H, $H_{Ar}$), 3.90 – 3.10 (br m, 1 H, B*H*). – **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 213 K): -99.1 (m, 2 F, P-*o*-$FC_6H_4$), -133.9 (m, 6 F, B-*o*-$C_6F_5$), -163.1 (m, 3 F, B-*p*-$C_6F_5$), -166.2 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P-NMR** (162 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -11.0 (d, $^1J_{P\text{-}H}$ = 525 Hz). - **$^{31}$P{$^1$H}-NMR** (162 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -11.0. – **$^{11}$B-NMR** (128 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -25.7 (d, $^1J_{B\text{-}H}$ = 83.6). – **$^{11}$B{$^1$H}-NMR** (128 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -25.7.

**P(2-F-$C_6H_4$)$_3$ (4) and B($C_6F_5$)$_3$ (NMR spectra page S51-57)**

**FLP + $H_2$ at rt: $^1$H-NMR** (400 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 7.54 – 7.42 (m, 3 H, $H_{Ar}$), 7.26 – 7.11 (m, 6 H, $H_{Ar}$), 7.08 – 6.96 (m, 3 H, $H_{Ar}$). – **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 298 K): -104.2 (m, 3 F, P-*o*-$FC_6H_4$), -127.9 (m, 6 F, B-*o*-$C_6F_5$), -143.6 (m, 3 F, B-*p*-$C_6F_5$), -160.8 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P{$^1$H}-NMR** (162 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -42.8 (q, $J_{P\text{-}F}$ = 57 Hz). – **$^{11}$B{$^1$H}-NMR** (128 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 59.0.

**[HP(2-F-$C_6H_4$)$_3$][HB($C_6F_5$)$_3$]: $^1$H-NMR** (400 MHz, $CD_2Cl_2$, 213 K): δ/ppm = 8.48 (d, $^1J_{P\text{-}H}$ = 540 Hz, 1 H, P*H*), 8.10 – 6.80 (m, 12 H, $H_{Ar}$), 3.90 – 3.10 (br m, 1 H, B*H*). - **$^1$H{$^{31}$P}-NMR** (400 MHz, $CD_2Cl_2$, 213 K): δ/ppm = 8.45 (s, 1 H, P*H*), 8.10 – 6.80 (m, 12 H, $H_{Ar}$), 3.90 – 3.10 (br m, 1 H, B*H*). – **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 213 K): -104.6 (m, 3 F, P-*o*-$FC_6H_4$), -134.0 (m, 6 F, B-*o*-$C_6F_5$), -163.1 (m, 3 F, B-*p*-$C_6F_5$), -166.2 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P-NMR** (162 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -15.3 (d, $^1J_{P\text{-}H}$ = 540 Hz). – **$^{31}$P{$^1$H }-NMR** (162 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -15.3. – **$^{11}$B-NMR** (128 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -25.5 (d, $^1J_{B\text{-}H}$ = 83.6 Hz). – **$^{11}$B{$^1$H}-NMR** (128 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -25.6.

**$P(2,6\text{-}F_2\text{-}C_6H_3)Ph_2$ (5) and $B(C_6F_5)_3$ (NMR spectra page S58-64)**

**FLP + $H_2$ at rt: $^1$H-NMR** (400 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 8.90 (br s, ~5% [$HP(2,6\text{-}F_2C_6H_3)Ph_2$ ]), 7.70 – 7.45 (m, 11H, $H_{Ar}$), 7.09 (dt, $J_{H\text{-}H}$ = 8.4 Hz, $J_{H\text{-}F}$ = 2.2 Hz, 2H, $H_m$ / $C_6H_3F_2$) – **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -98.0 (m, 2 F, P-*o*-$FC_6H_4$), -128.3 (m, 6 F, B-*o*-$C_6F_5$), -145.0 (m, 3 F, B-*p*-$C_6F_5$), -161.2 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P{$^1$H}-NMR** (162 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -22.6. – **$^{11}$B{$^1$H}-NMR** (128 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -53.9.

**[$HP(2,6\text{-}F_2C_6H_3)Ph_2$ ][$HB(C_6F_5)_3$] (60 %): $^1$H-NMR** (400 MHz, $CD_2Cl_2$, 233 K): δ/ppm = 9.50 – 7.50 (br s, 1H, P*H*), 8.00 – 7.00 (m, 13H, $H_{Ar}$), 4.00 – 3.00 (br m, 1H, B*H*). – **$^1$H{$^{31}$P}-NMR** (400 MHz, $CD_2Cl_2$, 213 K): δ/ppm = 8.90 (s, 1H, P*H*), 8.00 – 7.00 (m, 13H, $H_{Ar}$), 4.00 – 3.00 (br m, 1H, B*H*). **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 233 K): δ/ppm = -96.5 (m, 2 F, P-*o*-$FC_6H_4$), -134.0 (m, 6 F, B-*o*-$C_6F_5$), -162.7 (m, 3 F, B-*p*-$C_6F_5$), -166.5 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P-NMR** (162 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -13.8 (d, $^1J_{P\text{-}H}$ = 513 Hz). – **$^{31}$P{$^1$H }-NMR** (162 MHz, $CD_2Cl_2$, 213 K): δ/ppm = -13.8 – **$^{11}$B{$^1$H }-NMR** (128 MHz, $CD_2Cl_2$, 233 K): δ/ppm = -25.5.

**$P(2,6\text{-}F_2C_6H_3)_2Ph$ (6) and $B(C_6F_5)_3$ (NMR spectra page S64-71)**

**FLP + $H_2$ at rt: $^1$H-NMR** (400 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 7.56 (t, $J_{H\text{-}H}$ = 7.9 Hz, 2H, $H_p$ / $C_6H_3F_2$), 7.48 – 7.32 (m, 5H), 6.93 (t, $J_{H\text{-}H}$ = 7.9 Hz, 4H, $H_m$ / $C_6H_3F_2$). – **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -99.9 (m, 4 F, P-*o*-$F_2C_6H_3$), -127.9 (m, 6 F, B-*o*-$C_6F_5$), -143.6 (m, 3 F, B-*p*-$C_6F_5$), -160.8 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P-NMR** (162 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -51.0. – **$^{11}$B-NMR** (128 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 59.3.

**[$HP(2,6\text{-}F_2C_6H_3)_2Ph$ ][$HB(C_6F_5)_3$]: $^1$H-NMR** (400 MHz, $CD_2Cl_2$, 233 K): δ/ppm = 9.00 (br s, 1H, P*H*), 7.44 (m, 7H, $H_{Ar}$), 6.96 (m, 4H, $H_{Ar}$), 4.00 – 3.00 (br m, 1H, B*H*). - **$^1$H{$^{31}$P}-NMR** (400 MHz, $CD_2Cl_2$, 233 K): δ/ppm = 9.01 (s, 1H, P*H*), 7.44 (m, 7H, $H_{Ar}$), 6.96 (m, 4H, $H_{Ar}$), 4.00 – 3.00 (br m, 1H, B*H*). – **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -99.9 (m, 4 F, P-*o*-$F_2C_6H_3$), -133.8 (m, 6 F, B-*o*-$C_6F_5$), -163.5 (m, 3 F, B-*p*-$C_6F_5$), -166.4 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P-NMR** (162 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -8.83 (d, $^1J_{P\text{-}H}$ = 505 Hz). – **$^{11}$B-NMR** (128 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -25.5. – **$^{11}$B{$^1$H }-NMR** (128 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -25.5.
Activation product besides excess of free FLP.

**$P(2,6\text{-}F_2C_6H_3)_3$ (7) and $B(C_6F_5)_3$ (NMR spectra page S71-73)**

**FLP + $H_2$ at rt: $^1$H-NMR** (400 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 7.48 – 7.35 (m, 3H, $H_p$), 6.99 – 6.87 (m, 6H, $H_m$). – **$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$, 298 K): -101.5 (m, 6 F, P-*o*-$F_2C_6H_3$), -127.9 (m, 6 F, B-*o*-$C_6F_5$), -143.5 (m, 3 F, B-*p*-$C_6F_5$), -160.8 (m, 6 F, B-*m*-$C_6F_5$). – **$^{31}$P{$^1$H}-NMR** (162 MHz, $CD_2Cl_2$, 298 K): δ/ppm = -78.3. – **$^{11}$B{$^1$H}-NMR** (128 MHz, $CD_2Cl_2$, 298 K): δ/ppm = 59.2.

No significant change was observed upon lowering the temperature to – 110 °C.

## Kinetics of the hydrogenation of 1,1-diphenylethylene (9) and trimethyl(methallyl)silane (10) with phosphines 3 - 8

### General procedure for the kinetic runs of the catalytic hydrogenations

In a glove box, $B(C_6F_5)_3$ (**1**) (20 mol%), the phosphine (20 mol%) and the substrate (0.05 mmol, by micro syringe) were dissolved in $CD_2Cl_2$ (0.50 ml). The solution was transferred to a sealable *J* Young NMR tube (standard-size) equipped with a Teflon tap. The solution was measured by $^1H$ NMR to verify the substrate to catalyst ratio by signal integration. The solution was frozen (without freeze-pump-thaw), charged with $H_2$ at 77 K (the NMR tube was immersed into the liquid $N_2$ in a controlled depth (15 cm) and time (10 seconds) to create reproducible pressure) and subjected to continuous rotation in a modified rotary evaporator with 10 rpm for the given time at room temperature (room temperature was measured during runs and was in the range of 21 °C to 23 °C).[6] Due to the direct and loss-free substrate to product conversion (as determined by NMR with internal standard mesitylene and GC-MS) the relative signal integration ratio between the substrate and product (normalized $CH_2$ / $CH_3$ in case of 1,1-diphenyl ethylene, $CH_2$ / $CH_2$ in case of trimethyl(methallyl)silane) could be used as direct probe for the conversion. Every kinetic run was repeated at least three times to ensure consistency for a qualitative discussion of the reaction profile. *Vide infra* for representative runs (two runs for each phosphine) and mean data for every investigated phosphine (tables, time *vs.* conversion plot, linearized plot). Data analysis was performed using Microsoft Excel 2010; linear regression analysis was performed using the Data Analysis Tool pack. Mean graphs and relative rate constants were determined by fitting over all determined data points (determined over at least 2 runs with analogue conditions), logarithmical linearization (in case of first order behavior) and linear regression. Trivial error analysis (standard deviation, standard error of the mean, error bars) was not performed, due to the collection of conversion values (y-values) at variable times (x-values) for repeated runs, but considered to be dispensable for a qualitative discussion of the reaction profiles. All NMR measurements were performed with the common acquisition parameters (d1 = 1.0 sec, elongated relaxation delays proved to have no influence on the relative substrate to product signal ratio).

### *Hydrogenation of 1,1-Diphenyl ethylene (9, DPE)*

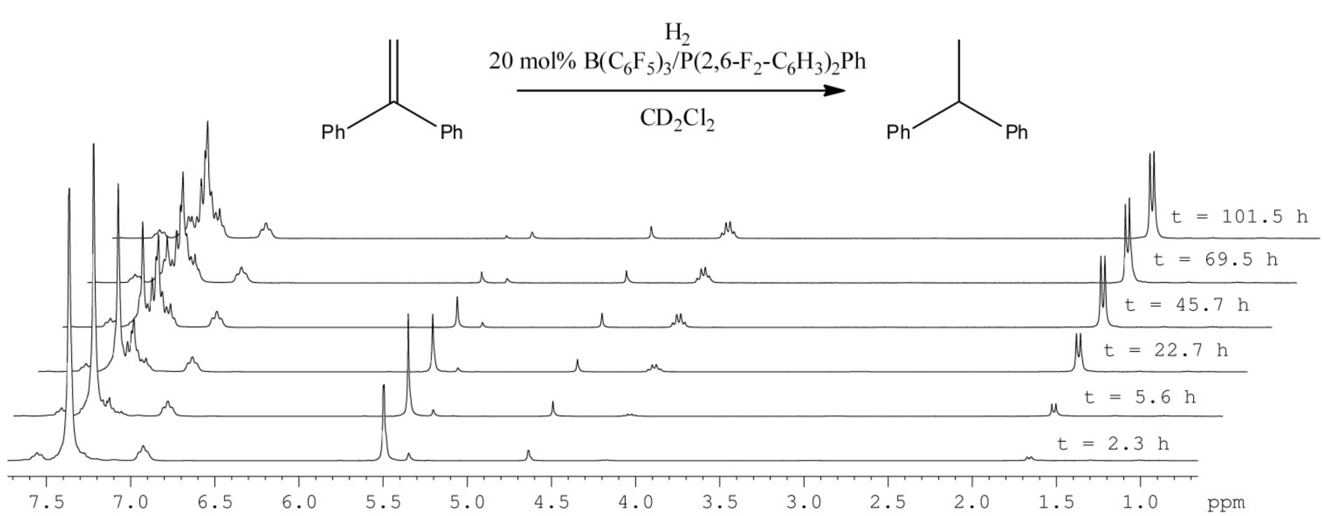
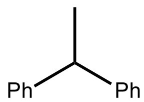



Figure 2: Hydrogenation of 1,1-diphenyl ethylene (representative example run with $P(2,6\text{-}F_2\text{-}C_6H_3)_2Ph$).

*1,1-Diphenylethane*: $^{1}$H NMR (400 MHz, $CD_2Cl_2$): δ = 7.31–7.15 (m, 10H, $H_{Ar}$), 4.16 (q, *J* = 7.3 Hz, 1H, C*H*), 1.64 (d, *J* = 7.3 Hz, 3H, C$H_3$) ppm. GC/MS (70 eV) = 182 (45), 167 (100), 152 (19), 77 (4).



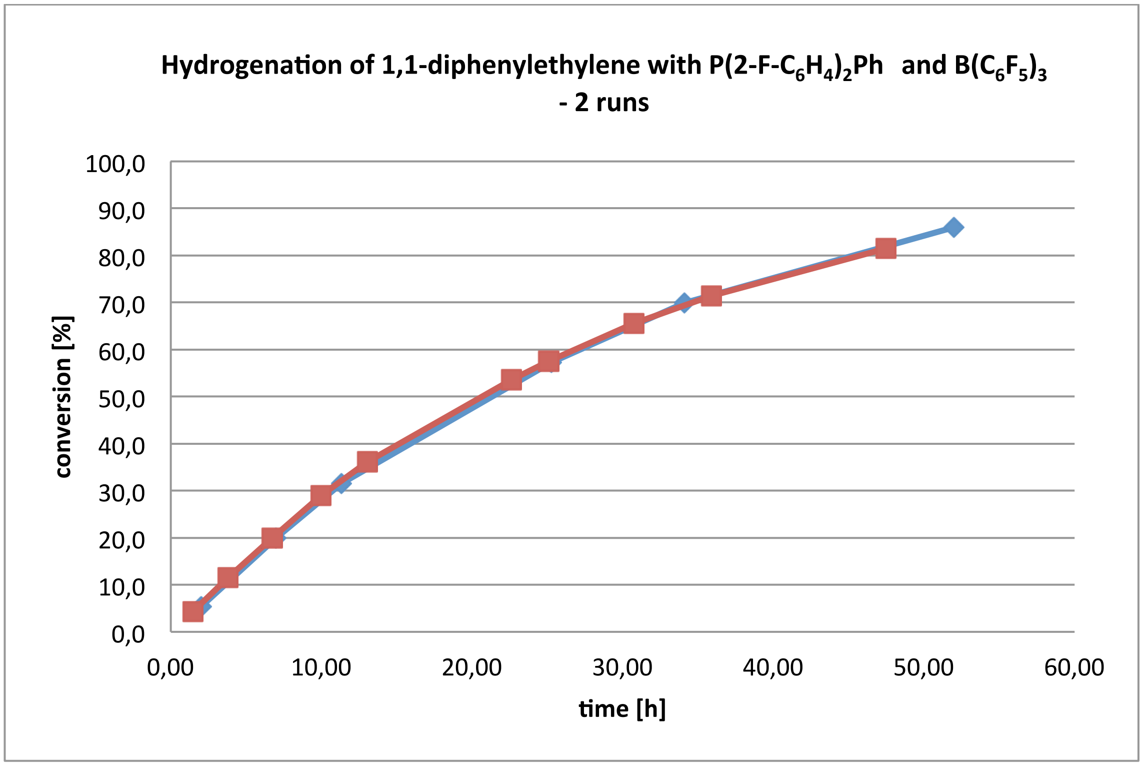

**Representative runs (two runs for each phosphine) and average data (determined from at least 2 runs) for every investigated phosphine (tables, time vs. conversion plot, linearized plot)**

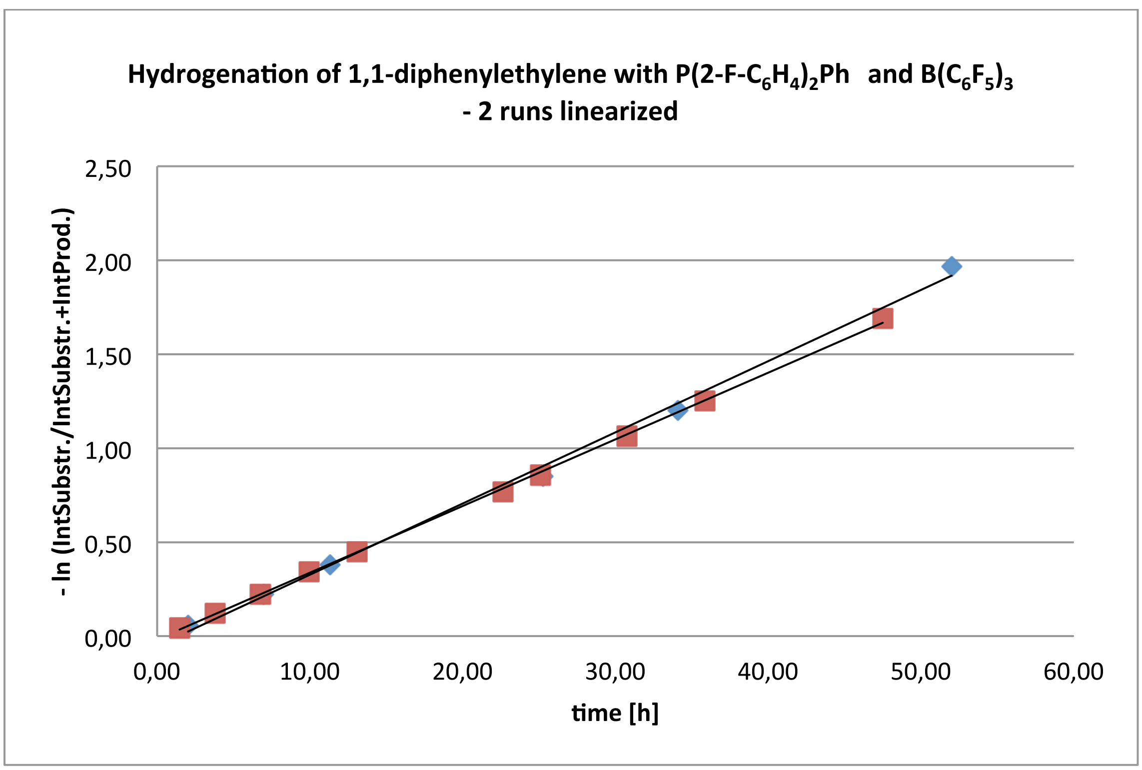
## ***Hydrogenation with P(2-F-$C_6H_4$)$_2$Ph* (3)**

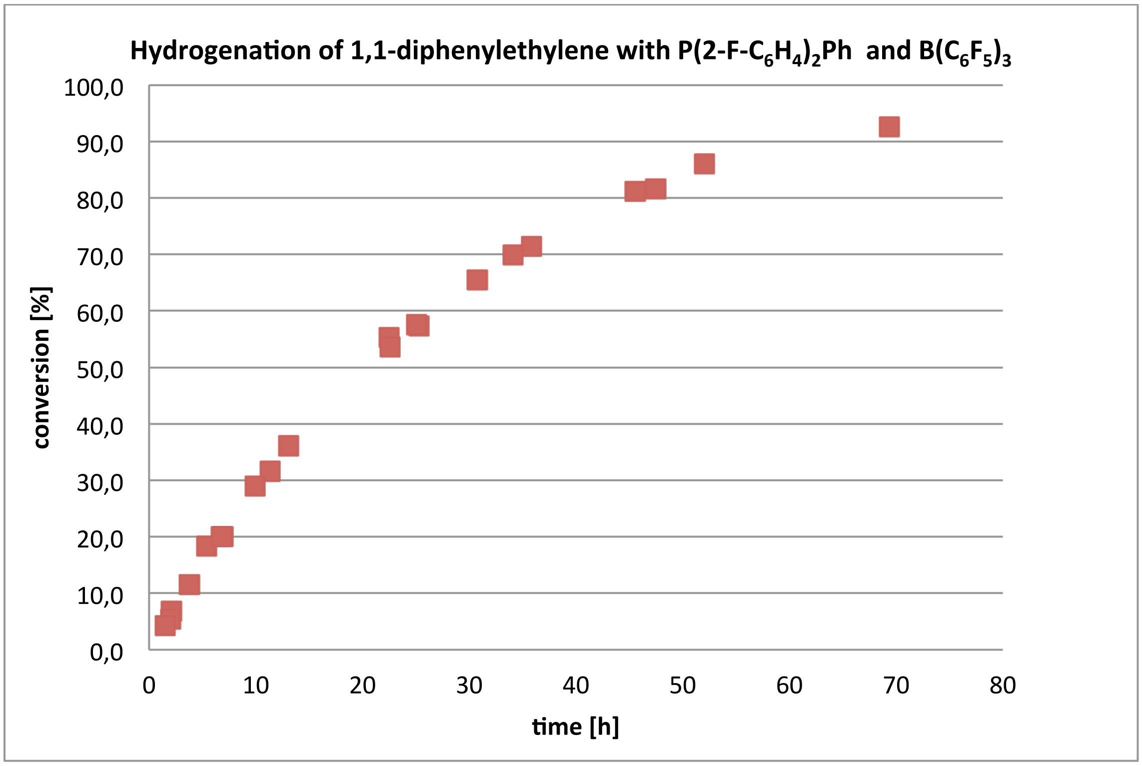
| Run | DPE [mg, mmol] | P(2-F-$C_6H_4$)$_2$Ph [mg, mmol] | B($C_6F_5$)$_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| II 1 | 9.0, 0.050 | 3.1, 0.010 | 5.1, 0.010 | 0.45 |
| II 2 | 9.0, 0.050 | 3.0, 0.010 | 5.2, 0.010 | 0.45 |

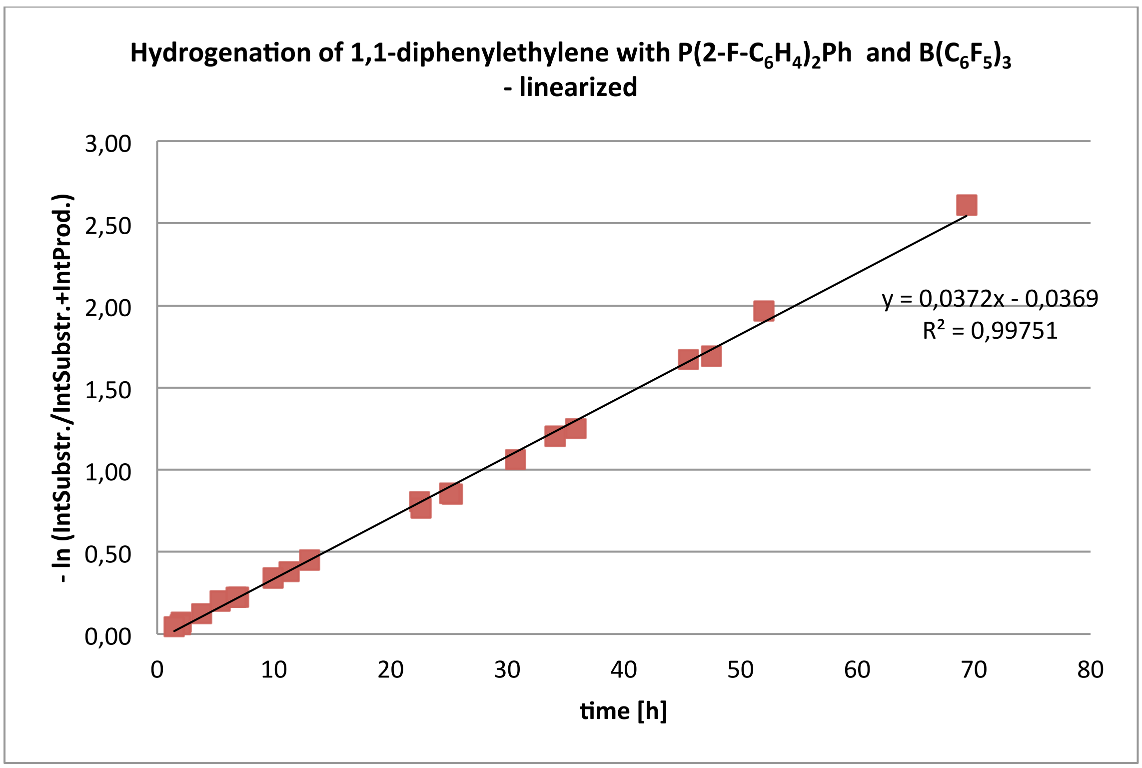
| run ID | Substr. $^{1}$H Integral | Prod. $^{1}$H Integral | Substr. $^{1}$H Integral $_{normalized}$ | Prod. $^{1}$H Integral $_{normalized}$ | conv. [%] | time [h] | "-ln($Int_{Substr.}$/$Int_{Substr.}$+$Int_{Prod.}$)" |
|---|---|---|---|---|---|---|---|
| II run 1-1 | 7,050 | 0,601 | 3,525 | 0,200 | 5,4 | 2,02 | 0,0553 |
| II run 1-2 | 6,205 | 2,323 | 3,103 | 0,774 | 20,0 | 6,97 | 0,2228 |
| II run 1-3 | 4,900 | 3,385 | 2,450 | 1,128 | 31,5 | 11,32 | 0,3788 |
| II run 1-4 | 3,427 | 6,893 | 1,713 | 2,298 | 57,3 | 25,27 | 0,8506 |
| II run 1-5 | 2,063 | 7,192 | 1,031 | 2,397 | 69,9 | 34,10 | 1,2013 |
| II run 1-6 | 1,139 | 10,498 | 0,570 | 3,499 | 86,0 | 52,00 | 1,9663 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| II run 2-1 | 14,817 | 1,000 | 7,408 | 0,333 | 4,3 | 1,47 | 0,0440 |
| II run 2-2 | 5,125 | 1,000 | 2,562 | 0,333 | 11,5 | 3,80 | 0,1223 |
| II run 2-3 | 2,672 | 1,000 | 1,336 | 0,333 | 20,0 | 6,75 | 0,2227 |
| II run 2-4 | 1,632 | 1,000 | 0,816 | 0,333 | 29,0 | 9,95 | 0,3426 |
| II run 2-5 | 1,176 | 1,000 | 0,588 | 0,333 | 36,2 | 13,08 | 0,4491 |
| II run 2-6 | 0,578 | 1,000 | 0,289 | 0,333 | 53,6 | 22,62 | 0,7669 |
| II run 2-7 | 0,492 | 1,000 | 0,246 | 0,333 | 57,5 | 25,08 | 0,8565 |
| II run 2-8 | 0,351 | 1,000 | 0,176 | 0,333 | 65,5 | 30,75 | 1,0645 |
| II run 2-9 | 0,267 | 1,000 | 0,134 | 0,333 | 71,4 | 35,87 | 1,2513 |
| II run 2-10 | 0,151 | 1,000 | 0,075 | 0,333 | 81,6 | 47,49 | 1,6903 |


Hydrogenation of 1,1-diphenylethylene with P(2-F-C6H4)2Ph and B(C6F5)3 - 2 runs
conversion [%]
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0,00
10,00
20,00
30,00
40,00
50,00
60,00
time [h]


Hydrogenation of 1,1-diphenylethylene with P(2-F-C6H4)2Ph and B(C6F5)3 - 2 runs linearized
- ln (IntSubstr./IntSubstr.+IntProd.)
2,50
2,00
1,50
1,00
0,50
0,00
0,00
10,00
20,00
30,00
40,00
50,00
60,00
time [h]

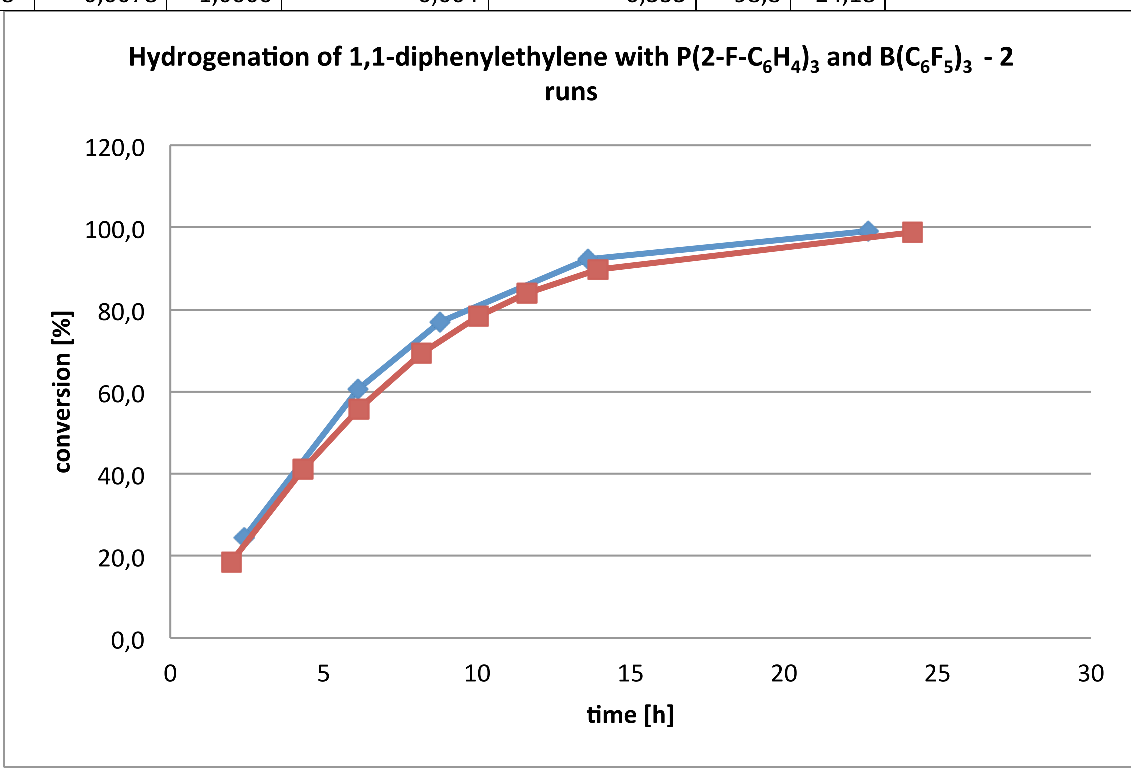

Hydrogenation of 1,1-diphenylethylene with P(2-F-C6H4)2Ph and B(C6F5)3
conversion [%]
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0
10
20
30
40
50
60
70
80
time [h]

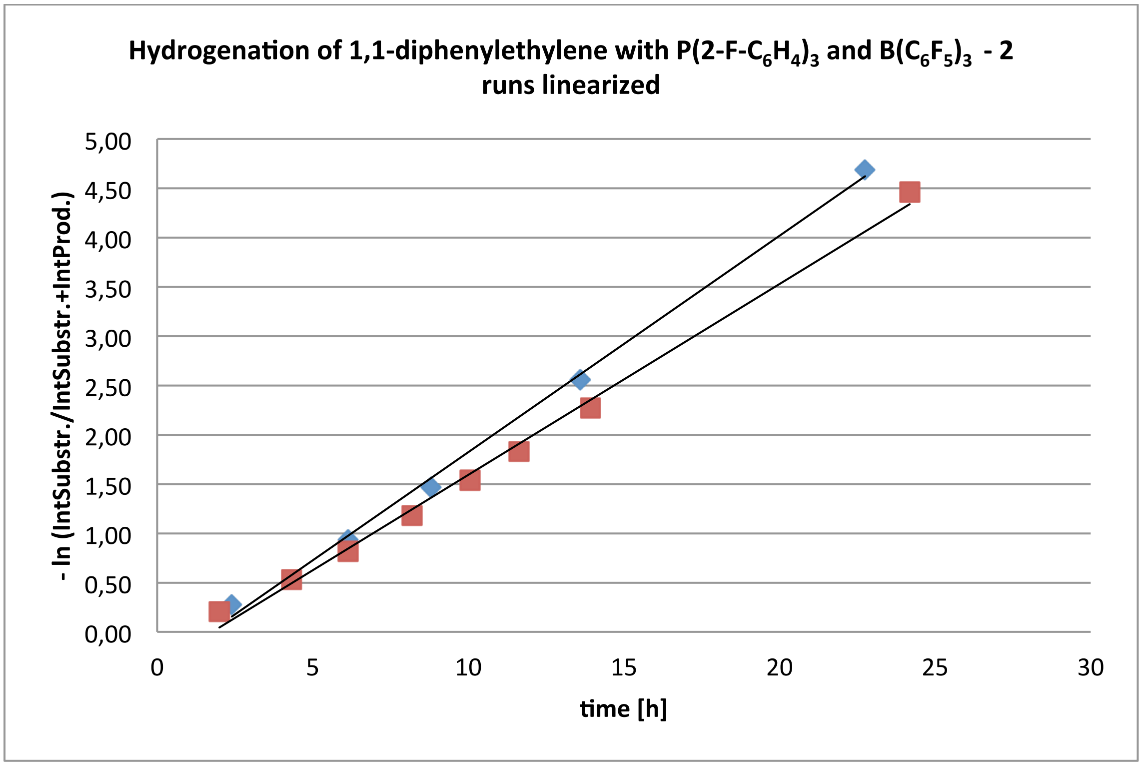

Hydrogenation of 1,1-diphenylethylene with P(2-F-C6H4)2Ph and B(C6F5)3
- linearized
- ln (IntSubstr./IntSubstr.+IntProd.)
3,00
2,50
2,00
1,50
1,00
0,50
0,00
0
10
20
30
40
50
60
70
80
time [h]
y = 0,0372x - 0,0369
R² = 0,99751

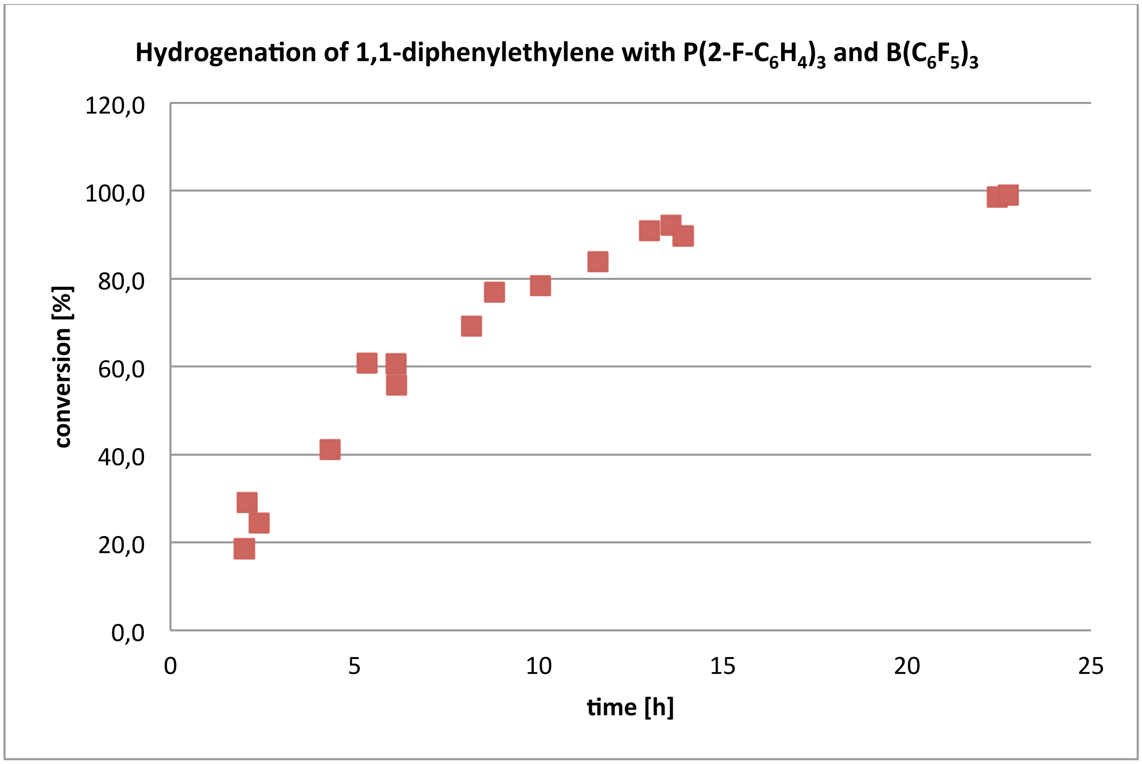
## *Hydrogenation with $P(2\text{-}F\text{-}C_6H_4)_3$* (4)

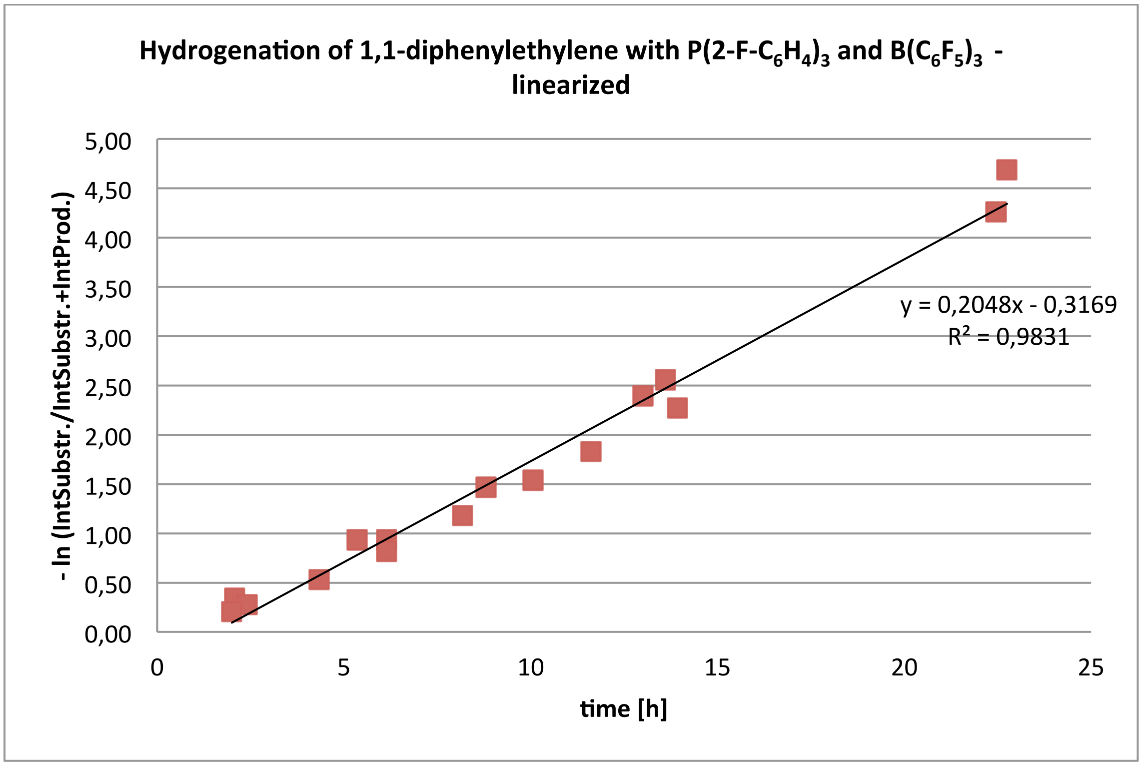
| Run | DPE [mg, mmol] | $P(2\text{-}F\text{-}C_6H_4)_3$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| III 1 | 6.4, 0.050 | 3.2, 0.010 | 5.2, 0.010 | 0.45 |
| III 2 | 6.4, 0.050 | 3.1, 0.010 | 5.0, 0.010 | 0.45 |

| run ID | Substr. $^1$H Integral | Prod. $^1$H Integral | Substr. $^1$H Integral $_{normalized}$ | Prod. $^1$H Integral $_{normalized}$ | conv. [%] | time [h] | "-ln(Int$_{Substr.}$/Int$_{Substr.}$+Int$_{Prod.}$)" |
|---|---|---|---|---|---|---|---|
| III run 1-1 | 8,9102 | 4,3031 | 4,455 | 1,434 | 24,4 | 2,4 | 0,2791 |
| III run 1-2 | 4,0298 | 9,3164 | 2,015 | 3,105 | 60,6 | 6,13 | 0,9327 |
| III run 1-3 | 4,1451 | 20,6878 | 2,073 | 6,896 | 76,9 | 8,8 | 1,4649 |
| III run 1-4 | 1,5095 | 26,9042 | 0,755 | 8,968 | 92,2 | 13,6 | 2,5558 |
| III run 1-5 | 0,2388 | 38,6606 | 0,119 | 12,887 | 99,1 | 22,75 | 4,6907 |
| | | | | | | | |
| III run 2-1 | 2,9256 | 1,0000 | 1,463 | 0,333 | 18,6 | 2,00 | 0,2053 |
| III run 2-2 | 0,9535 | 1,0000 | 0,477 | 0,333 | 41,1 | 4,33 | 0,5301 |
| III run 2-3 | 0,5290 | 1,0000 | 0,265 | 0,333 | 55,8 | 6,13 | 0,8155 |
| III run 2-4 | 0,2958 | 1,0000 | 0,148 | 0,333 | 69,3 | 8,18 | 1,1798 |
| III run 2-5 | 0,1832 | 1,0000 | 0,092 | 0,333 | 78,4 | 10,05 | 1,5345 |
| III run 2-6 | 0,1276 | 1,0000 | 0,064 | 0,333 | 83,9 | 11,62 | 1,8285 |
| III run 2-7 | 0,0767 | 1,0000 | 0,038 | 0,333 | 89,7 | 13,93 | 2,2713 |
| III run 2-8 | 0,0078 | 1,0000 | 0,004 | 0,333 | 98,8 | 24,18 | 4,4598 |




Hydrogenation of 1,1-diphenylethylene with P(2-F-C6H4)3 and B(C6F5)3 - 2 runs linearized
- ln (IntSubstr./IntSubstr.+IntProd.)
5,00
4,50
4,00
3,50
3,00
2,50
2,00
1,50
1,00
0,50
0,00
0
5
10
15
20
25
30
time [h]

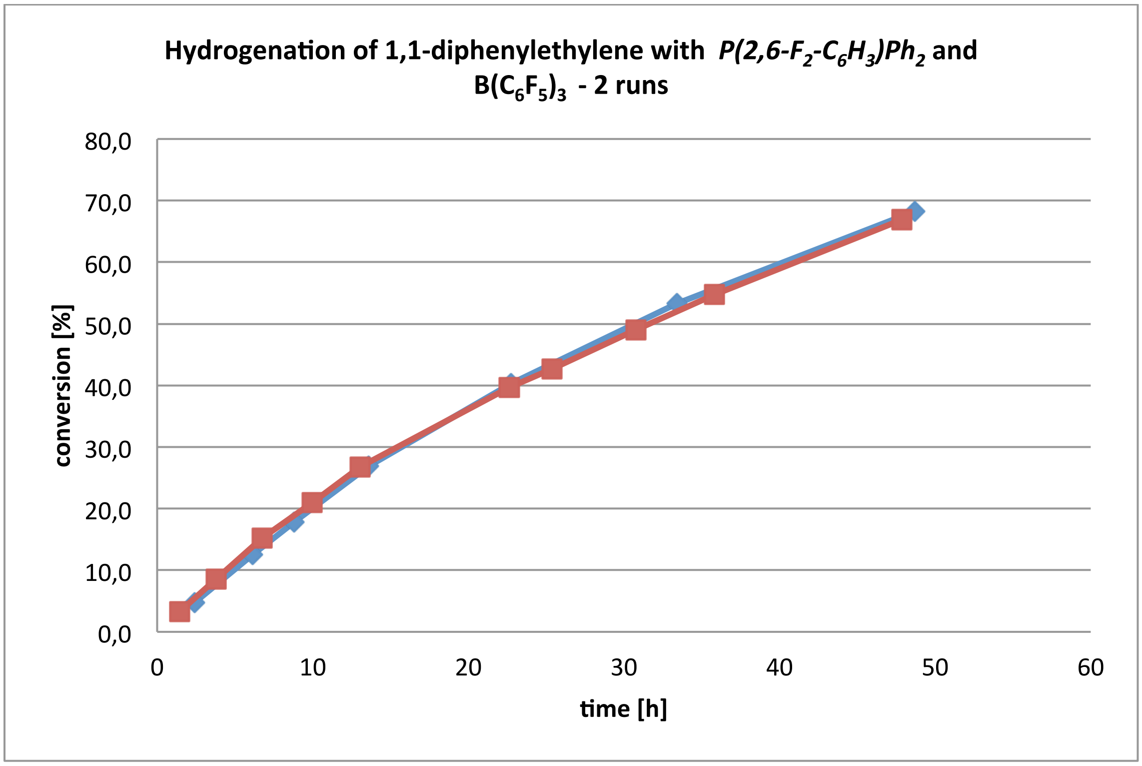

Hydrogenation of 1,1-diphenylethylene with P(2-F-C6H4)3 and B(C6F5)3
conversion [%]
120,0
100,0
80,0
60,0
40,0
20,0
0,0
0
5
10
15
20
25
time [h]

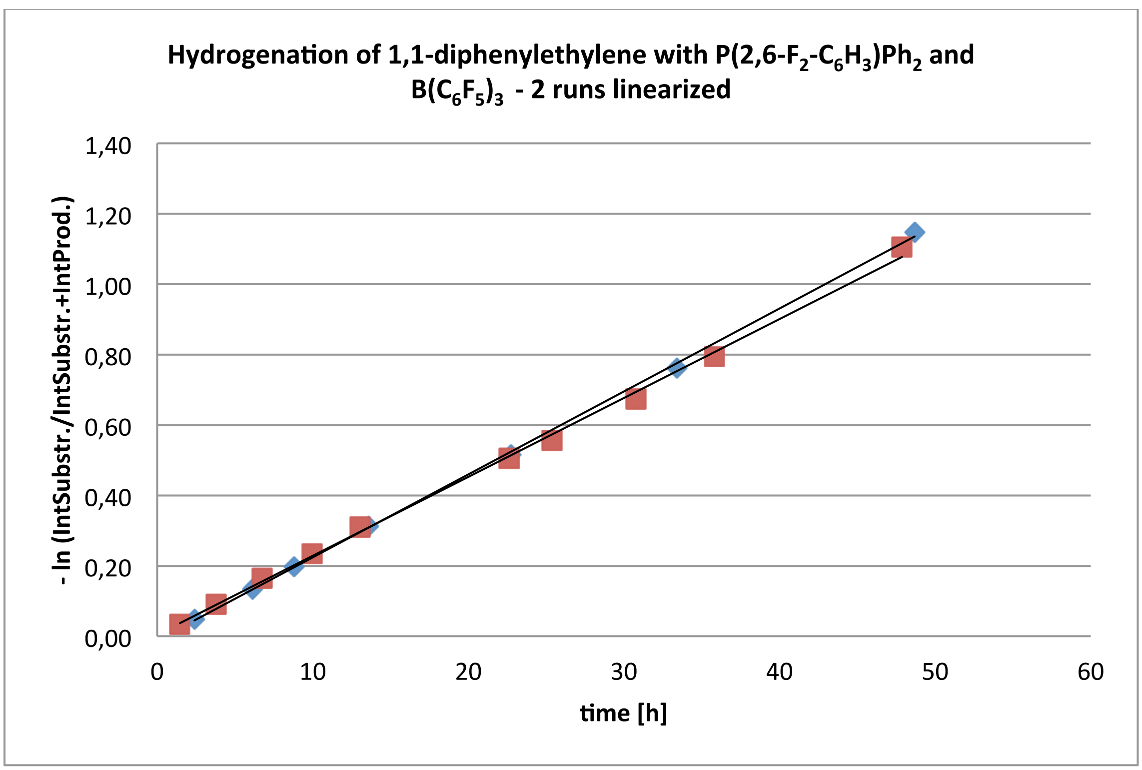


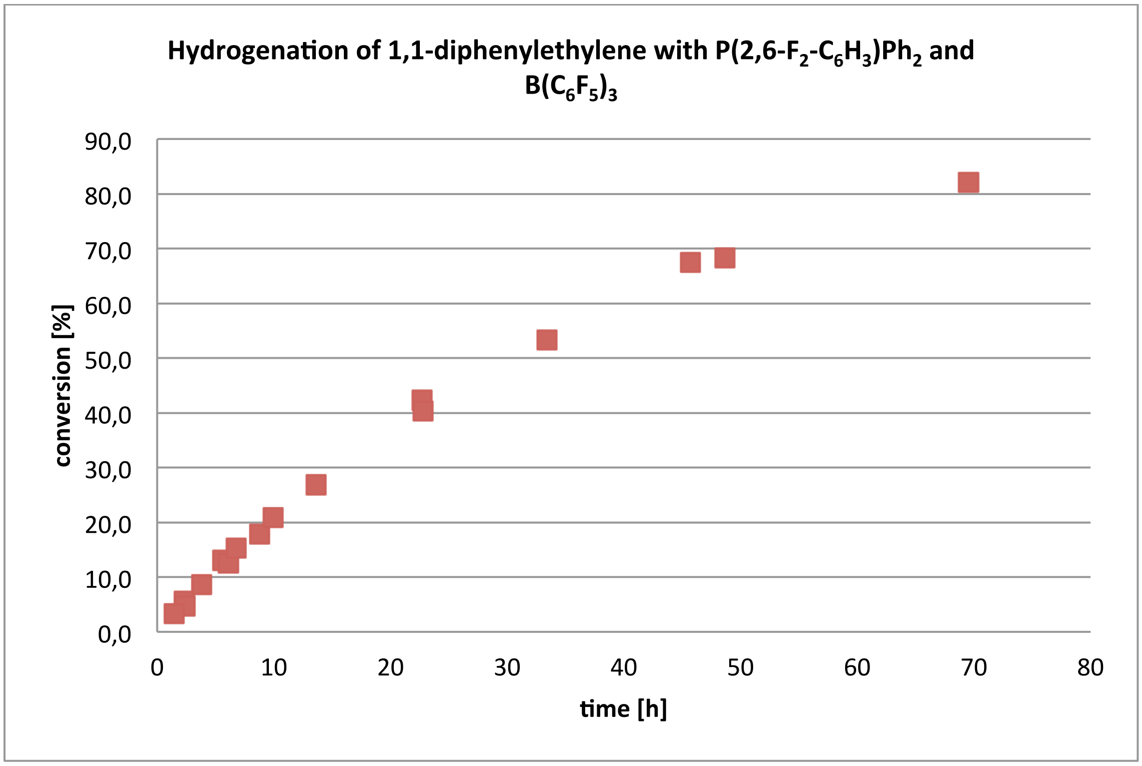

## *Hydrogenation with $P(2,6\text{-}F_2\text{-}C_6H_3)Ph_2$* (5)

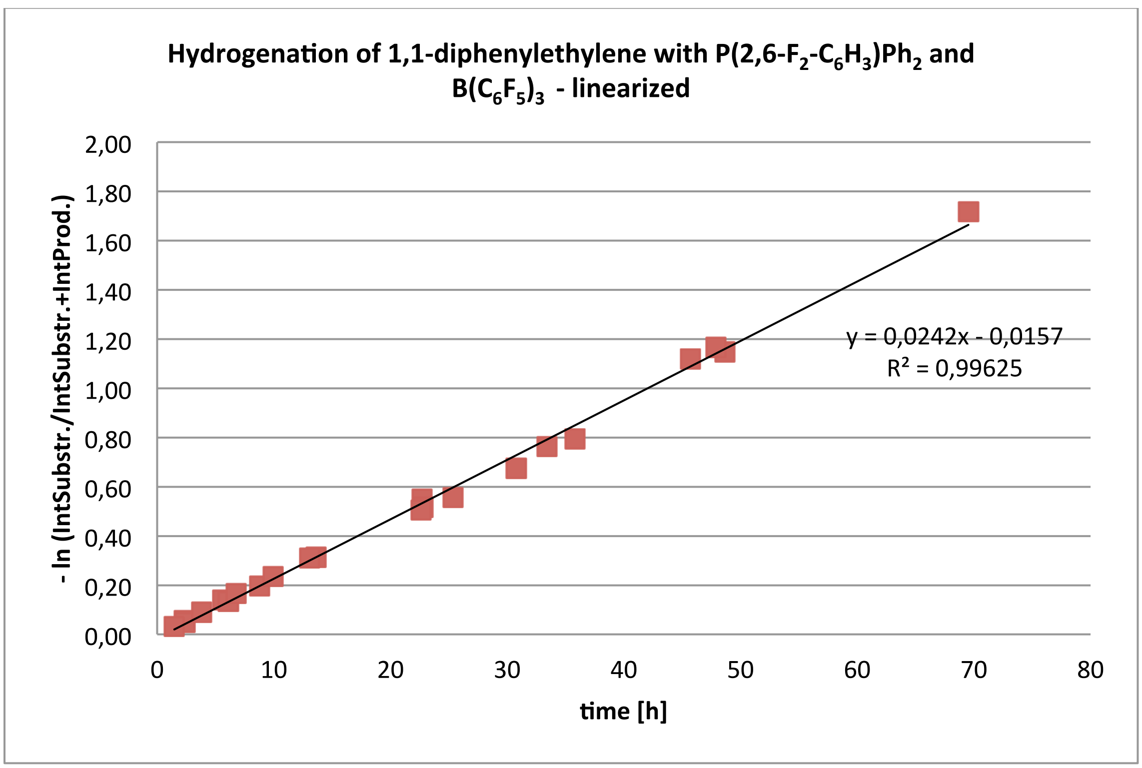
| Run | DPE [mg, mmol] | $P(2,6\text{-}F_2\text{-}C_6H_3)Ph_2$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| IV 1 | 9.0, 0.050 | 2.9, 0.010 | 5.0, 0.010 | 0.45 |
| IV 2 | 9.0, 0.050 | 2.8, 0.010 | 5.0, 0.010 | 0.45 |

| run ID | Substr. $^1H$ Integral | Prod. $^1H$ Integral | Substr. $^1H$ Integral $_{normalized}$ | Prod. $^1H$ Integral $_{normalized}$ | conv. [%] | time [h] | "-ln(Int$_{Substr.}$/Int$_{Substr.}$+Int$_{Prod.}$)" |
|---|---|---|---|---|---|---|---|
| IV run 1-1 | 13,1318 | 0,9748 | 6,566 | 0,325 | 4,7 | 2,4 | 0,0483 |
| IV run 1-2 | 13,6345 | 2,9368 | 6,817 | 0,979 | 12,6 | 6,13 | 0,1342 |
| IV run 1-3 | 11,0431 | 3,6068 | 5,522 | 1,202 | 17,9 | 8,8 | 0,1970 |
| IV run 1-4 | 12,8529 | 7,0694 | 6,426 | 2,356 | 26,8 | 13,6 | 0,3124 |
| IV run 1-5 | 11,3141 | 11,4744 | 5,657 | 3,825 | 40,3 | 22,75 | 0,5165 |
| IV run 1-6 | 4,6616 | 7,9877 | 2,331 | 2,663 | 53,3 | 33,42 | 0,7619 |
| IV run 1-7 | 2,8436 | 9,1623 | 1,422 | 3,054 | 68,2 | 48,68 | 1,1468 |
| | | | | | | | |
| IV run 2-1 | 19,5805 | 1,0000 | 9,790 | 0,333 | 3,3 | 1,467 | 0,0335 |
| IV run 2-2 | 7,0673 | 1,0000 | 3,534 | 0,333 | 8,6 | 3,8 | 0,0901 |
| IV run 2-3 | 3,7073 | 1,0000 | 1,854 | 0,333 | 15,2 | 6,75 | 0,1654 |
| IV run 2-4 | 2,5223 | 1,0000 | 1,261 | 0,333 | 20,9 | 9,95 | 0,2345 |
| IV run 2-5 | 1,8274 | 1,0000 | 0,914 | 0,333 | 26,7 | 13,067 | 0,3110 |
| IV run 2-6 | 1,0153 | 1,0000 | 0,508 | 0,333 | 39,6 | 22,617 | 0,5048 |
| IV run 2-7 | 0,8970 | 1,0000 | 0,449 | 0,333 | 42,6 | 25,367 | 0,5557 |
| IV run 2-8 | 0,6931 | 1,0000 | 0,347 | 0,333 | 49,0 | 30,767 | 0,6739 |
| IV run 2-9 | 0,5502 | 1,0000 | 0,275 | 0,333 | 54,8 | 35,833 | 0,7938 |
| IV run 2-10 | 0,3021 | 1,0000 | 0,165 | 0,333 | 66,9 | 47,867 | 1,1053 |


Hydrogenation of 1,1-diphenylethylene with P(2,6-F2-C6H3)Ph2 and B(C6F5)3 - 2 runs
conversion [%]
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0
10
20
30
40
50
60
time [h]


Hydrogenation of 1,1-diphenylethylene with P(2,6-F2-C6H3)Ph2 and B(C6F5)3 - 2 runs linearized
- ln (IntSubstr./IntSubstr.+IntProd.)
1,40
1,20
1,00
0,80
0,60
0,40
0,20
0,00
0
10
20
30
40
50
60
time [h]


Hydrogenation of 1,1-diphenylethylene with P(2,6-F2-C6H3)Ph2 and B(C6F5)3
conversion [%]
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0
10
20
30
40
50
60
70
80
time [h]


Hydrogenation of 1,1-diphenylethylene with P(2,6-F2-C6H3)Ph2 and B(C6F5)3 - linearized
- ln (IntSubstr./IntSubstr.+IntProd.)
2,00
1,80
1,60
1,40
1,20
1,00
0,80
0,60
0,40
0,20
0,00
0
10
20
30
40
50
60
70
80
time [h]
y = 0,0242x - 0,0157
R² = 0,99625

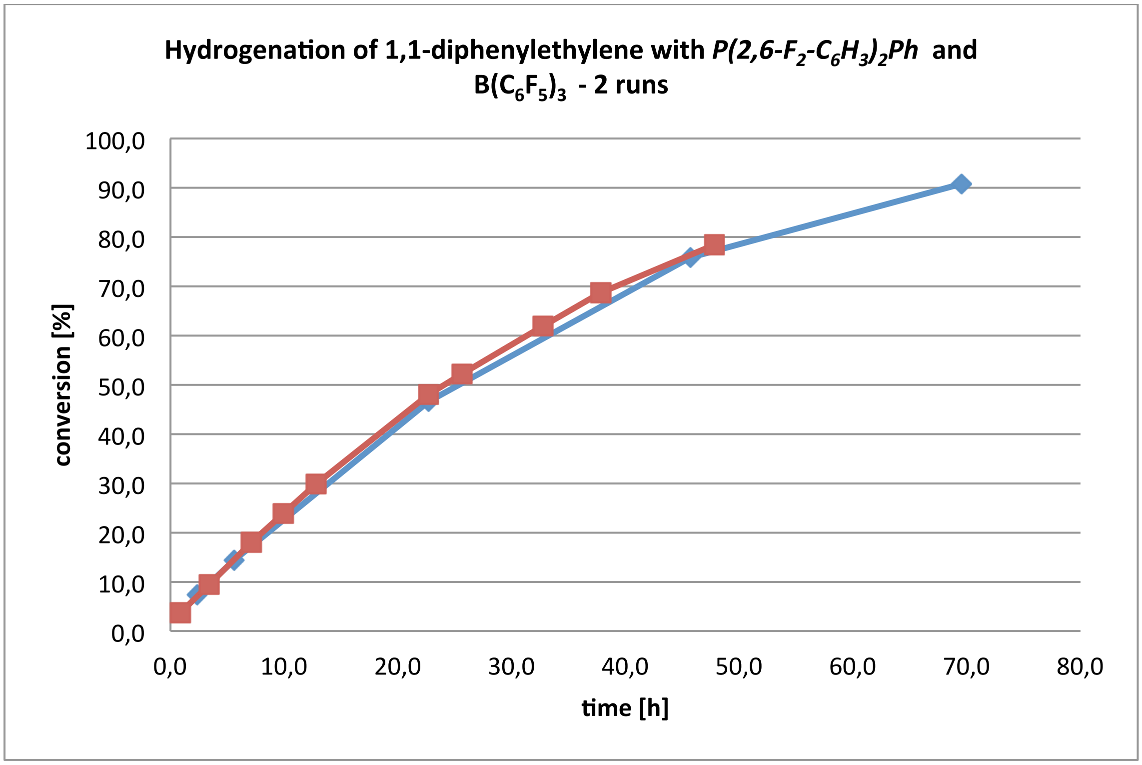
Electronic Supplementary Material (ESI) for Chemical Science
This journal is © The Royal Society of Chemistry 2013

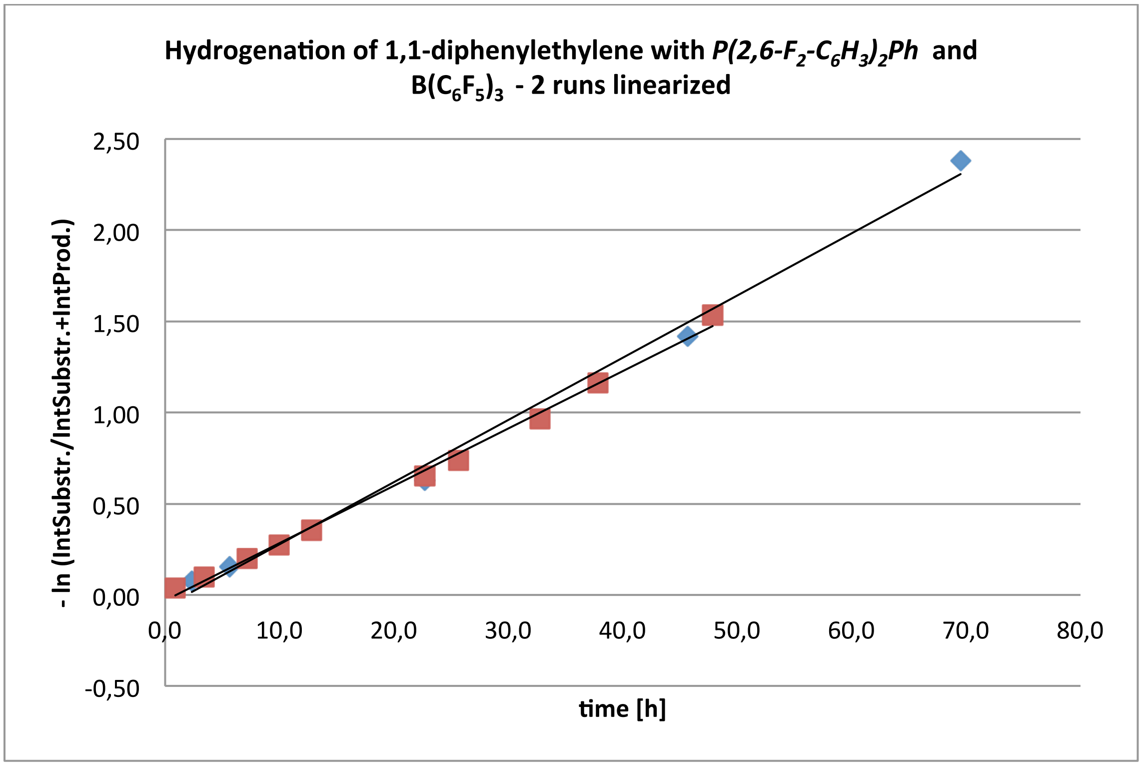


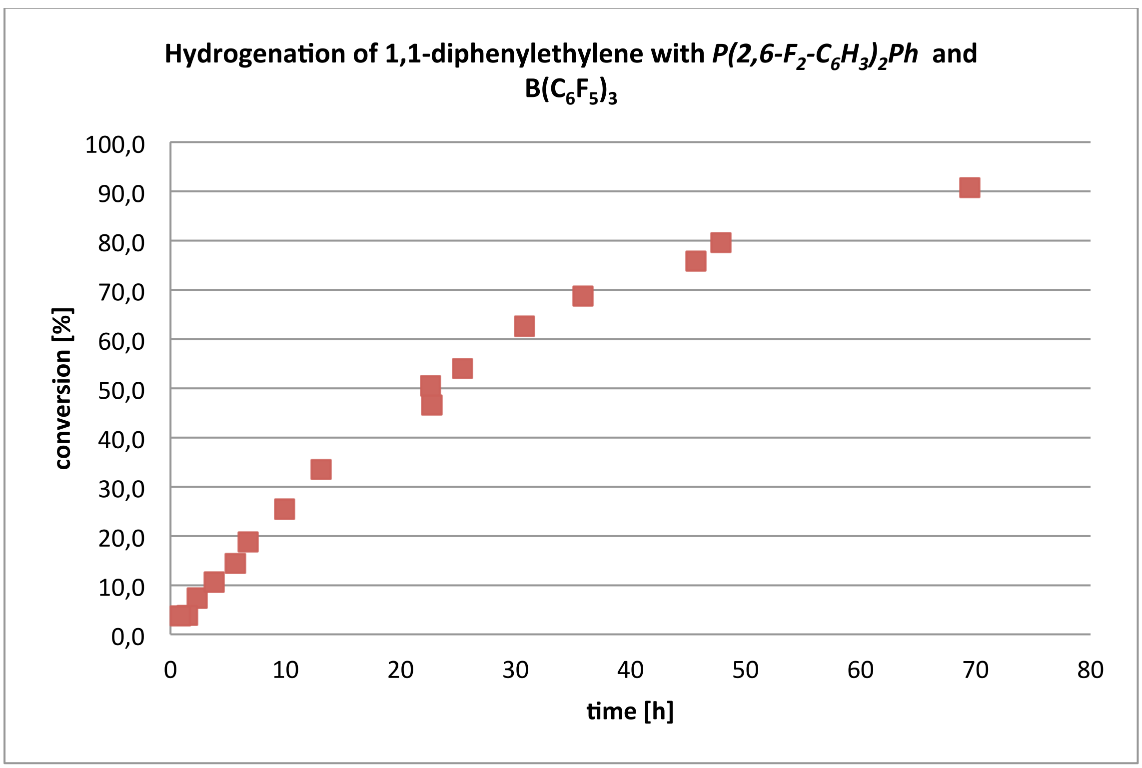
## ***Hydrogenation with $P(2,6\text{-}F_2\text{-}C_6H_3)_2Ph$* (6)**

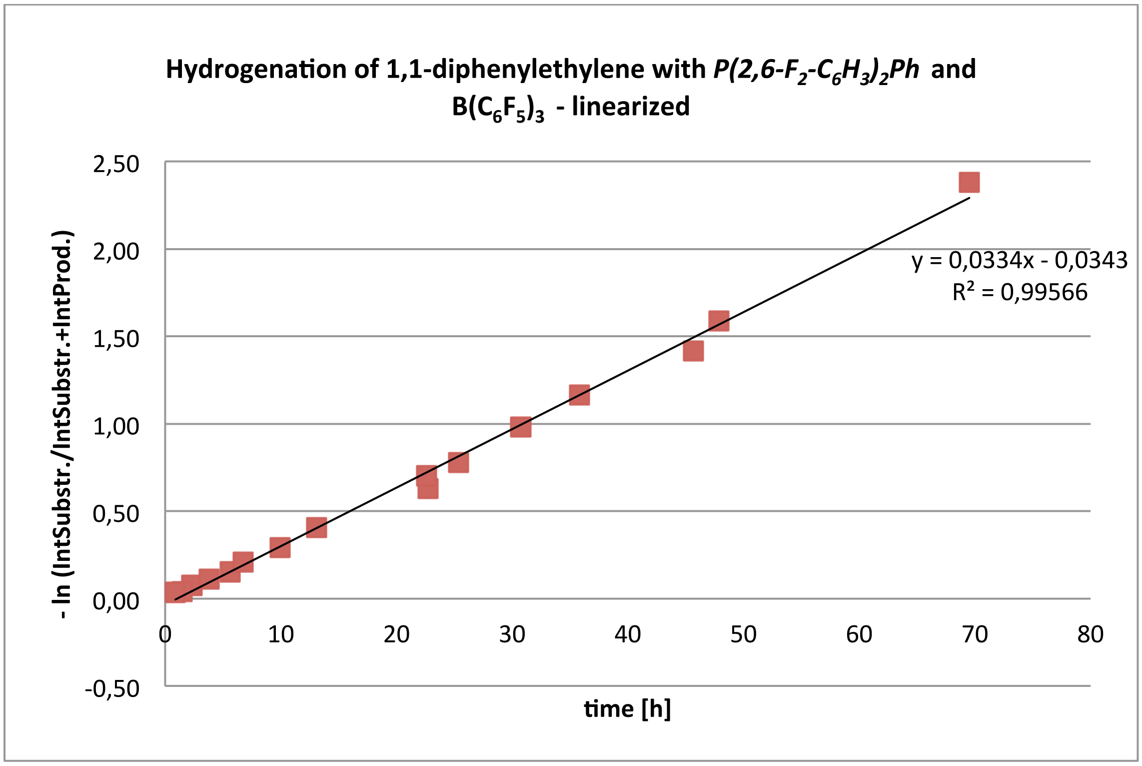
| Run | DPE [mg, mmol] | $P(2,6\text{-}F_2\text{-}C_6H_3)_2Ph$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| V 1 | 9.0, 0.050 | 3.3, 0.010 | 5.2, 0.010 | 0.45 |
| V 2 | 9.0, 0.050 | 3.4, 0.010 | 5.1, 0.010 | 0.45 |

| run ID | Substr. $^1H$ Integral | Prod. $^1H$ Integral | Substr. $^1H$ Integral $_{normalized}$ | Prod. $^1H$ Integral $_{normalized}$ | conv. [%] | time [h] | "-ln($Int_{Substr.}$/$Int_{Substr.}$+$Int_{Prod.}$)" |
|---|---|---|---|---|---|---|---|
| V run 1-1 | 9,151 | 1,083 | 4,575 | 0,361 | 7,3 | 2,3 | 0,0759 |
| V run 1-2 | 11,031 | 2,771 | 5,515 | 0,924 | 14,3 | 5,6 | 0,1548 |
| V run 1-3 | 11,313 | 14,828 | 5,657 | 4,943 | 46,6 | 22,7 | 0,6279 |
| V run 1-4 | 5,428 | 25,459 | 2,714 | 8,486 | 75,8 | 45,7 | 1,4175 |
| V run 1-5 | 1,832 | 26,963 | 0,916 | 8,988 | 90,8 | 69,5 | 2,3806 |
| | | | | | | | |
| V run 2-1 | 17,566 | 1,000 | 8,783 | 0,333 | 3,7 | 0,9 | 0,0372 |
| V run 2-2 | 6,423 | 1,000 | 3,212 | 0,333 | 9,4 | 3,4 | 0,0987 |
| V run 2-3 | 3,032 | 1,000 | 1,516 | 0,333 | 18,0 | 7,1 | 0,1987 |
| V run 2-4 | 2,121 | 1,000 | 1,061 | 0,333 | 23,9 | 9,9 | 0,2733 |
| V run 2-5 | 1,564 | 1,000 | 0,782 | 0,333 | 29,9 | 12,8 | 0,3550 |
| V run 2-6 | 0,723 | 1,000 | 0,362 | 0,333 | 48,0 | 22,7 | 0,6533 |
| V run 2-7 | 0,612 | 1,000 | 0,306 | 0,333 | 52,1 | 25,6 | 0,7367 |
| V run 2-8 | 0,410 | 1,000 | 0,205 | 0,333 | 61,9 | 32,8 | 0,9651 |
| V run 2-9 | 0,303 | 1,000 | 0,152 | 0,333 | 68,7 | 37,9 | 1,1623 |
| V run 2-10 | 0,183 | 1,000 | 0,092 | 0,333 | 78,4 | 47,9 | 1,5345 |




Hydrogenation of 1,1-diphenylethylene with P(2,6-F2-C6H3)2Ph and B(C6F5)3 - 2 runs linearized
2,50
2,00
1,50
1,00
0,50
0,00
-0,50
0,0
10,0
20,0
30,0
40,0
50,0
60,0
70,0
80,0
- ln (IntSubstr./IntSubstr.+IntProd.)
time [h]

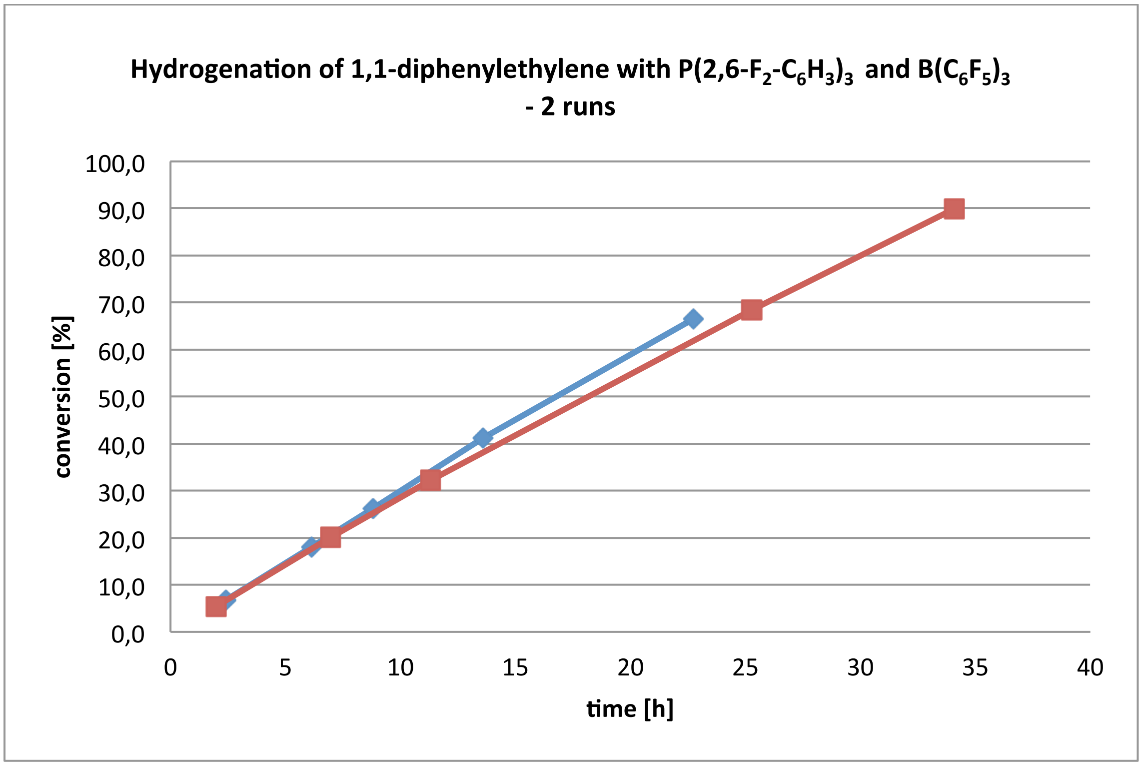

Hydrogenation of 1,1-diphenylethylene with P(2,6-F2-C6H3)2Ph and B(C6F5)3
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0
10
20
30
40
50
60
70
80
conversion [%]
time [h]

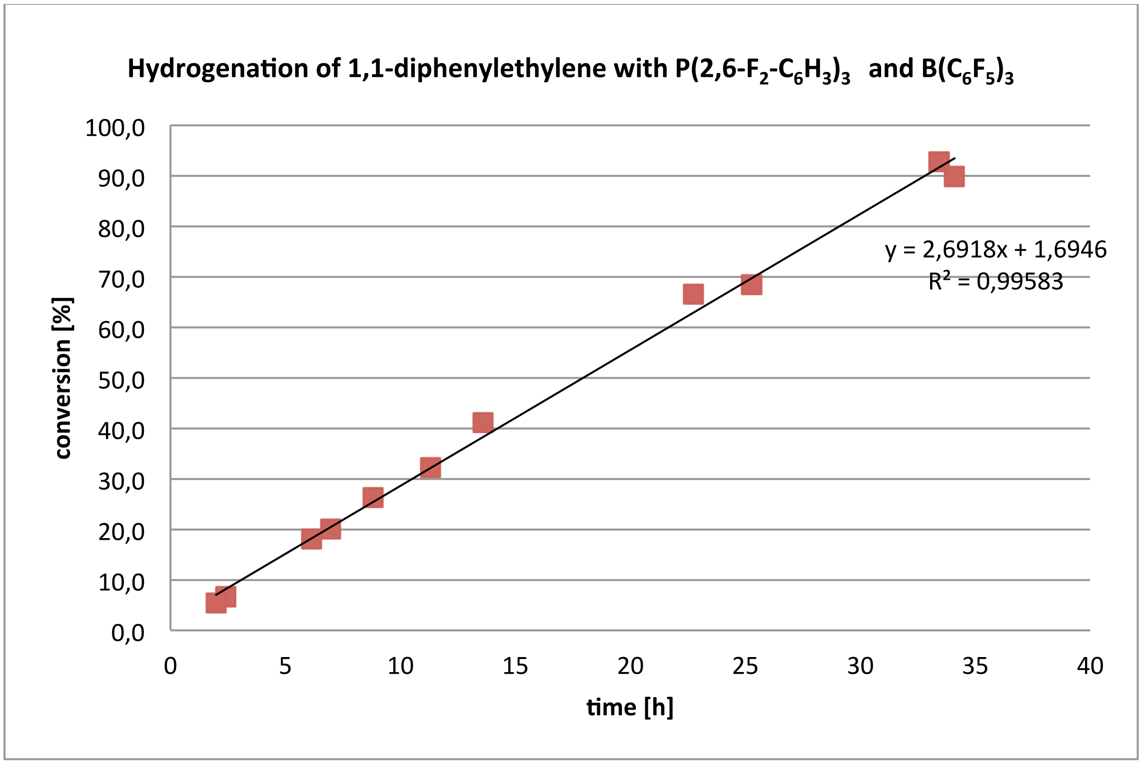


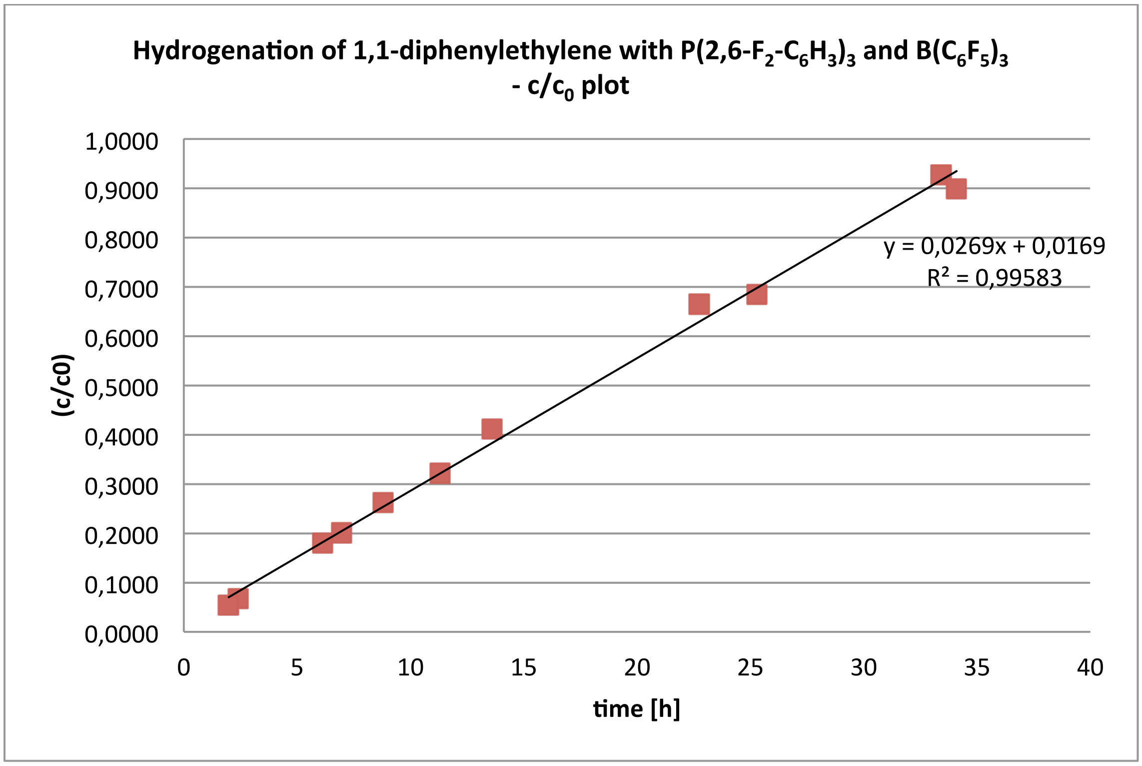

***Hydrogenation with $P(2,6\text{-}F_2\text{-}C_6H_3)_3$ (7)***

| Run | DPE [mg, mmol] | $P(2,6\text{-}F_2\text{-}C_6H_3)_3$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| VI 1 | 9.0, 0.050 | 3.8, 0.010 | 5.2, 0.010 | 0.45 |
| VI 2 | 9.0, 0.050 | 3.7, 0.010 | 5.1, 0.010 | 0.45 |

| run ID | Substr. $^1$H Integral | Prod. $^1$H Integral | Substr. $^1$H Integral $_{normalized}$ | Prod. $^1$H Integral $_{normalized}$ | conv. [%] | time [h] | "($Int_{Prod}/Int_{Substr.}+Int_{Prod.}$)" |
|---|---|---|---|---|---|---|---|
| VI run 1-1 | 12,7965 | 1,3806 | 6,398 | 0,460 | 6,7 | 2,4 | 0,0671 |
| VI run 1-2 | 13,8360 | 4,5756 | 6,918 | 1,525 | 18,1 | 6,13 | 0,1806 |
| VI run 1-3 | 11,3542 | 6,0619 | 5,677 | 2,021 | 26,2 | 8,8 | 0,2625 |
| VI run 1-4 | 10,6267 | 11,1515 | 5,313 | 3,717 | 41,2 | 13,6 | 0,4116 |
| VI run 1-5 | 8,5324 | 25,4377 | 4,266 | 8,479 | 66,5 | 22,75 | 0,6653 |
| VI run 1-6 | 0,8385 | 16,0613 | 0,419 | 5,354 | 92,7 | 33,42 | 0,9274 |
| | | | | | | | |
| VI run 2-1 | 11,6887 | 1,0045 | 5,844 | 0,335 | 5,4 | 1,98 | 0,0542 |
| VI run 2-2 | 11,7839 | 4,4324 | 5,892 | 1,477 | 20,0 | 6,97 | 0,2005 |
| VI run 2-3 | 9,1248 | 6,5113 | 4,562 | 2,170 | 32,2 | 11,32 | 0,3224 |
| VI run 2-4 | 4,5853 | 14,8920 | 2,293 | 4,964 | 68,4 | 25,27 | 0,6841 |
| VI run 2-5 | 1,6515 | 22,0783 | 0,826 | 7,359 | 89,9 | 34,1 | 0,8991 |


Hydrogenation of 1,1-diphenylethylene with P(2,6-F2-C6H3)3 and B(C6F5)3
- 2 runs
conversion [%]
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0
5
10
15
20
25
30
35
40
time [h]

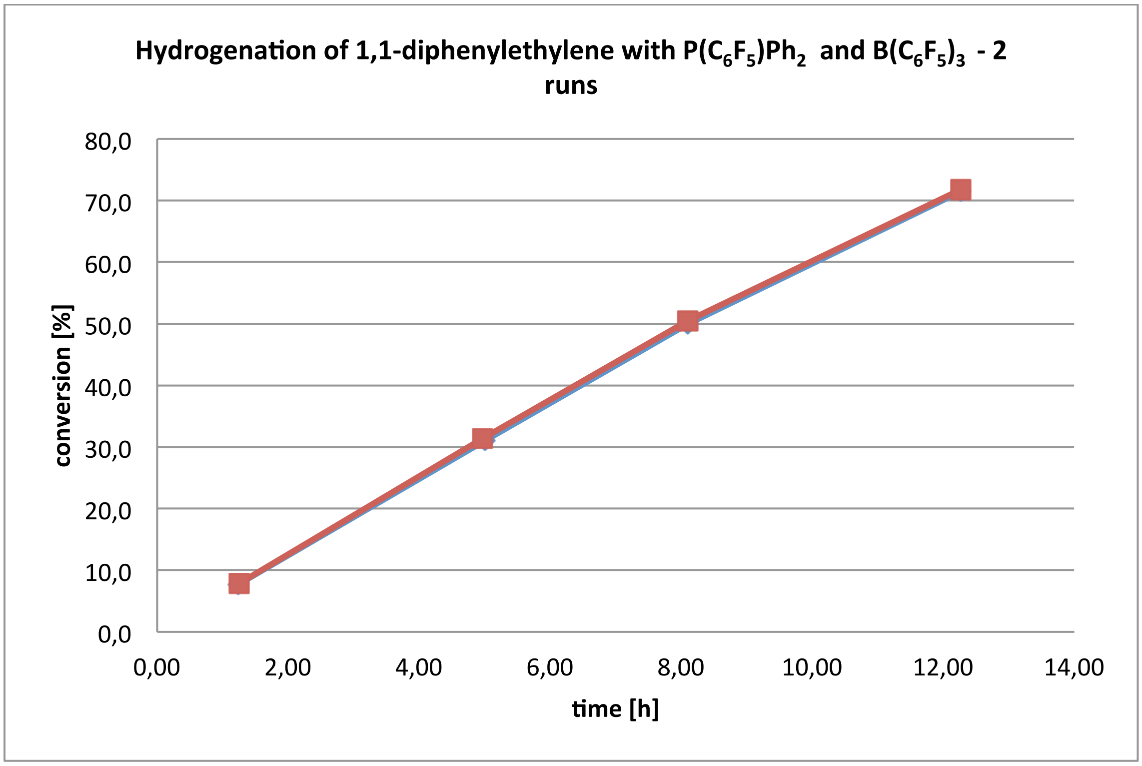

Hydrogenation of 1,1-diphenylethylene with P(2,6-F2-C6H3)3 and B(C6F5)3
conversion [%]
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0
5
10
15
20
25
30
35
40
time [h]
y = 2,6918x + 1,6946
R² = 0,99583

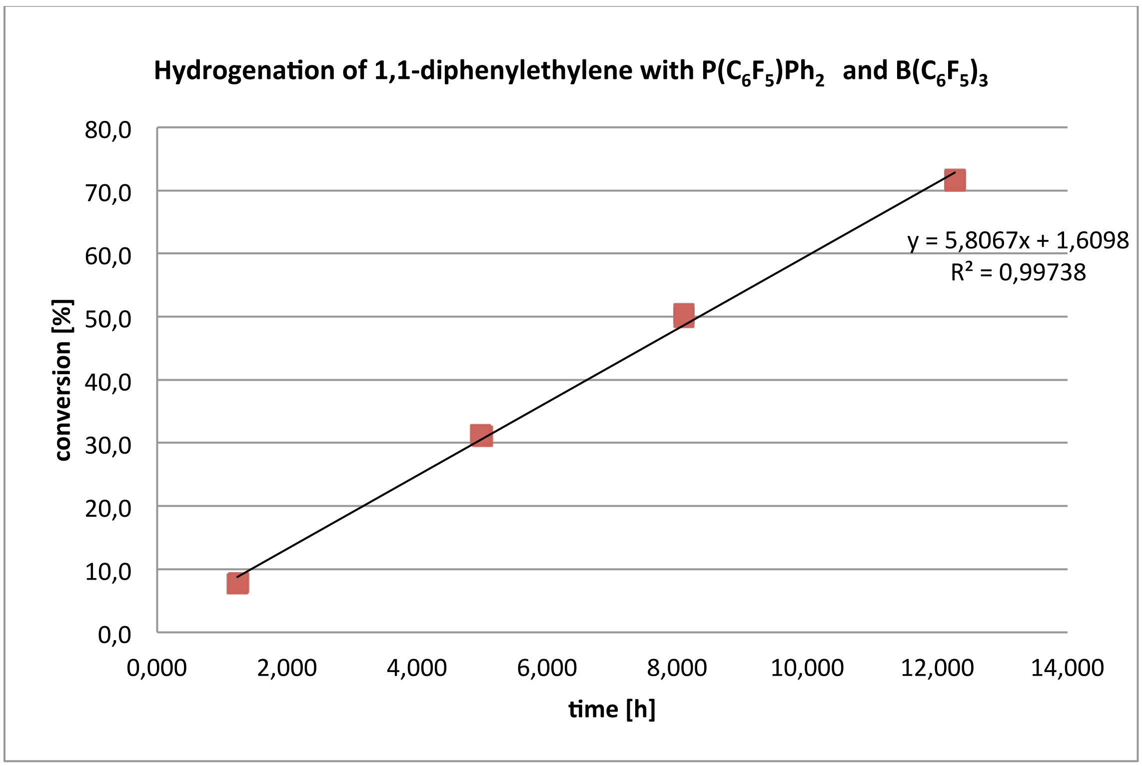


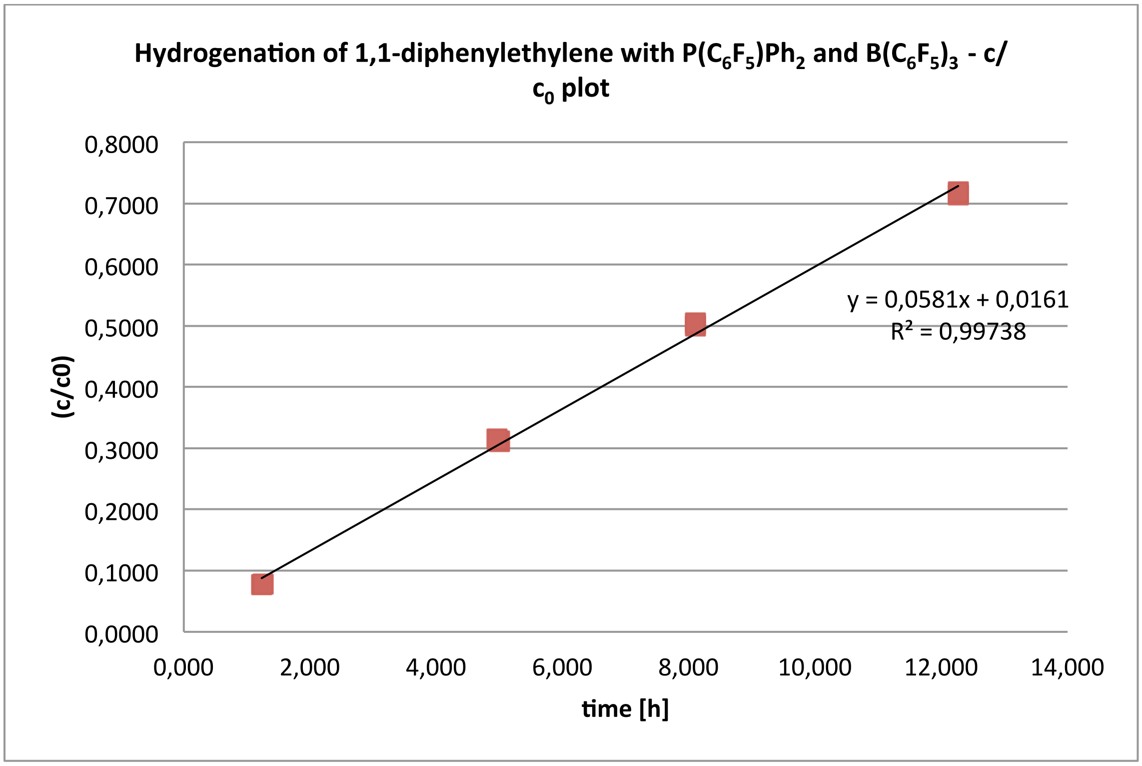

***Hydrogenation with $P(C_6F_5)Ph_2$* (8)**

| Run | DPE [mg, mmol] | $P(C_6F_5)Ph_2$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| VII 1 | 9.0, 0.050 | 3.5, 0.010 | 5.1, 0.010 | 0.45 |
| VII 2 | 9.0, 0.050 | 3.5, 0.010 | 5.1, 0.010 | 0.45 |

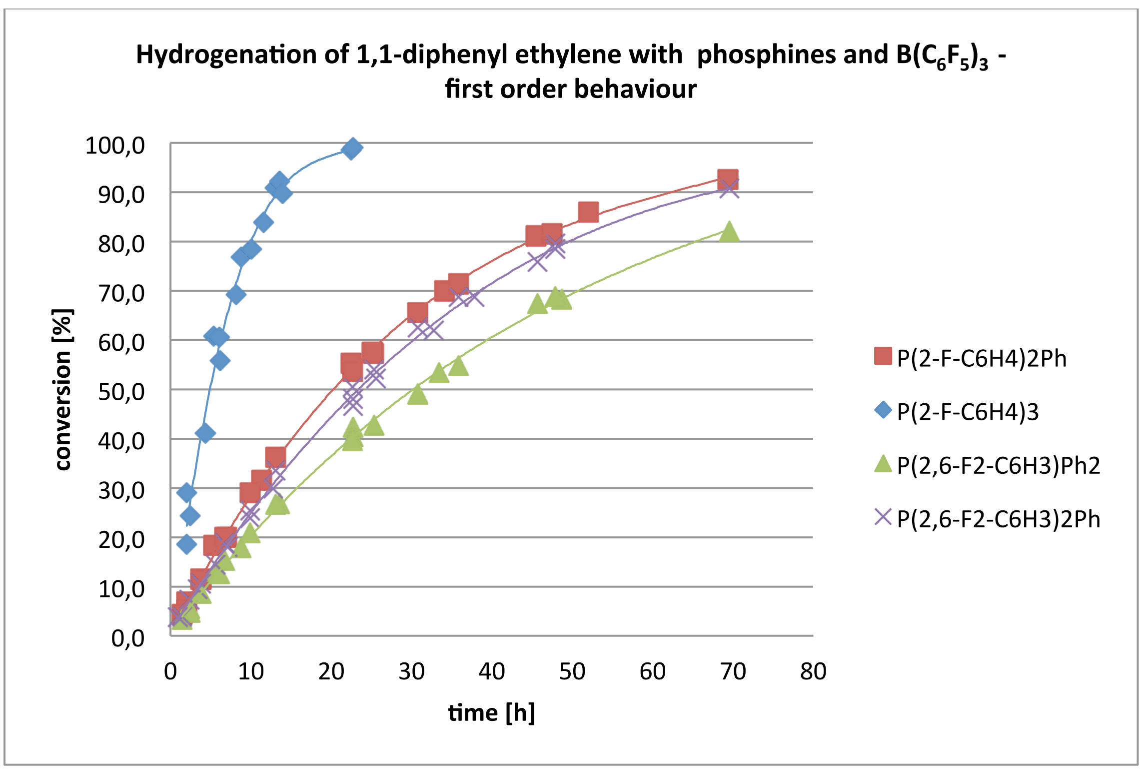
| run ID | Substr. $^1$H Integral | Prod. $^1$H Integral | Substr. $^1$H Integral $_{normalized}$ | Prod. $^1$H Integral $_{normalized}$ | conv. [%] | time [h] | "($Int_{Prod}/Int_{Substr.}+Int_{Prod.}$)" |
|---|---|---|---|---|---|---|---|
| VII run 1-1 | 8,021 | 1,000 | 4,011 | 0,333 | 7,7 | 1,23 | 0,0767 |
| VII run 1-2 | 1,478 | 1,000 | 0,739 | 0,333 | 31,1 | 5,00 | 0,3109 |
| VII run 1-3 | 0,668 | 1,000 | 0,334 | 0,333 | 49,9 | 8,10 | 0,4994 |
| VII run 1-4 | 0,267 | 1,000 | 0,133 | 0,333 | 71,4 | 12,27 | 0,7144 |
| | | | | | | | |
| VII run 2-1 | 7,835 | 1,000 | 3,917 | 0,333 | 7,8 | 1,25 | 0,0784 |
| VII run 2-2 | 1,457 | 1,000 | 0,728 | 0,333 | 31,4 | 4,97 | 0,3140 |
| VII run 2-3 | 0,653 | 1,000 | 0,326 | 0,333 | 50,5 | 8,10 | 0,5053 |
| VII run 2-4 | 0,262 | 1,000 | 0,131 | 0,333 | 71,8 | 12,27 | 0,7179 |

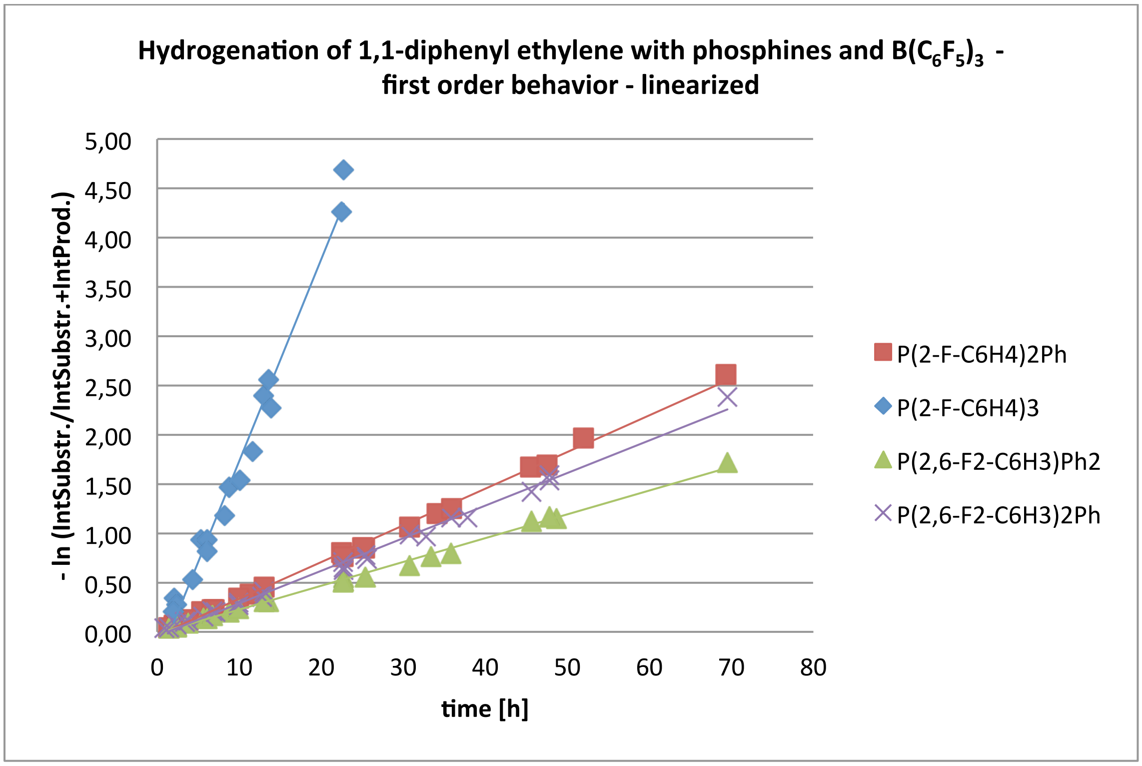

Hydrogenation of 1,1-diphenylethylene with P(C6F5)Ph2 and B(C6F5)3 - 2 runs
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
conversion [%]
0,00
2,00
4,00
6,00
8,00
10,00
12,00
14,00
time [h]

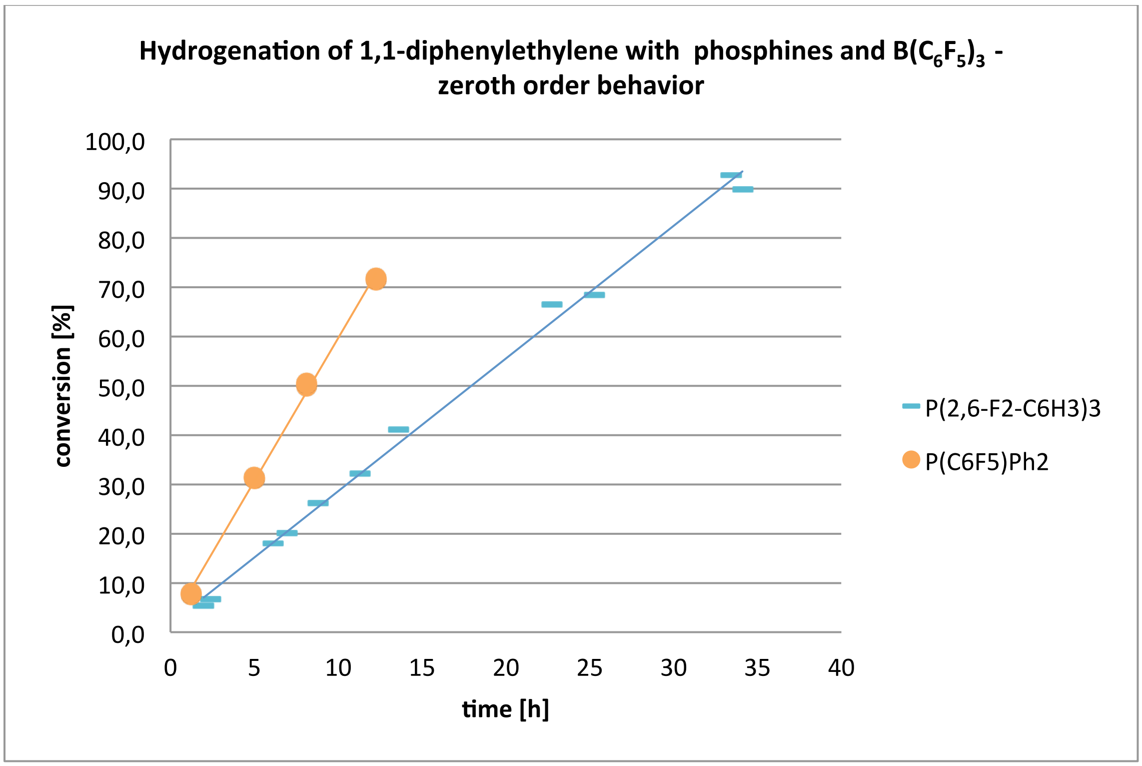

Hydrogenation of 1,1-diphenylethylene with P(C6F5)Ph2 and B(C6F5)3
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
conversion [%]
y = 5,8067x + 1,6098
R² = 0,99738
0,000
2,000
4,000
6,000
8,000
10,000
12,000
14,000
time [h]




***<u>Comparison of all phosphines in the hydrogenation of 1,1-diphenyl ethylene</u>***




Hydrogenation of 1,1-diphenyl ethylene with phosphines and B(C6F5)3 - first order behavior - linearized
- ln (IntSubstr./IntSubstr.+IntProd.)
5,00
4,50
4,00
3,50
3,00
2,50
2,00
1,50
1,00
0,50
0,00
0
10
20
30
40
50
60
70
80
time [h]
P(2-F-C6H4)2Ph
P(2-F-C6H4)3
P(2,6-F2-C6H3)Ph2
P(2,6-F2-C6H3)2Ph


Hydrogenation of 1,1-diphenylethylene with phosphines and B(C6F5)3 - zeroth order behavior
conversion [%]
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0
5
10
15
20
25
30
35
40
time [h]
P(2,6-F2-C6H3)3
P(C6F5)Ph2

## *Hydrogenation of trimethyl(methallyl)silane (10, TMAS)*

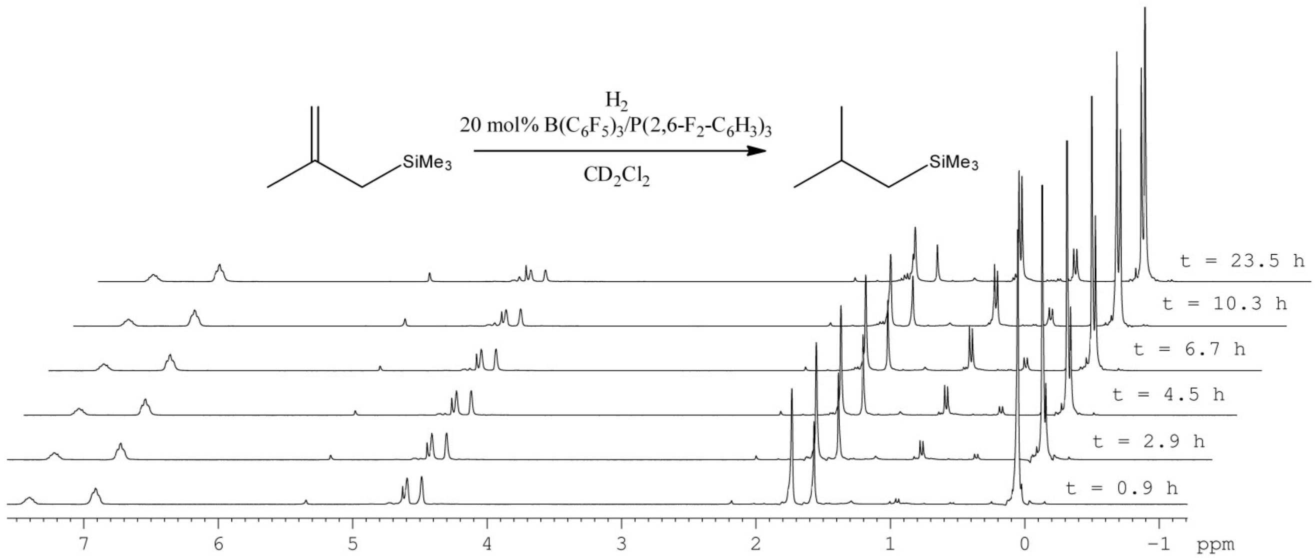
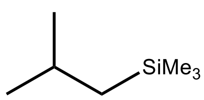



Figure 3: Hydrogenation of trimethyl(methallyl)silane (representative example run with $P(2,6\text{-}F_2\text{-}C_6H_3)_3$).

*Isobutyltrimethylsilane*: $^1$H NMR (300 MHz, $CD_2Cl_2$): δ = 1.76 (m, 1H, C*H*), 0.93 (d, $J$ = 6.5 Hz, 6H, C$H_3$), 0.52 (d, $J$ = 6.7 Hz, 2H, C$H_2$), 0.00 (s, 9H, $SiMe_3$) ppm. GC/MS (70 eV) = 130 (5), 115 (100), 73 (40).

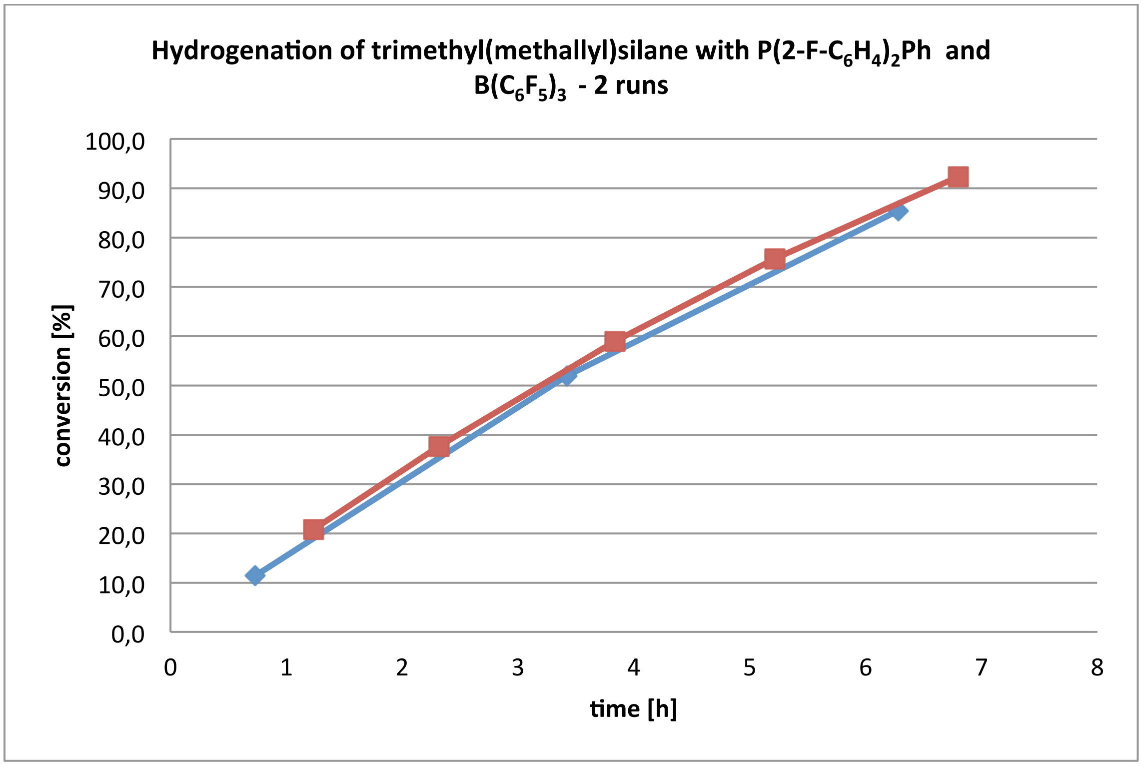


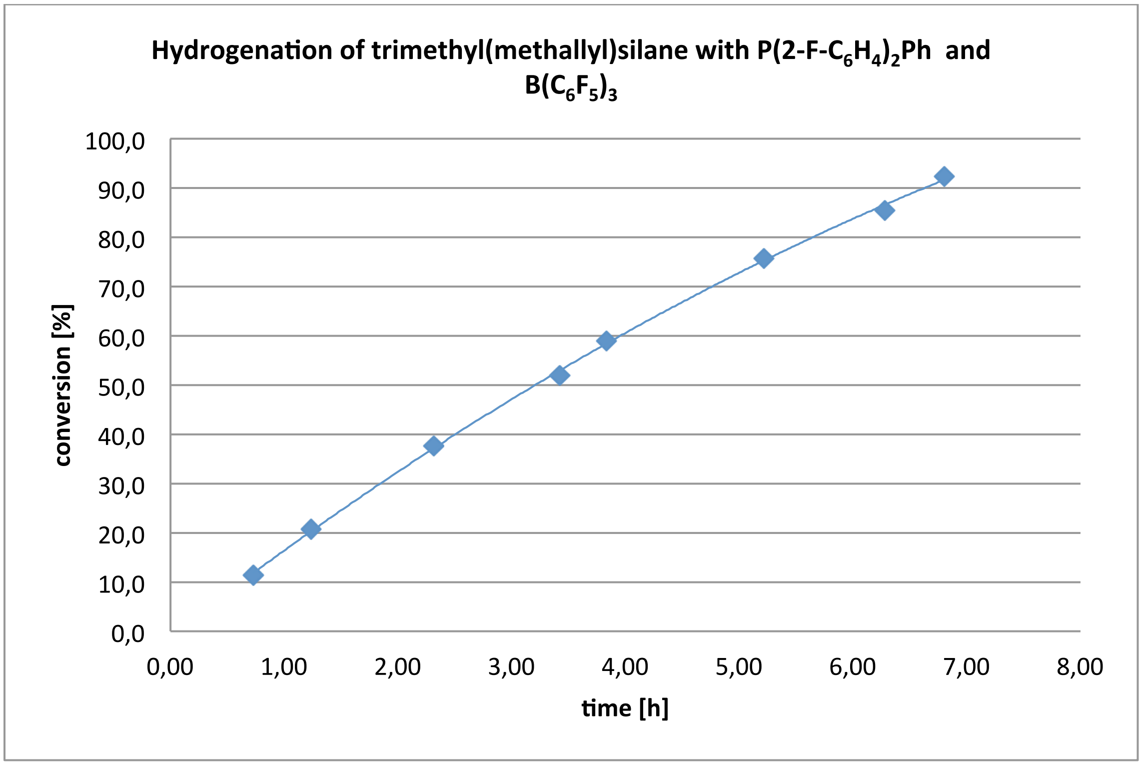

***Representative runs (two runs for each phosphine) and mean data (determined from at least 2 runs) for every investigated phosphine (tables, time vs. conversion plot)***

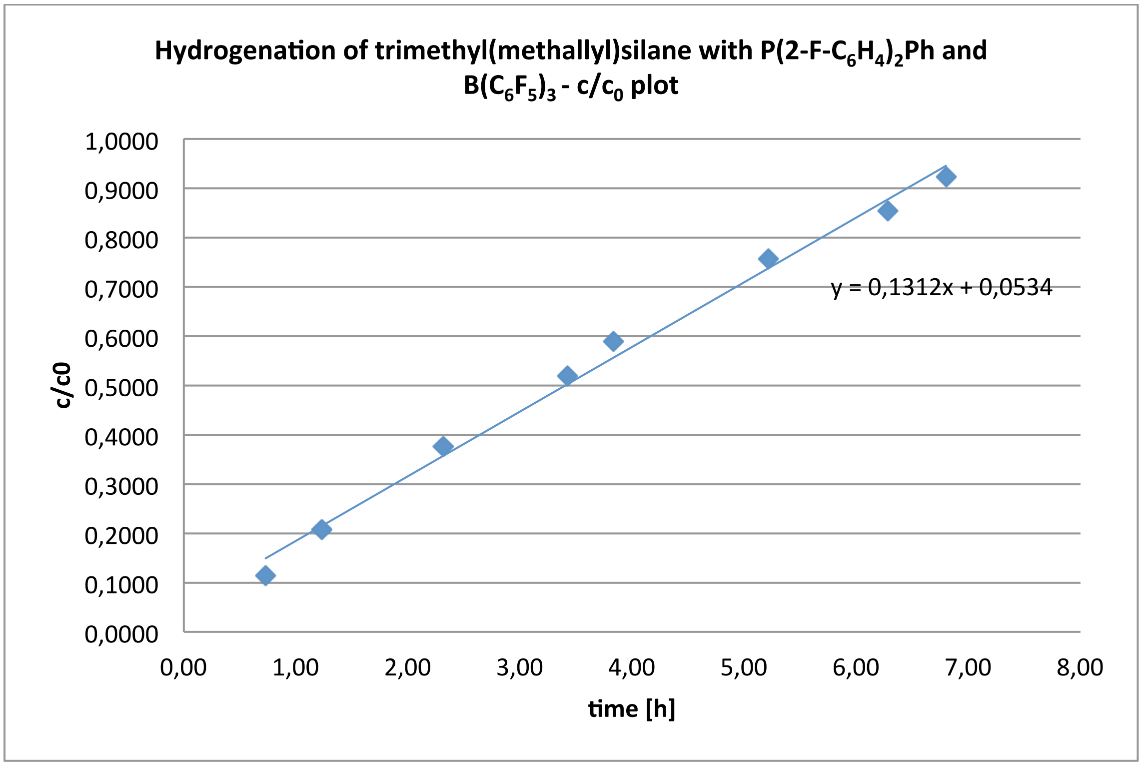
### ***Hydrogenation with $P(2\text{-}F\text{-}C_6H_4)_2Ph$* (3)**

| Run | TMAS [mg, mmol] | $P(2\text{-}F\text{-}C_6H_4)Ph_2$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| II 1 | 6.4, 0.050 | 2.9, 0.010 | 5.0, 0.010 | 0.45 |
| II 2 | 6.4, 0.050 | 3.0, 0.010 | 5.1, 0.010 | 0.45 |

| run ID | Substrate $^1$H Integral | Product $^1$H Integral | conv. [%] | time [h] | "($Int_{Prod}/Int_{Substr.}+Int_{Prod.}$)" |
|---|---|---|---|---|---|
| II run 1-1 | 1,0000 | 0,1277 | 11,3 | 0,73 | 0,1132 |
| II run 1-2 | 1,0000 | 1,0802 | 51,9 | 3,42 | 0,5193 |
| II run 1-3 | 1,0000 | 5,8782 | 85,5 | 6,28 | 0,8546 |
| | | | | | |
| II run 2-1 | 1,0000 | 0,2622 | 20,8 | 1,23 | 0,2077 |
| II run 2-2 | 1,0000 | 0,6039 | 37,7 | 2,32 | 0,3765 |
| II run 2-3 | 1,0000 | 1,4328 | 58,9 | 3,83 | 0,5890 |
| II run 2-4 | 1,0000 | 3,1135 | 75,7 | 5,22 | 0,7569 |
| II run 2-5 | 1,0000 | 12,0672 | 92,3 | 6,80 | 0,9235 |


Hydrogenation of trimethyl(methallyl)silane with P(2-F-C6H4)2Ph and B(C6F5)3 - 2 runs
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
conversion [%]
0
1
2
3
4
5
6
7
8
time [h]


Hydrogenation of trimethyl(methallyl)silane with P(2-F-C6H4)2Ph and B(C6F5)3
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
conversion [%]
0,00
1,00
2,00
3,00
4,00
5,00
6,00
7,00
8,00
time [h]



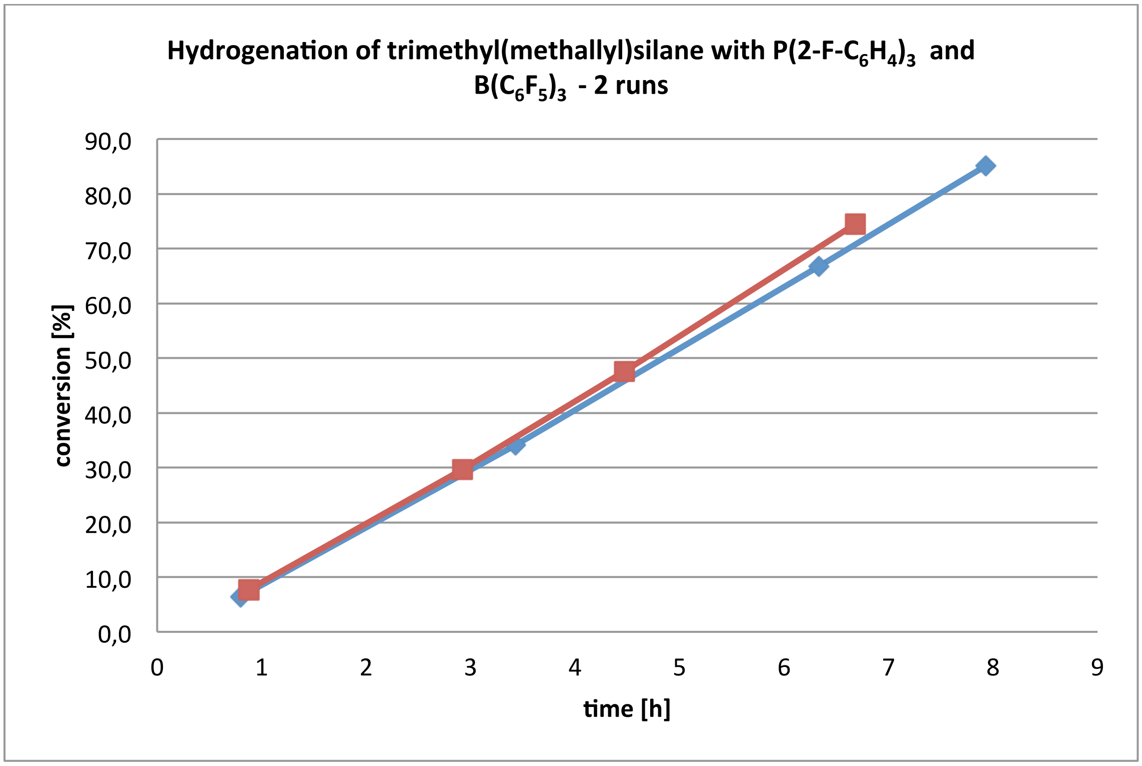

***Hydrogenation with $P(2\text{-}F\text{-}C_6H_4)_3$*** **(4)**

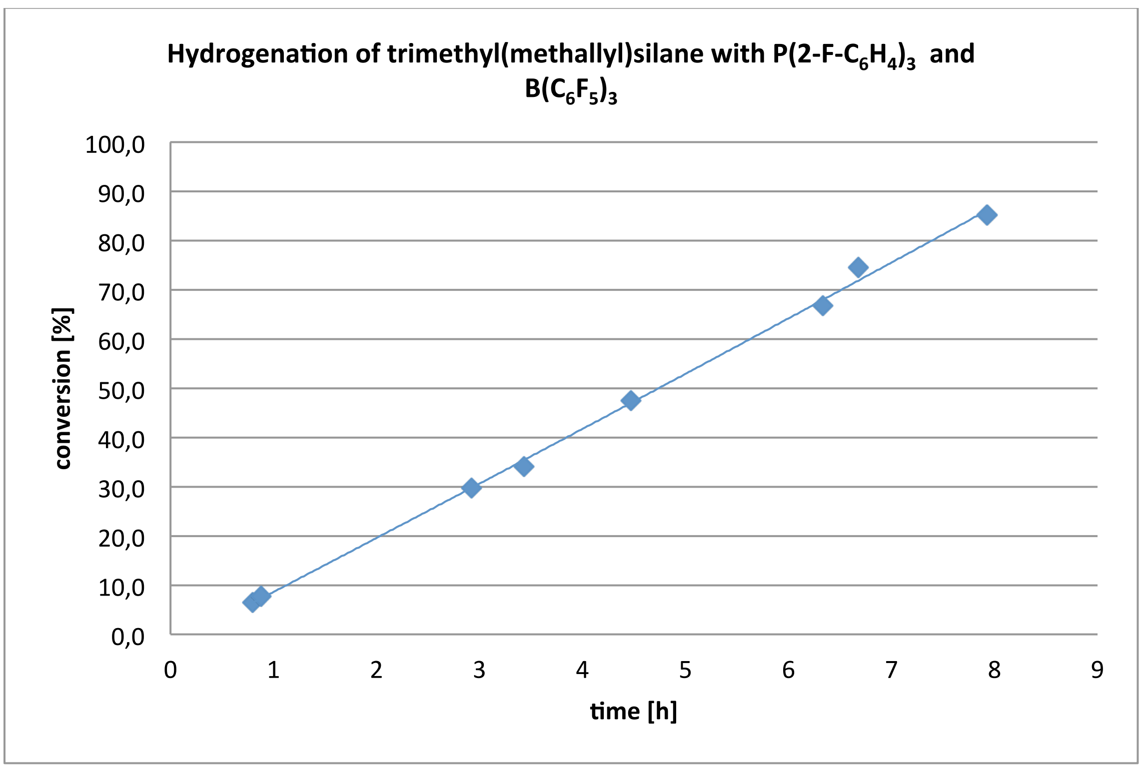
| Run | TMAS [mg, mmol] | $P(2\text{-}F\text{-}C_6H_4)_3$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| III 1 | 6.4, 0.050 | 3.0, 0.010 | 5.0, 0.010 | 0.45 |
| III 2 | 6.4, 0.050 | 3.2, 0.010 | 5.1, 0.010 | 0.45 |

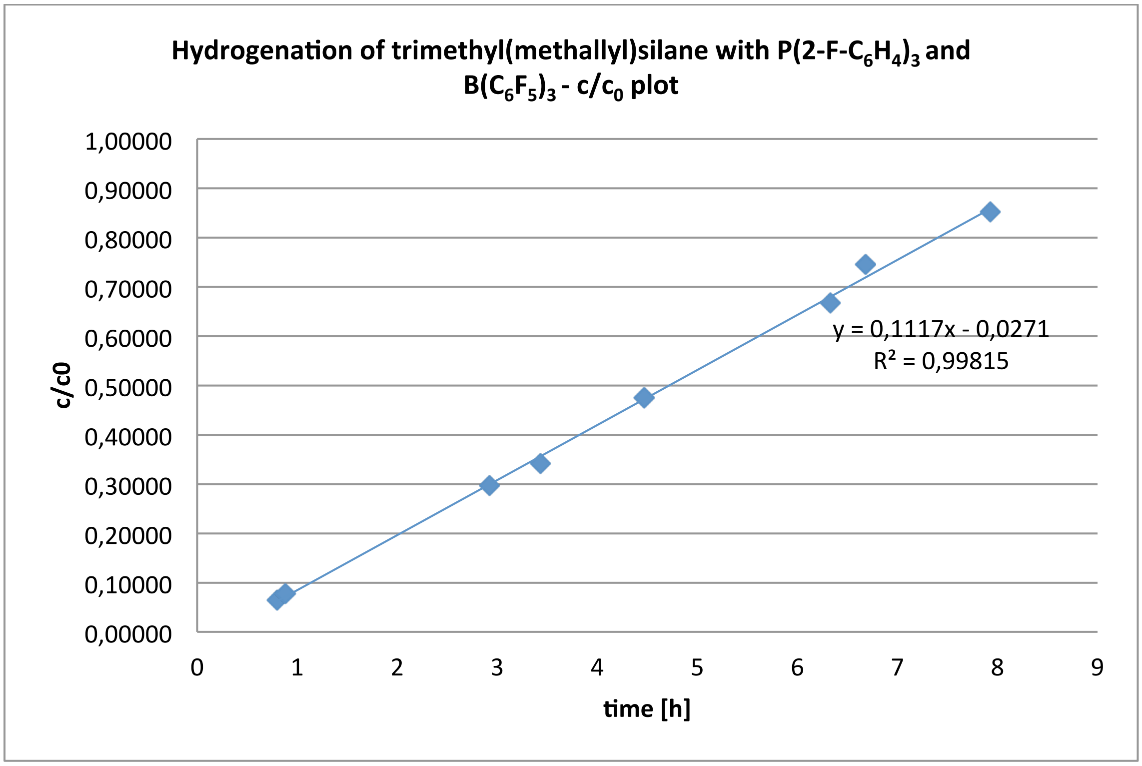
| run ID | Substrate $^1$H Integral | Product $^1$H Integral | conv. [%] | time [h] | "($Int_{Prod}/Int_{Substr.}+Int_{Prod.}$)" |
|---|---|---|---|---|---|
| III run 1-1 | 1,0000 | 0,0684 | 6,4 | 0,8 | 0,06402 |
| III run 1-2 | 1,0000 | 0,5177 | 34,1 | 3,43 | 0,34111 |
| III run 1-3 | 1,0000 | 2,0095 | 66,8 | 6,33 | 0,66772 |
| III run 1-4 | 1,0000 | 5,7227 | 85,1 | 7,93 | 0,85125 |
| | | | | | |
| III run 2-1 | 1,0000 | 0,0836 | 7,7 | 0,88 | 0,07715 |
| III run 2-2 | 1,0000 | 0,4214 | 29,6 | 2,92 | 0,29647 |
| III run 2-3 | 1,0000 | 0,9066 | 47,6 | 4,47 | 0,47551 |
| III run 2-4 | 1,0000 | 2,9175 | 74,5 | 6,68 | 0,74474 |

Electronic Supplementary Material (ESI) for Chemical Science



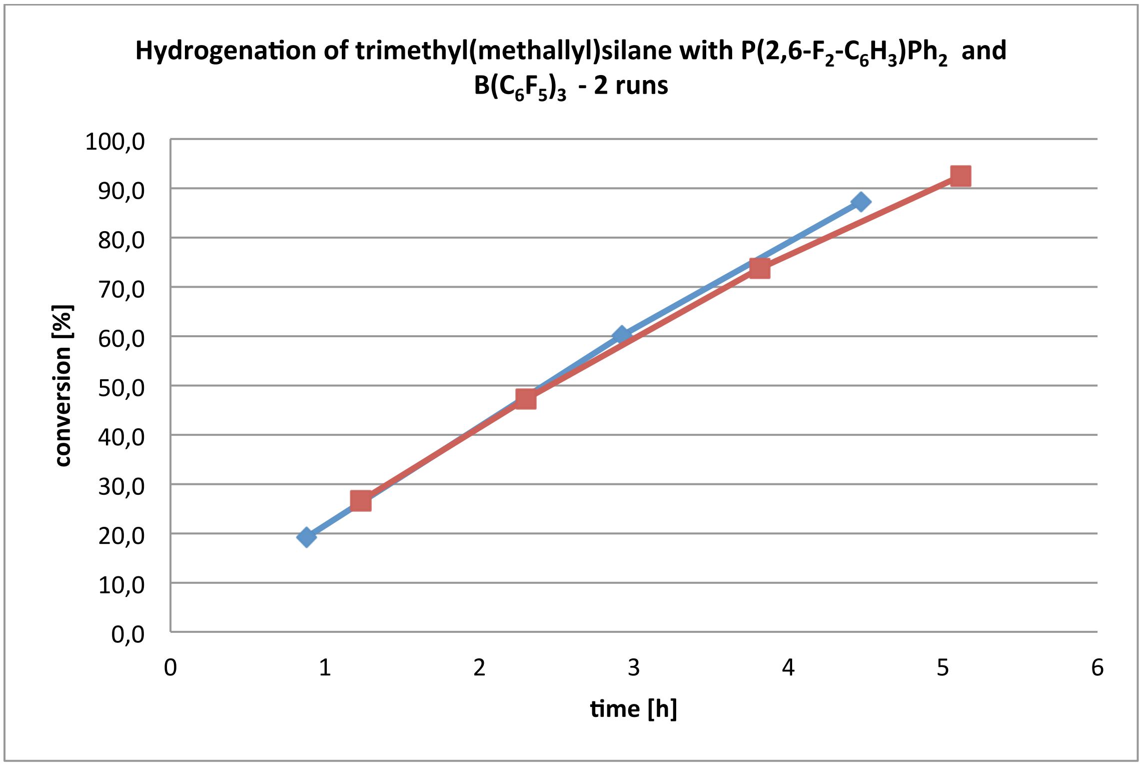



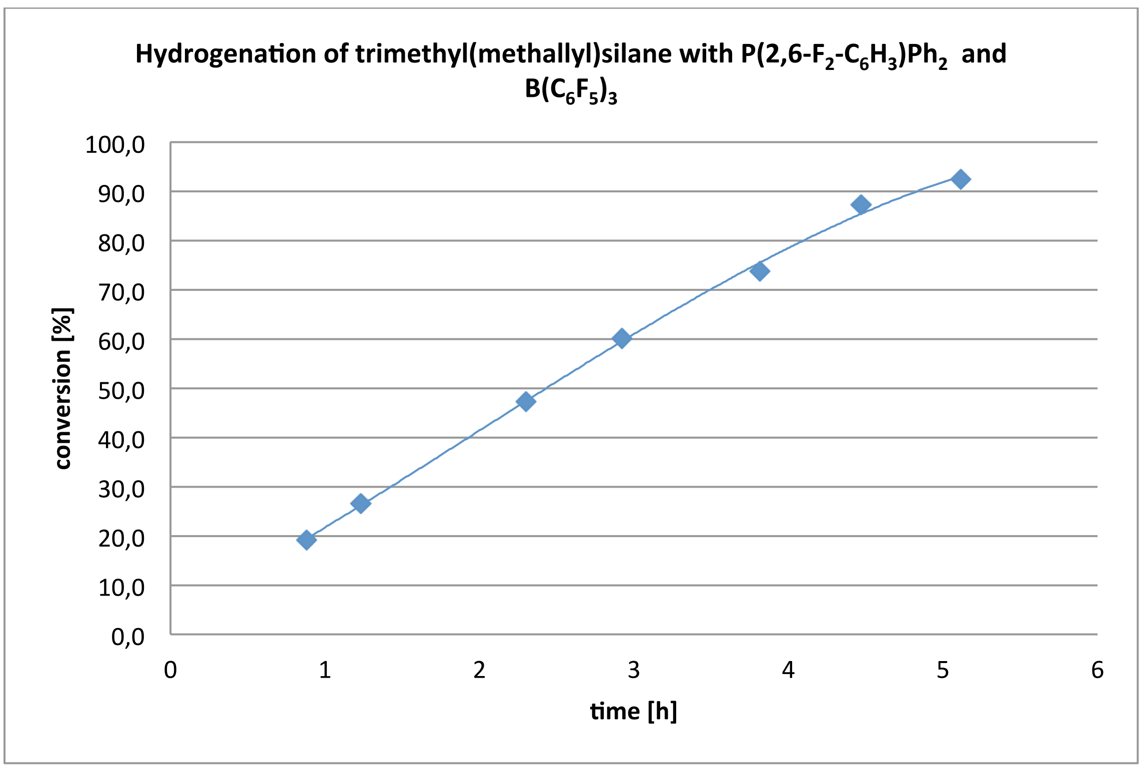


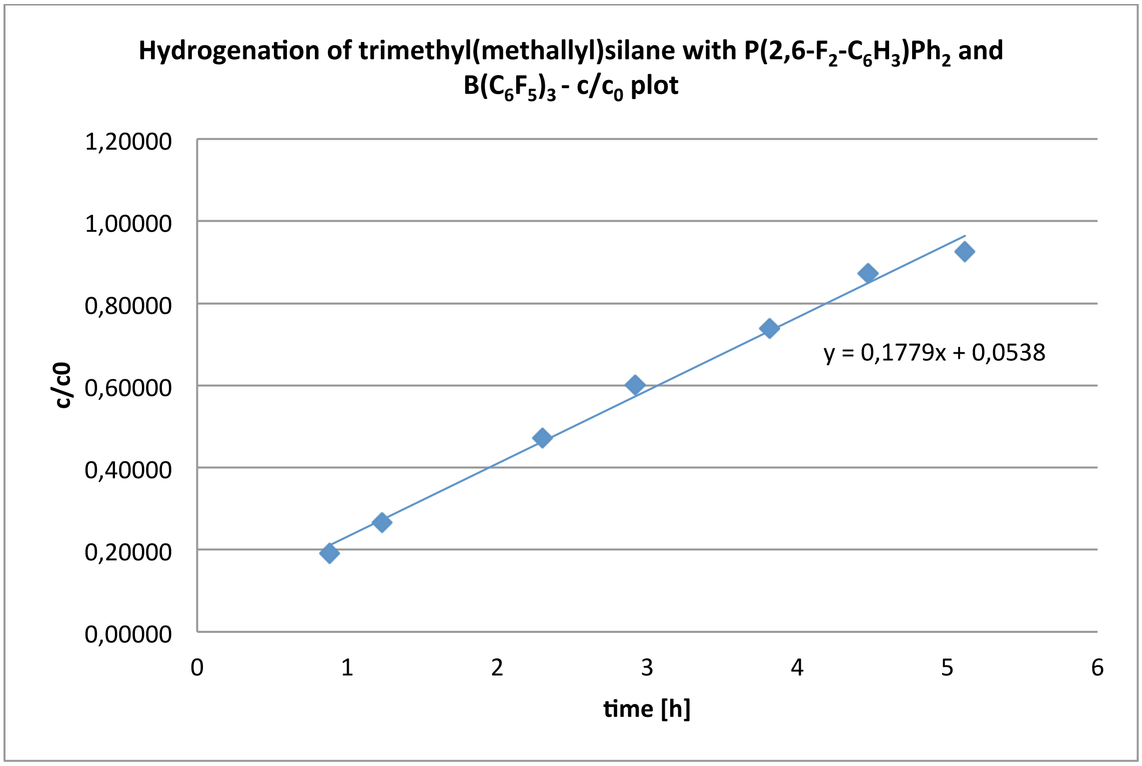

***Hydrogenation with P(2,6-F$_2$-C$_6$H$_3$)Ph$_2$* (5)**

| Run | TMAS [mg, mmol] | P(2,6-$F_2$-$C_6H_3$)$Ph_2$ [mg, mmol] | B($C_6F_5$)$_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| IV 1 | 6.4, 0.050 | 2.8, 0.010 | 5.2, 0.010 | 0.45 |
| IV 2 | 6.4, 0.050 | 2.9, 0.010 | 5.1, 0.010 | 0.45 |

| run ID | Substrate $^1$H Integral | Product $^1$H Integral | conv. [%] | time [h] | "($Int_{Prod}$/$Int_{Substr.}$+$Int_{Prod.}$)" |
|---|---|---|---|---|---|
| IV run 1-1 | 1,0000 | 0,2372 | 19,2 | 0,88 | 0,19172 |
| IV run 1-2 | 1,0000 | 1,5058 | 60,1 | 2,92 | 0,60093 |
| IV run 1-3 | 1,0000 | 6,8315 | 87,2 | 4,47 | 0,87231 |
| | | | | | |
| IV run 2-1 | 1,0000 | 0,3614 | 26,5 | 1,23 | 0,26546 |
| IV run 2-2 | 1,0000 | 0,8957 | 47,2 | 2,30 | 0,47249 |
| IV run 2-3 | 1,0000 | 2,8130 | 73,8 | 3,82 | 0,73774 |
| IV run 2-4 | 1,0000 | 12,3742 | 92,5 | 5,12 | 0,92523 |


Hydrogenation of trimethyl(methallyl)silane with $P(2,6\text{-}F_2\text{-}C_6H_3)Ph_2$ and $B(C_6F_5)_3$ - 2 runs
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
conversion [%]
0
1
2
3
4
5
6
time [h]

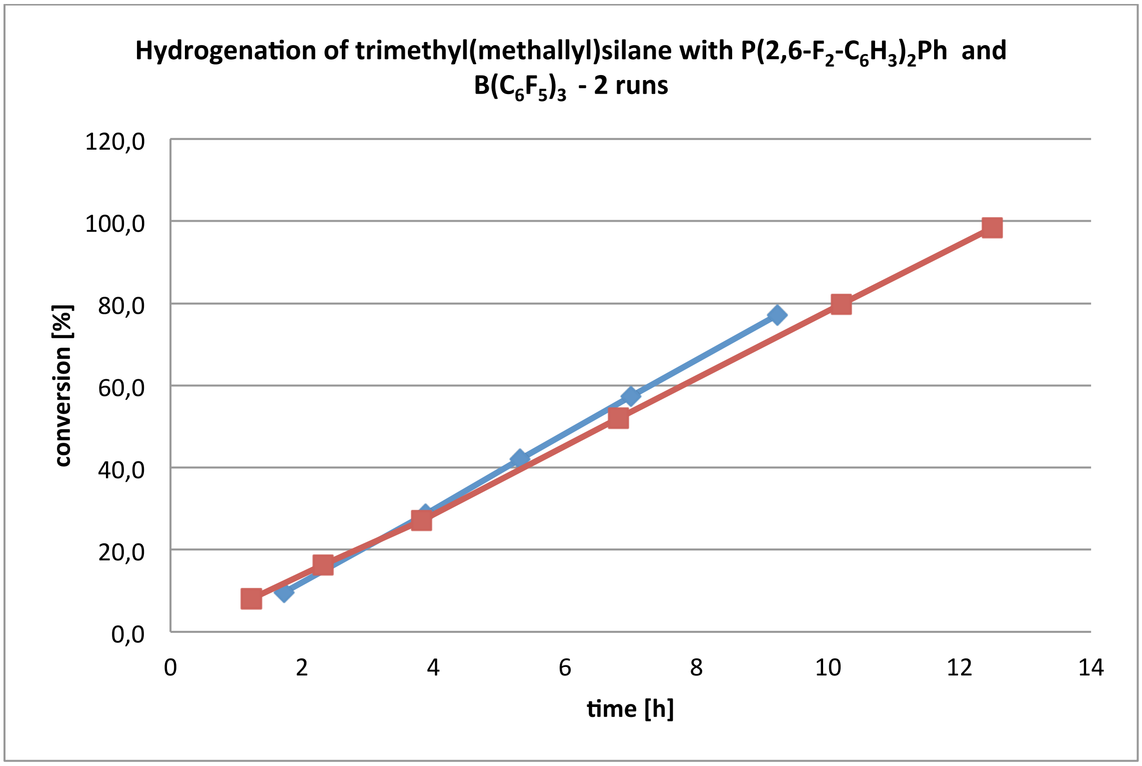

Hydrogenation of trimethyl(methallyl)silane with $P(2,6\text{-}F_2\text{-}C_6H_3)Ph_2$ and $B(C_6F_5)_3$
100,0
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
conversion [%]
0
1
2
3
4
5
6
time [h]

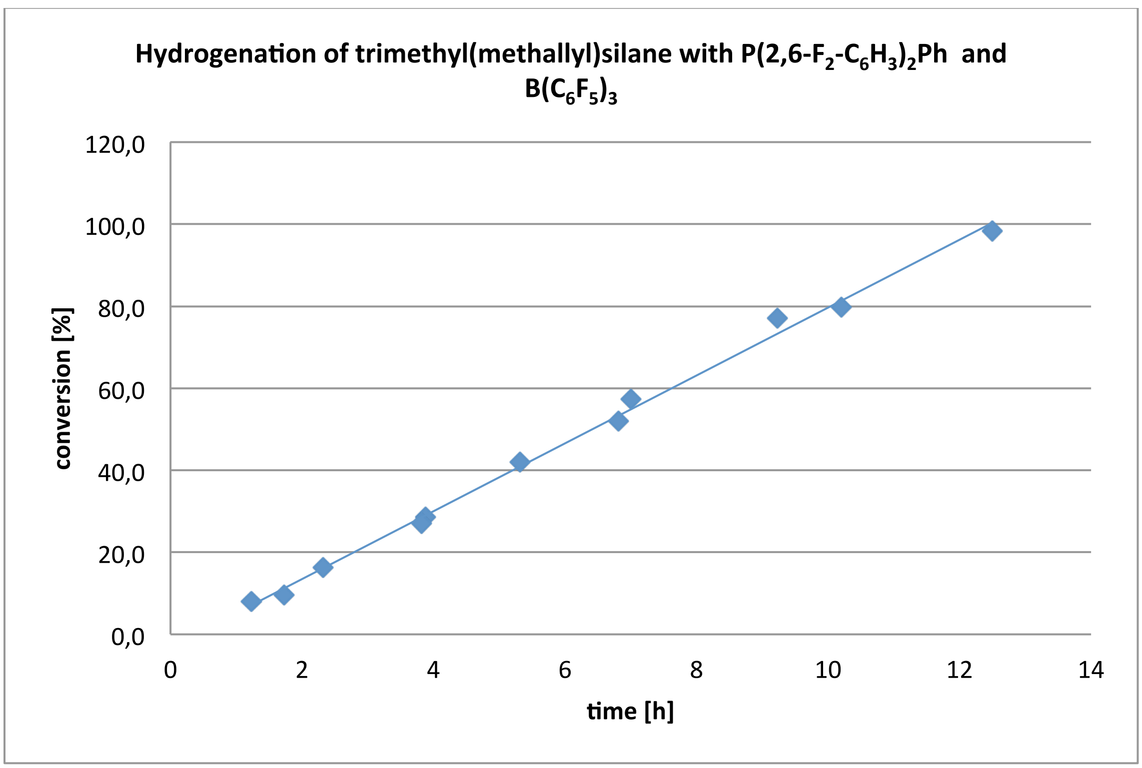


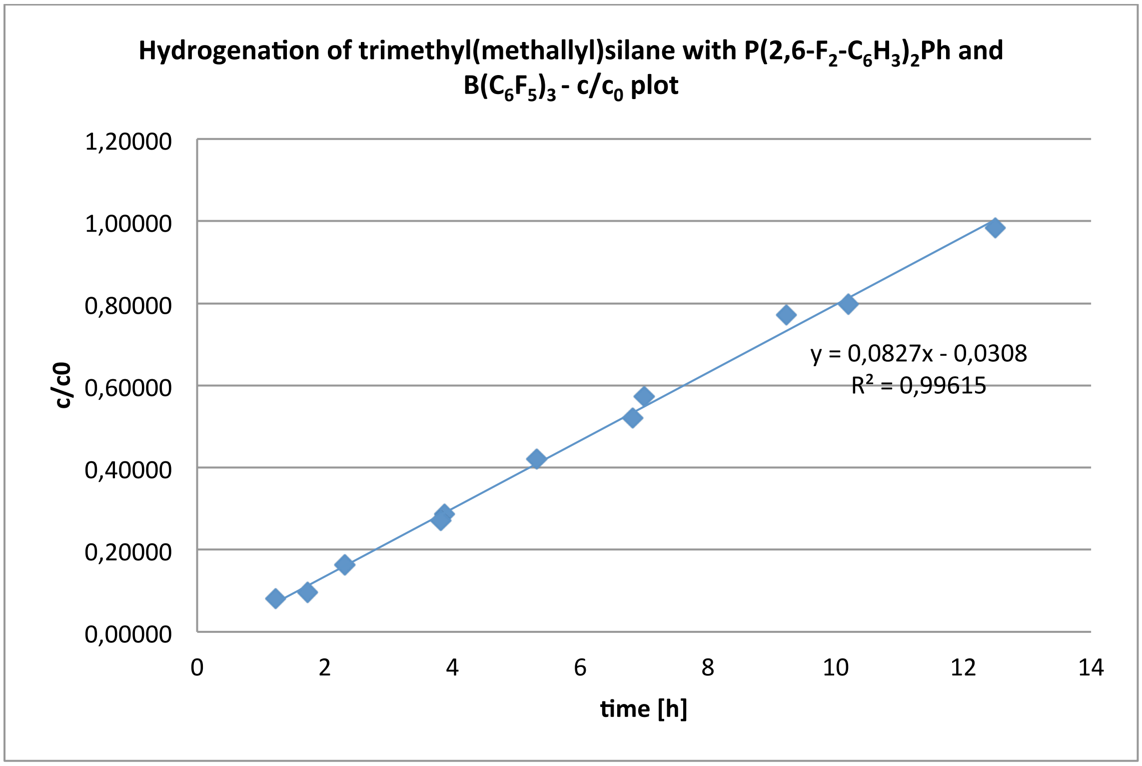

***Hydrogenation with $P(2,6\text{-}F_2\text{-}C_6H_3)_2Ph$ (6)***

| Run | TMAS [mg, mmol] | $P(2,6\text{-}F_2\text{-}C_6H_3)_2Ph$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| V 1 | 6.4, 0.050 | 3.2, 0.010 | 5.1, 0.010 | 0.45 |
| V 2 | 6.4, 0.050 | 3.4, 0.010 | 5.1, 0.010 | 0.45 |

| run ID | Substrate $^1$H Integral | Product $^1$H Integral | conv. [%] | time [h] | "($Int_{Prod}/Int_{Substr.}+Int_{Prod.}$)" |
|---|---|---|---|---|---|
| V run 1-1 | 1,0000 | 0,1063 | 9,6 | 1,73 | 0,09609 |
| V run 1-2 | 1,0000 | 0,4002 | 28,6 | 3,88 | 0,28582 |
| V run 1-3 | 1,0000 | 0,7260 | 42,1 | 5,32 | 0,42063 |
| V run 1-4 | 1,0000 | 1,3441 | 57,3 | 7 | 0,57340 |
| V run 1-5 | 1,0000 | 3,3639 | 77,1 | 9,23 | 0,77085 |
| | | | | | |
| V run 2-1 | 1,0000 | 0,0867 | 8,0 | 1,233 | 0,07978 |
| V run 2-2 | 1,0000 | 0,1943 | 16,3 | 2,317 | 0,16269 |
| V run 2-3 | 1,0000 | 0,3699 | 27,0 | 3,817 | 0,27002 |
| V run 2-4 | 1,0000 | 1,0814 | 52,0 | 6,817 | 0,51955 |
| V run 2-5 | 1,0000 | 3,9420 | 79,8 | 10,200 | 0,79765 |
| V run 2-6 | 1,0000 | 60,0000 | 98,4 | 12,500 | 0,98361 |


Hydrogenation of trimethyl(methallyl)silane with P(2,6-F2-C6H3)2Ph and B(C6F5)3 - 2 runs
conversion [%]
120,0
100,0
80,0
60,0
40,0
20,0
0,0
0
2
4
6
8
10
12
14
time [h]

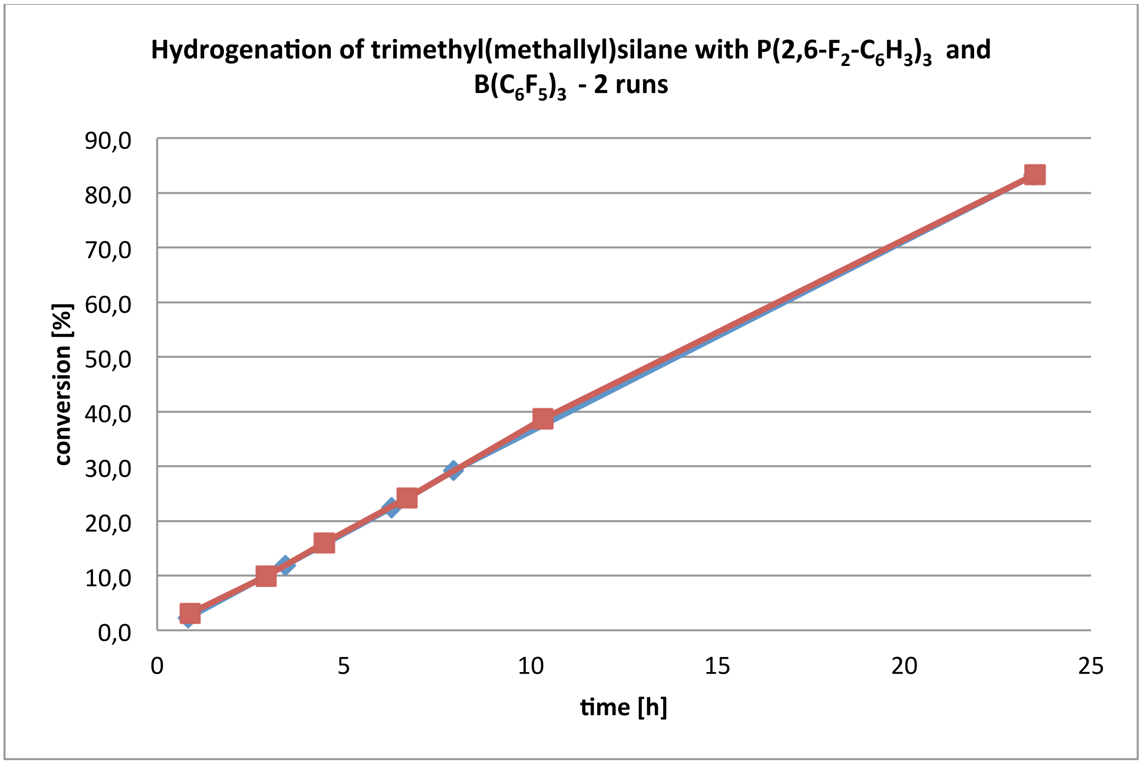

Hydrogenation of trimethyl(methallyl)silane with P(2,6-F2-C6H3)2Ph and B(C6F5)3
conversion [%]
120,0
100,0
80,0
60,0
40,0
20,0
0,0
0
2
4
6
8
10
12
14
time [h]

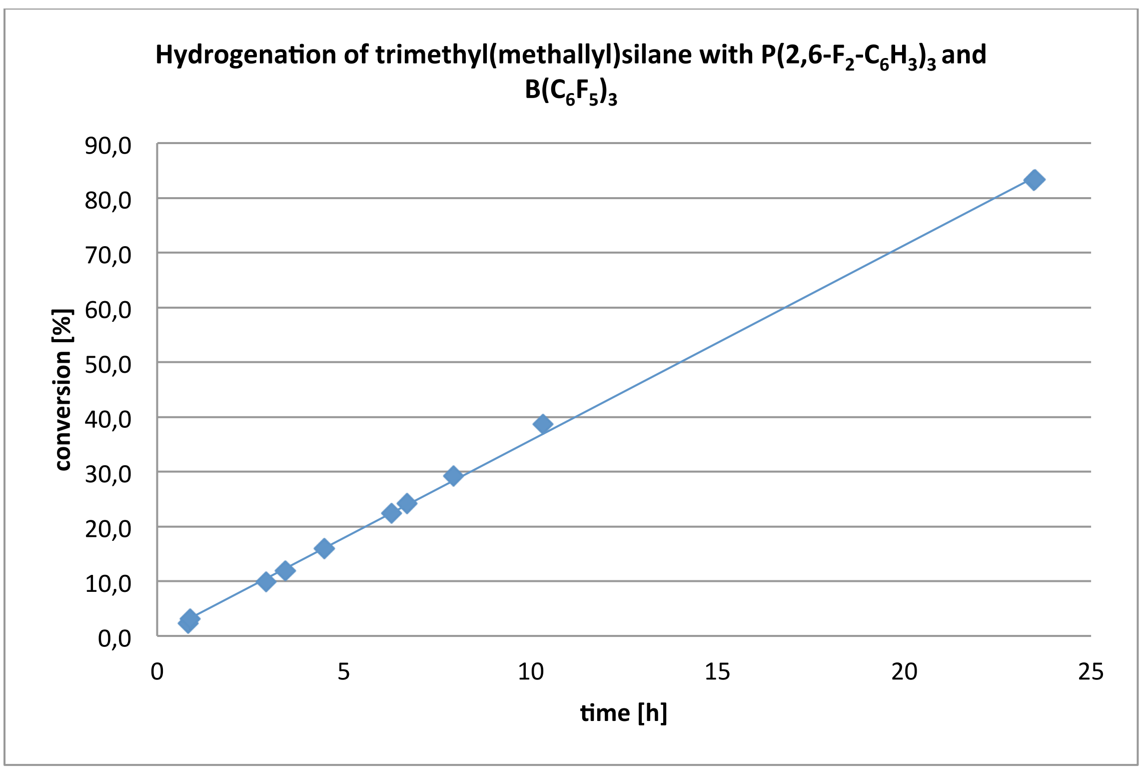


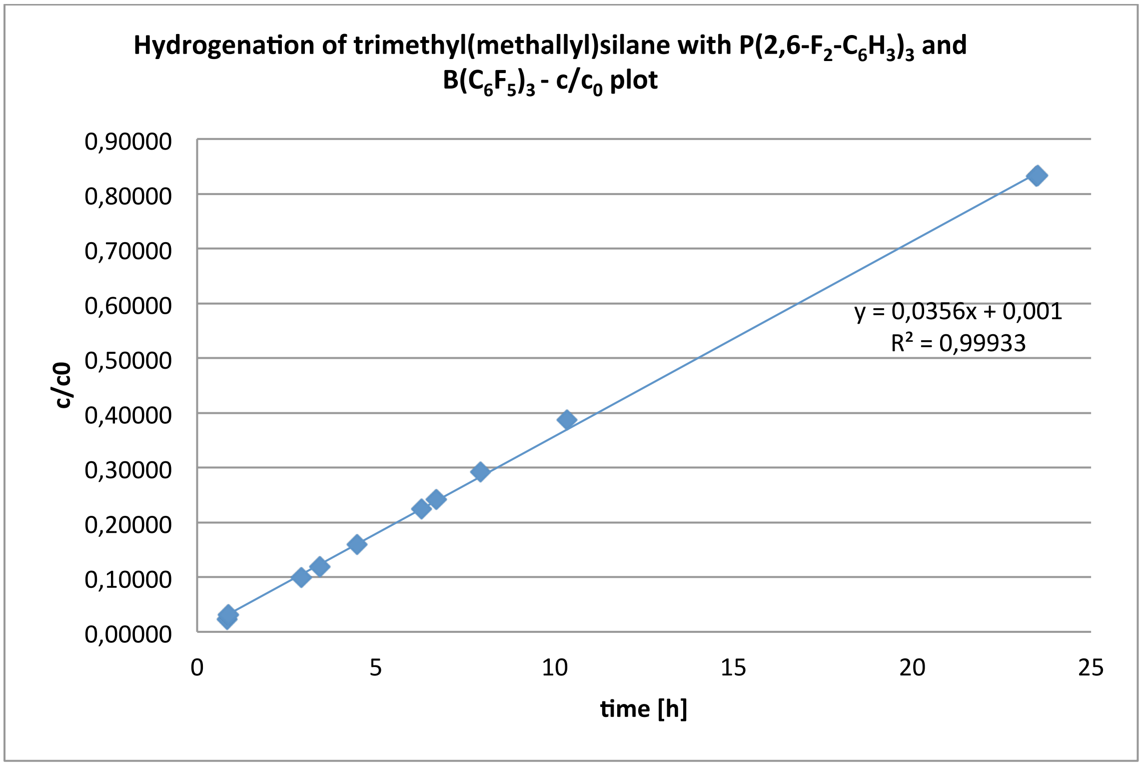

***Hydrogenation with $P(2,6\text{-}F_2\text{-}C_6H_3)_3$ (7)***

| Run | TMAS [mg, mmol] | $P(2,6\text{-}F_2\text{-}C_6H_3)_3$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| VI 1 | 6.4, 0.050 | 3.7, 0.010 | 5.2, 0.010 | 0.45 |
| VI 2 | 6.4, 0.050 | 3.7, 0.010 | 5.2, 0.010 | 0.45 |

| run ID | Substrate $^1$H Integral | Product $^1$H Integral | conversion [%] | time [h] | "($Int_{Prod}/Int_{Substr.}+Int_{Prod.}$)" |
|---|---|---|---|---|---|
| VI run 1-1 | 1,0000 | 0,0235 | 2,3 | 0,83 | 0,02296 |
| VI run 1-2 | 1,0000 | 0,1353 | 11,9 | 3,43 | 0,11918 |
| VI run 1-3 | 1,0000 | 0,2892 | 22,4 | 6,28 | 0,22433 |
| VI run 1-4 | 1,0000 | 0,4126 | 29,2 | 7,93 | 0,29209 |
| VI run 1-5 | 1,0000 | 4,9640 | 83,2 | 23,47 | 0,83233 |
| | | | | | |
| VI run 2-1 | 1,0000 | 0,0319 | 3,1 | 0,88 | 0,03091 |
| VI run 2-2 | 1,0000 | 0,1104 | 9,9 | 2,92 | 0,09942 |
| VI run 2-3 | 1,0000 | 0,1900 | 16,0 | 4,47 | 0,15966 |
| VI run 2-4 | 1,0000 | 0,3193 | 24,2 | 6,68 | 0,24202 |
| VI run 2-5 | 1,0000 | 0,6304 | 38,7 | 10,33 | 0,38665 |
| VI run 2-6 | 1,0000 | 4,9846 | 83,3 | 23,5 | 0,83290 |


Hydrogenation of trimethyl(methallyl)silane with P(2,6-F2-C6H3)3 and B(C6F5)3 - 2 runs
conversion [%]
time [h]
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0
5
10
15
20
25

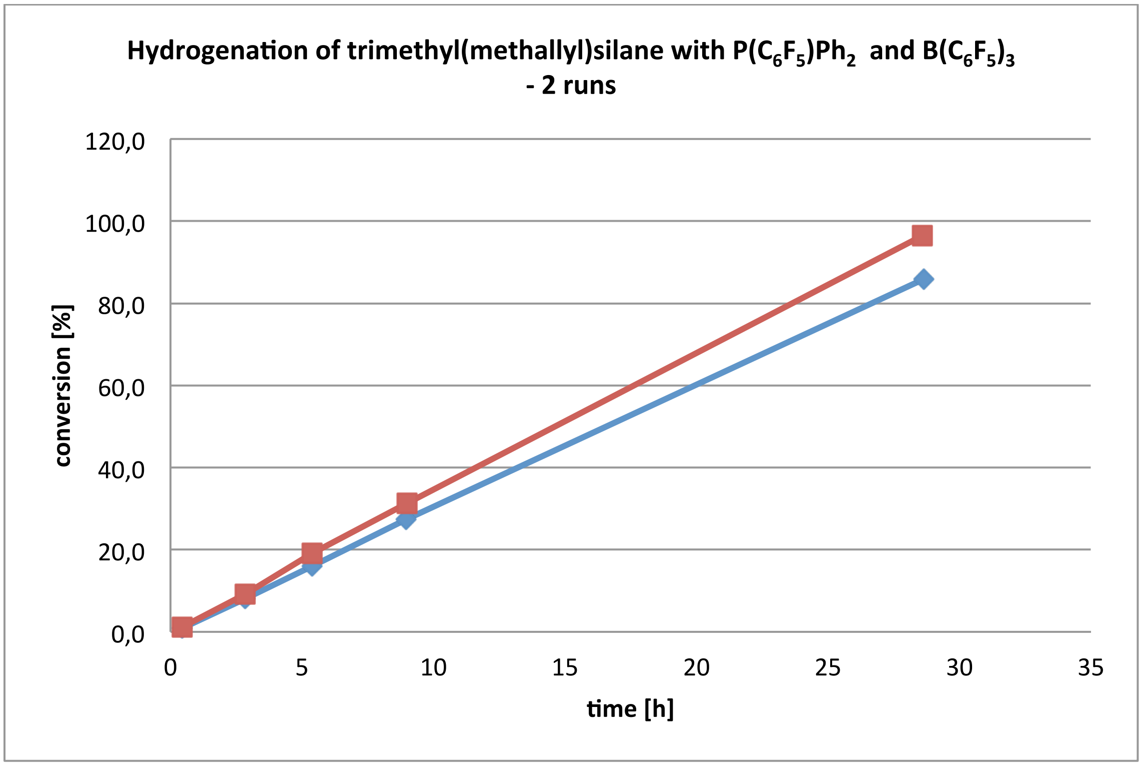

Hydrogenation of trimethyl(methallyl)silane with P(2,6-F2-C6H3)3 and B(C6F5)3
conversion [%]
time [h]
90,0
80,0
70,0
60,0
50,0
40,0
30,0
20,0
10,0
0,0
0
5
10
15
20
25

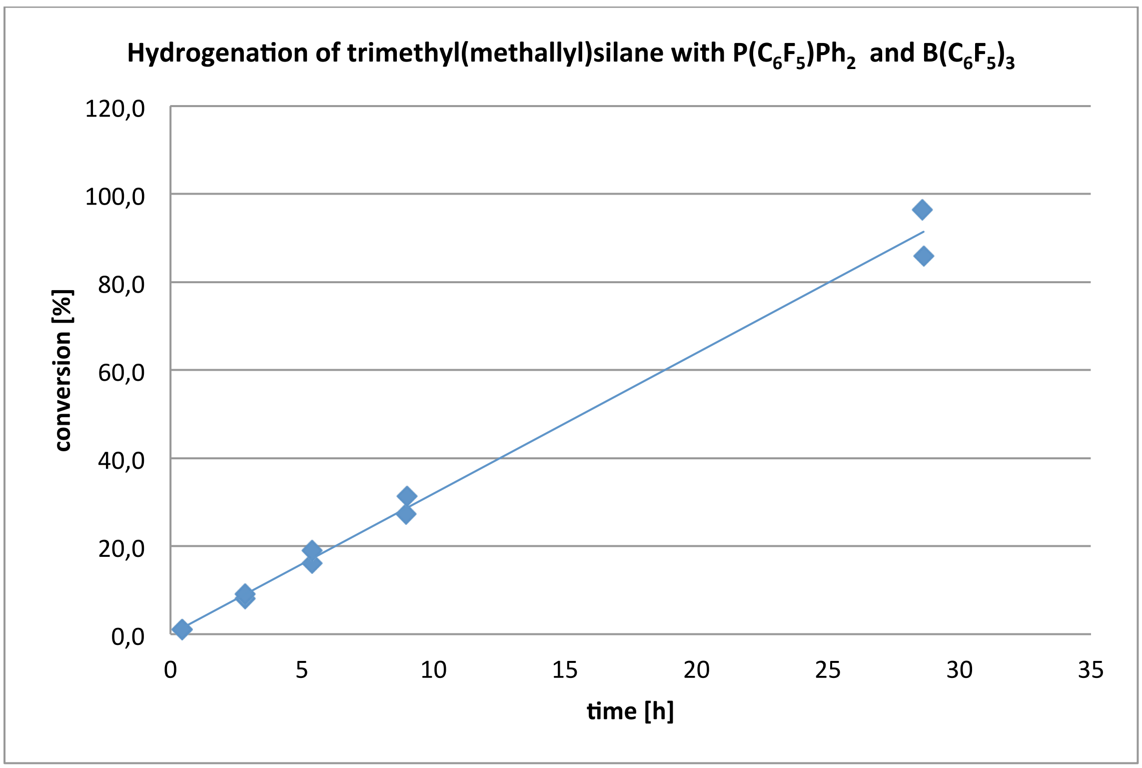


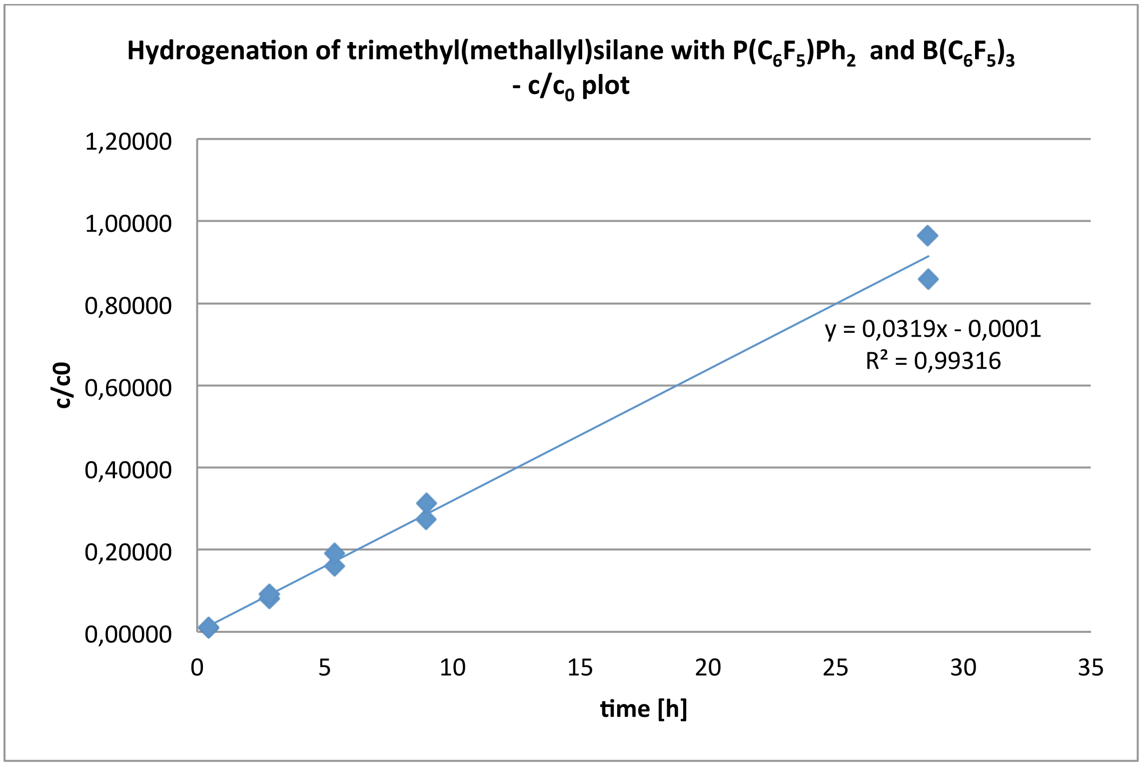

***Hydrogenation with $P(C_6F_5)Ph_2$* (8)**

| Run | TMAS [mg, mmol] | $P(C_6F_5)Ph_2$ [mg, mmol] | $B(C_6F_5)_3$ [mg, mmol] | $CD_2Cl_2$ [ml] |
|---|---|---|---|---|
| VII 1 | 6.4, 0.050 | 3.6, 0.010 | 5.3, 0.010 | 0.45 |
| VII 2 | 6.4, 0.050 | 3.4, 0.010 | 5.1, 0.010 | 0.45 |

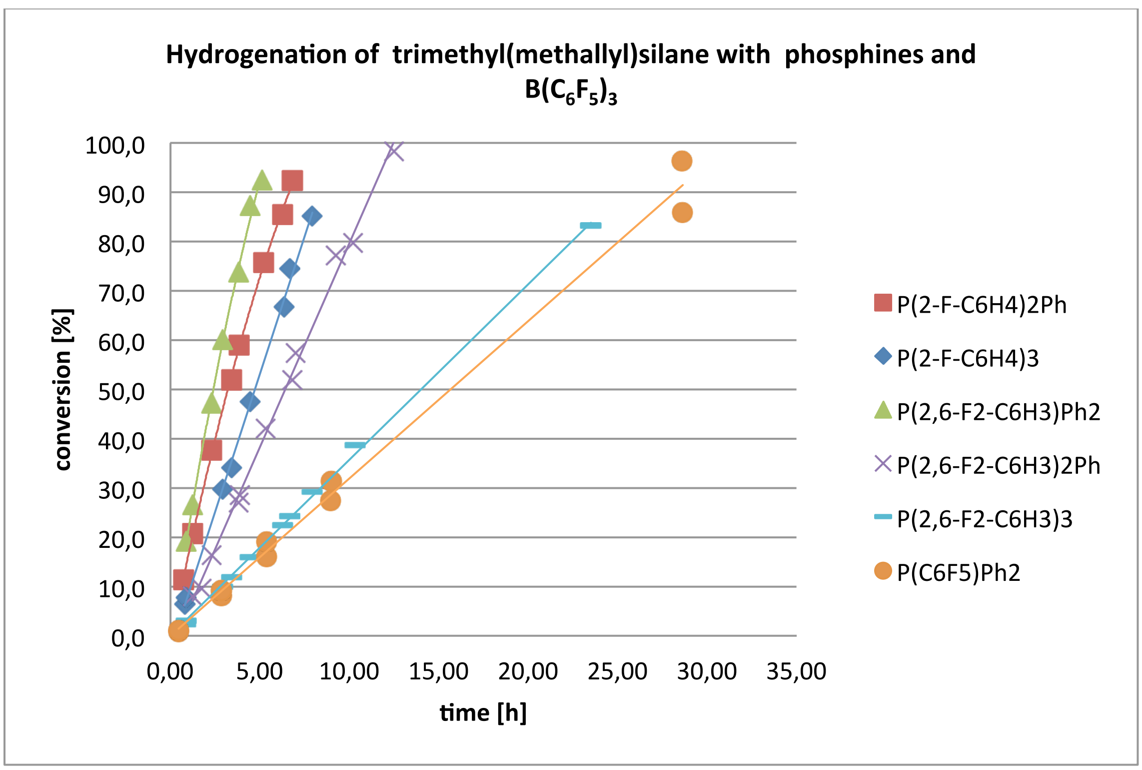
| run ID | Substrate $^1$H Integral | Product $^1$H Integral | conversion [%] | time [h] | "$(Int_{Prod}/Int_{Substr.}+Int_{Prod.})$" |
|---|---|---|---|---|---|
| VII run 1-1 | 1,0000 | 0,0091 | 0,9 | 0,45 | 0,00902 |
| VII run 1-2 | 1,0000 | 0,0879 | 8,1 | 2,833 | 0,08080 |
| VII run 1-3 | 1,0000 | 0,1913 | 16,1 | 5,383 | 0,16058 |
| VII run 1-4 | 1,0000 | 0,3762 | 27,3 | 8,967 | 0,27336 |
| VII run 1-5 | 1,0000 | 6,0897 | 85,9 | 28,633 | 0,85895 |
| | | | | | |
| VII run 2-1 | 1,0000 | 0,0112 | 1,1 | 0,45 | 0,01108 |
| VII run 2-2 | 1,0000 | 0,1011 | 9,2 | 2,833 | 0,09182 |
| VII run 2-3 | 1,0000 | 0,2356 | 19,1 | 5,383 | 0,19068 |
| VII run 2-4 | 1,0000 | 0,4563 | 31,3 | 8,983 | 0,31333 |
| VII run 2-5 | 1,0000 | 26,9384 | 96,4 | 28,6 | 0,96421 |


Hydrogenation of trimethyl(methallyl)silane with P(C6F5)Ph2 and B(C6F5)3 - 2 runs
conversion [%]
0,0
20,0
40,0
60,0
80,0
100,0
120,0
time [h]
0
5
10
15
20
25
30
35

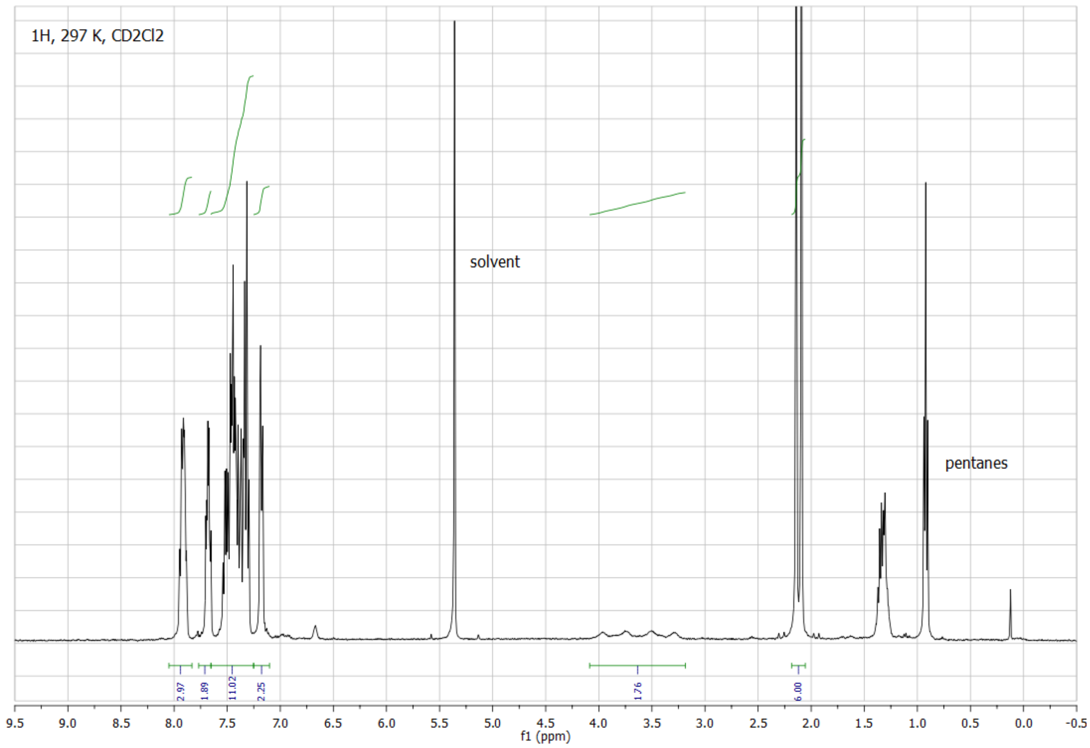

Hydrogenation of trimethyl(methallyl)silane with P(C6F5)Ph2 and B(C6F5)3
conversion [%]
0,0
20,0
40,0
60,0
80,0
100,0
120,0
time [h]
0
5
10
15
20
25
30
35

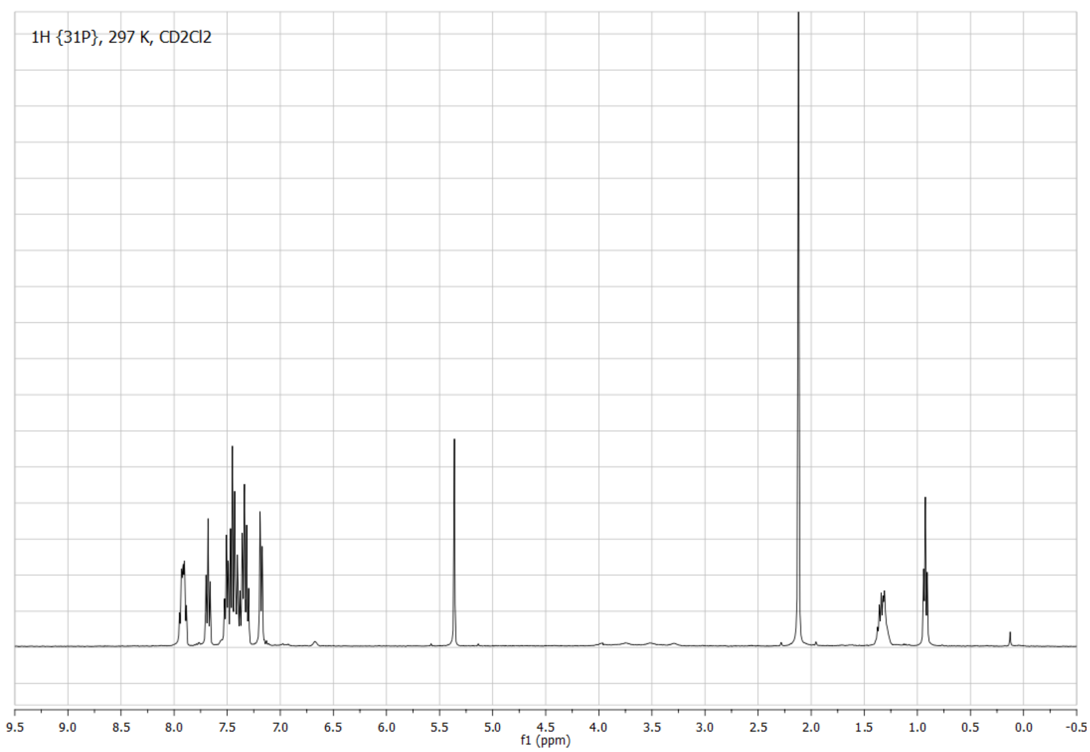


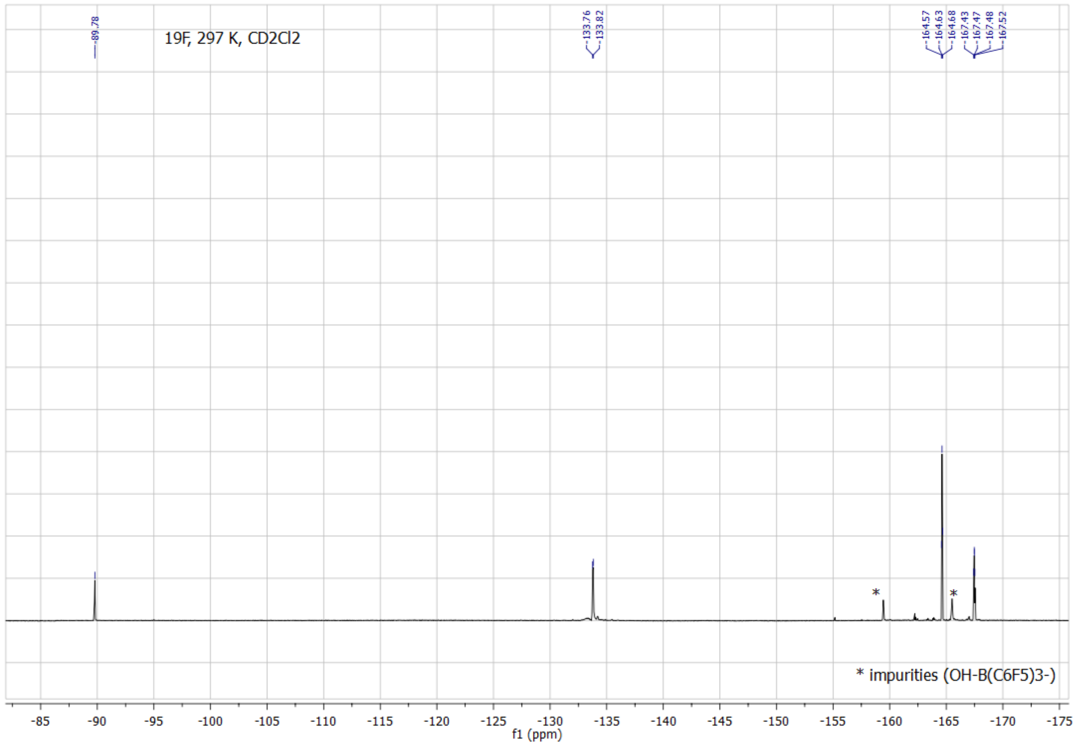

***Comparison of all phosphines in the hydrogenation of trimethyl(methallyl)silane***

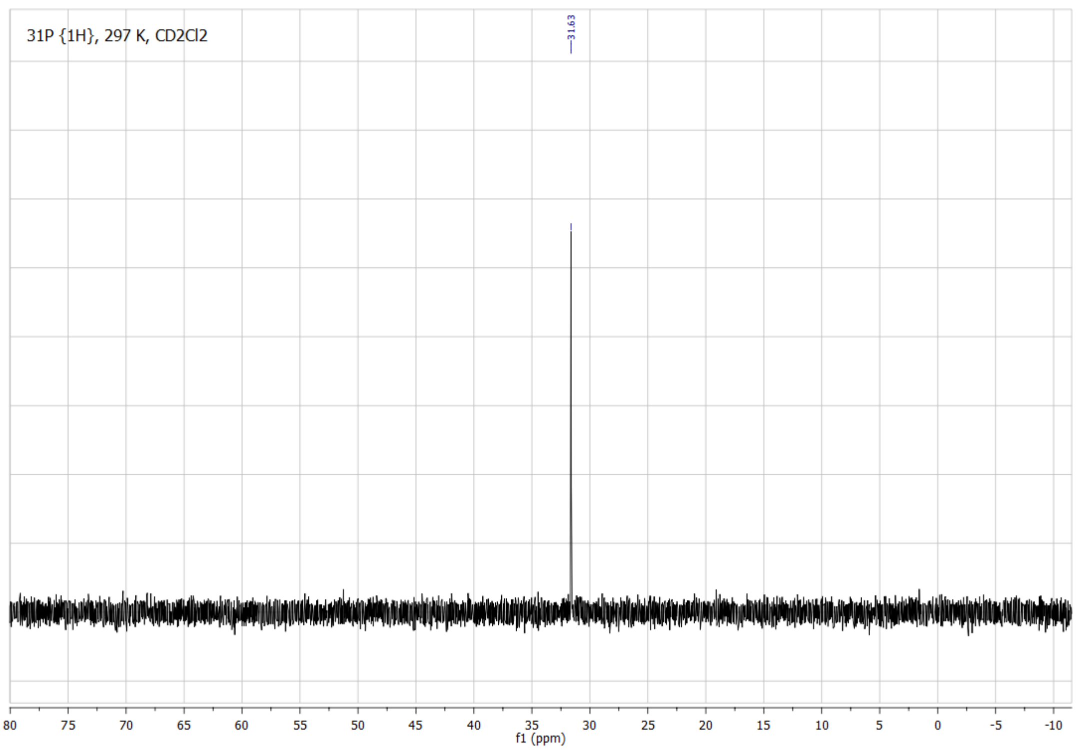


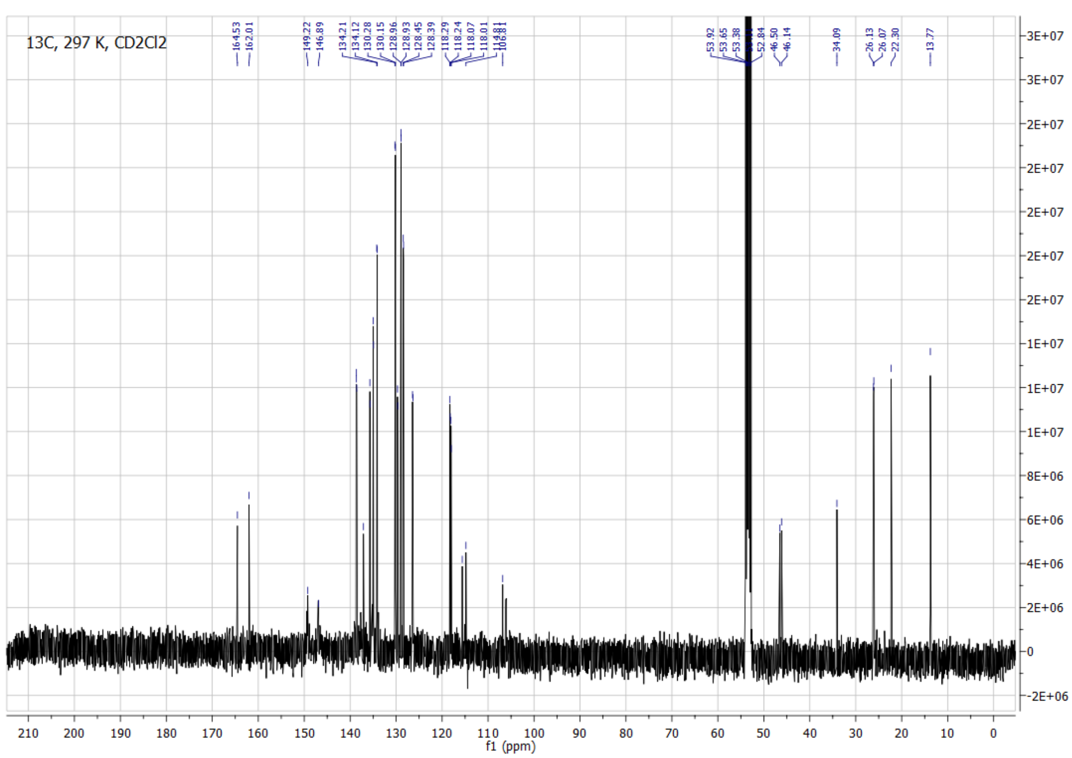
## $^{1}H$, $^{19}F$, $^{31}P$, $^{11}B$ and $^{13}C$ NMR spectra of intermediate 12

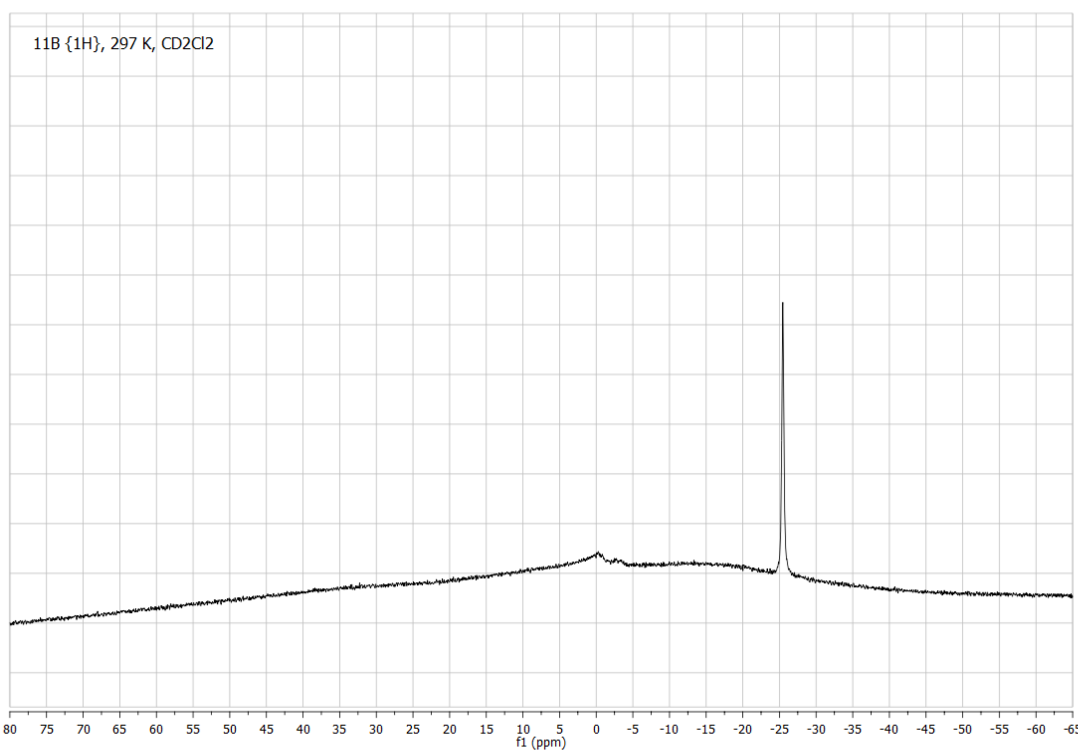


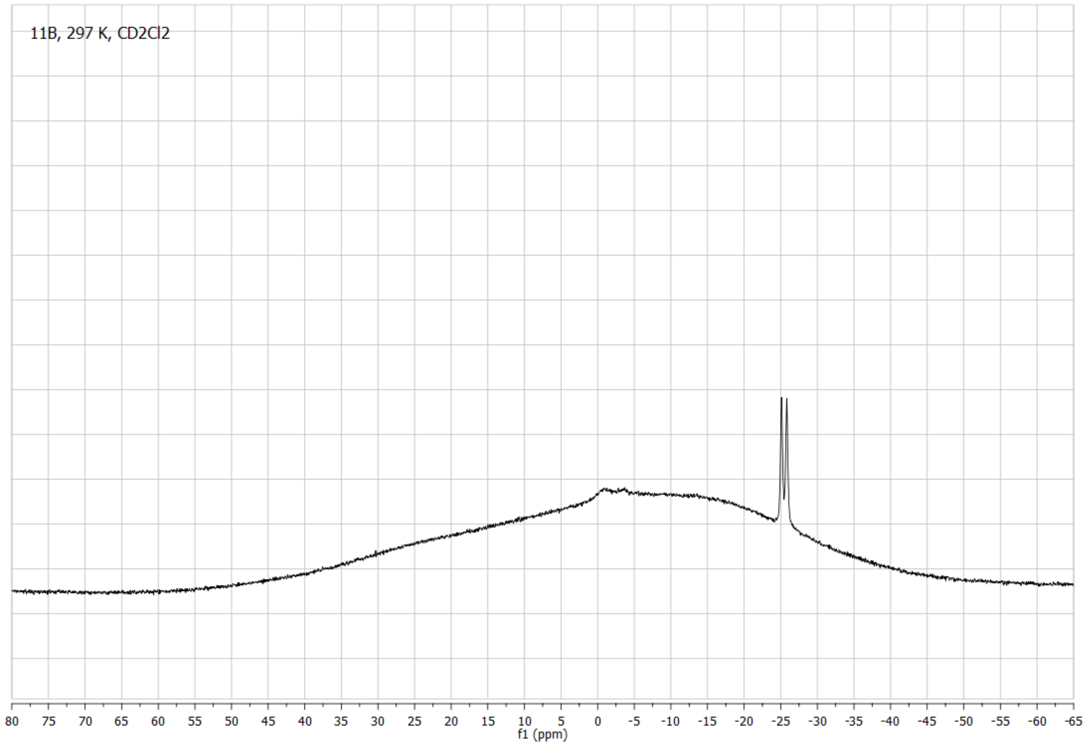




19F, 297 K, CD2Cl2
-89.78
-133.76
-133.82
-164.57
-164.63
-164.68
-167.43
-167.47
-167.48
-167.52
* impurities (OH-B(C6F5)3-)
f1 (ppm)


31P {1H}, 297 K, CD2Cl2
31.63
f1 (ppm)


13C, 297 K, CD2Cl2
f1 (ppm)

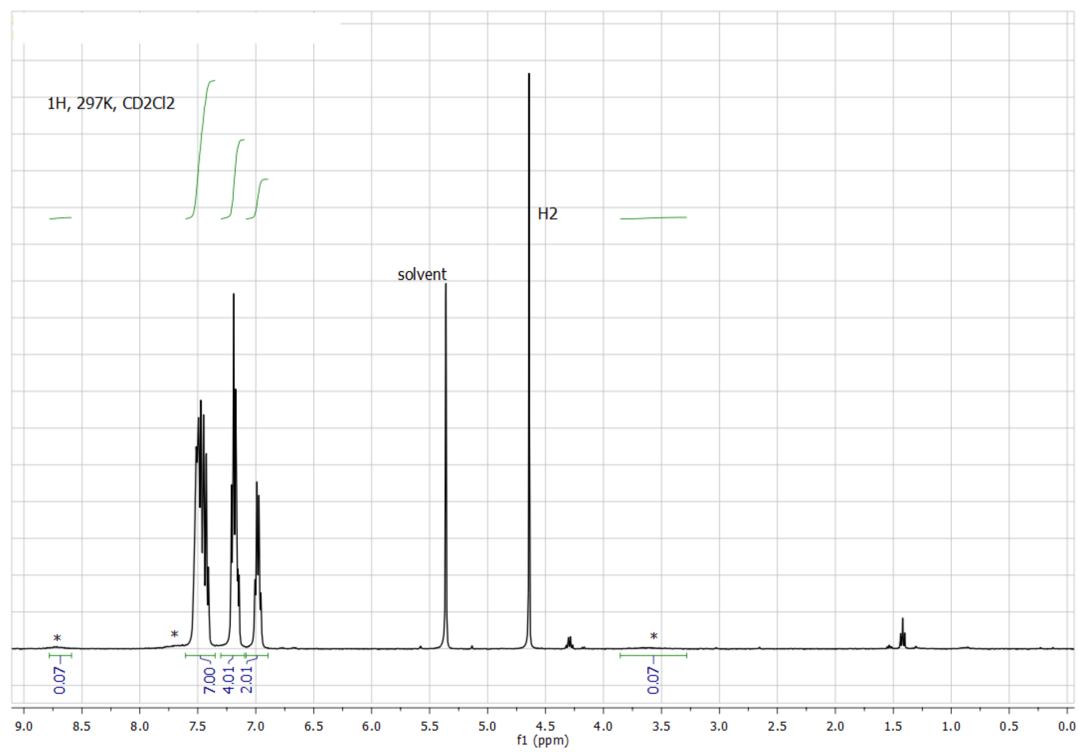

11B {1H}, 297 K, CD2Cl2
f1 (ppm)

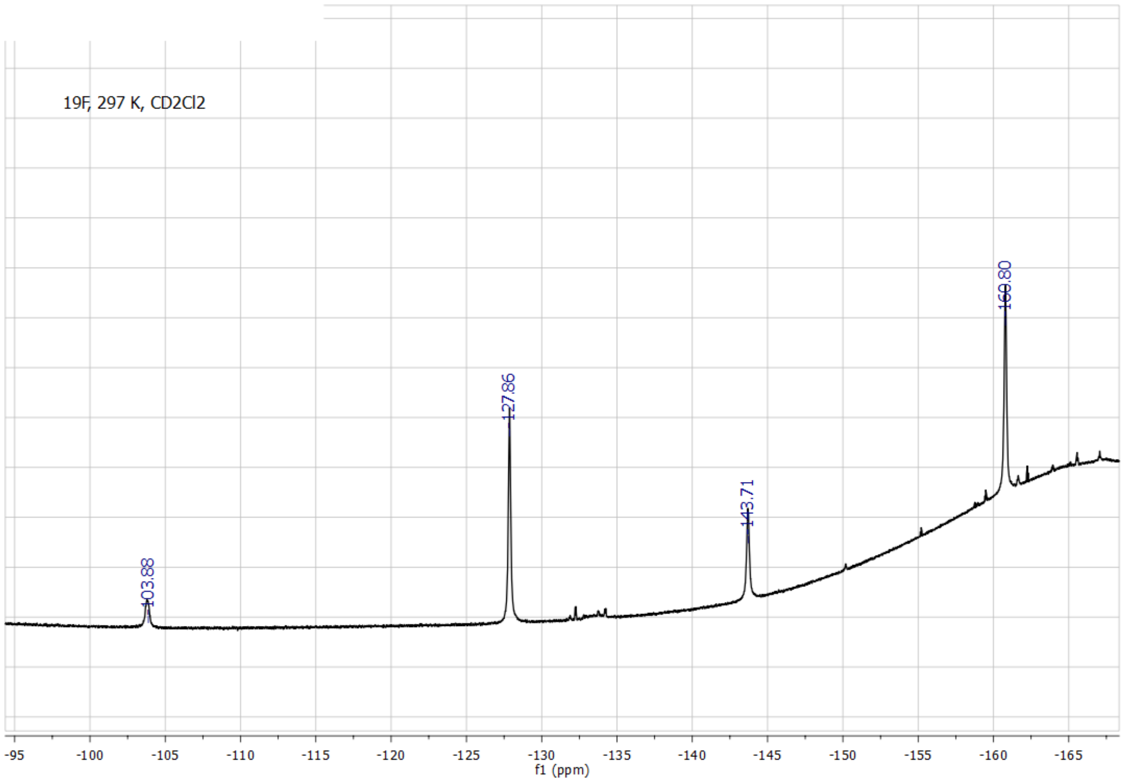


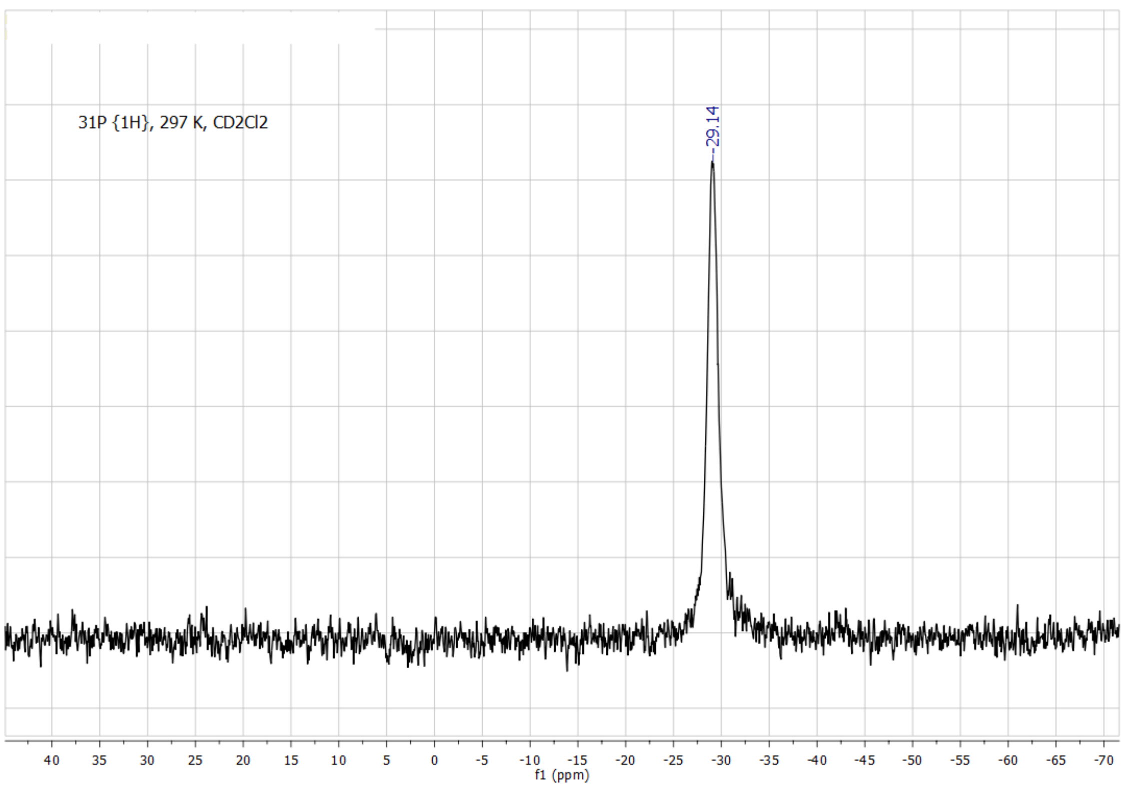

## $^{1}H$, $^{19}F$, $^{31}P$ and $^{11}B$ NMR spectra of low temperature $H_2$-activation with phosphines 3-7

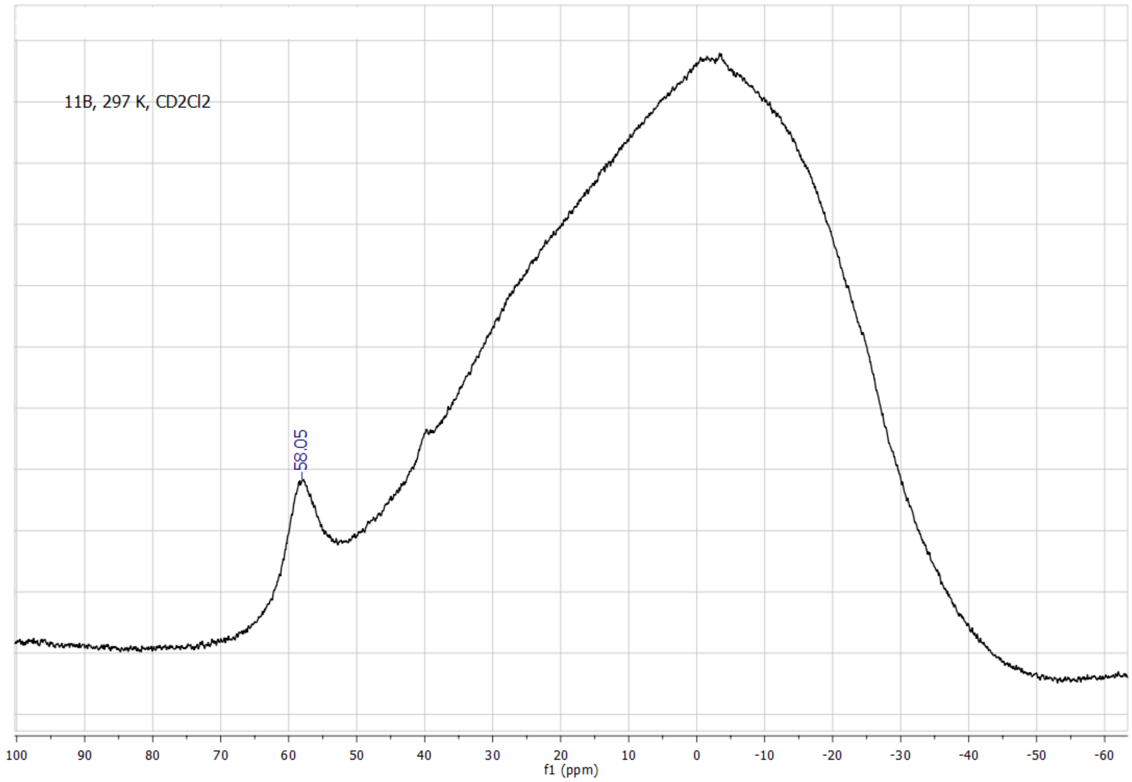
### $P(2\text{-}F\text{-}C_6H_4)_2Ph$ (3) and $B(C_6F_5)_3$ (1)

**FLP + $H_2$ at rt**

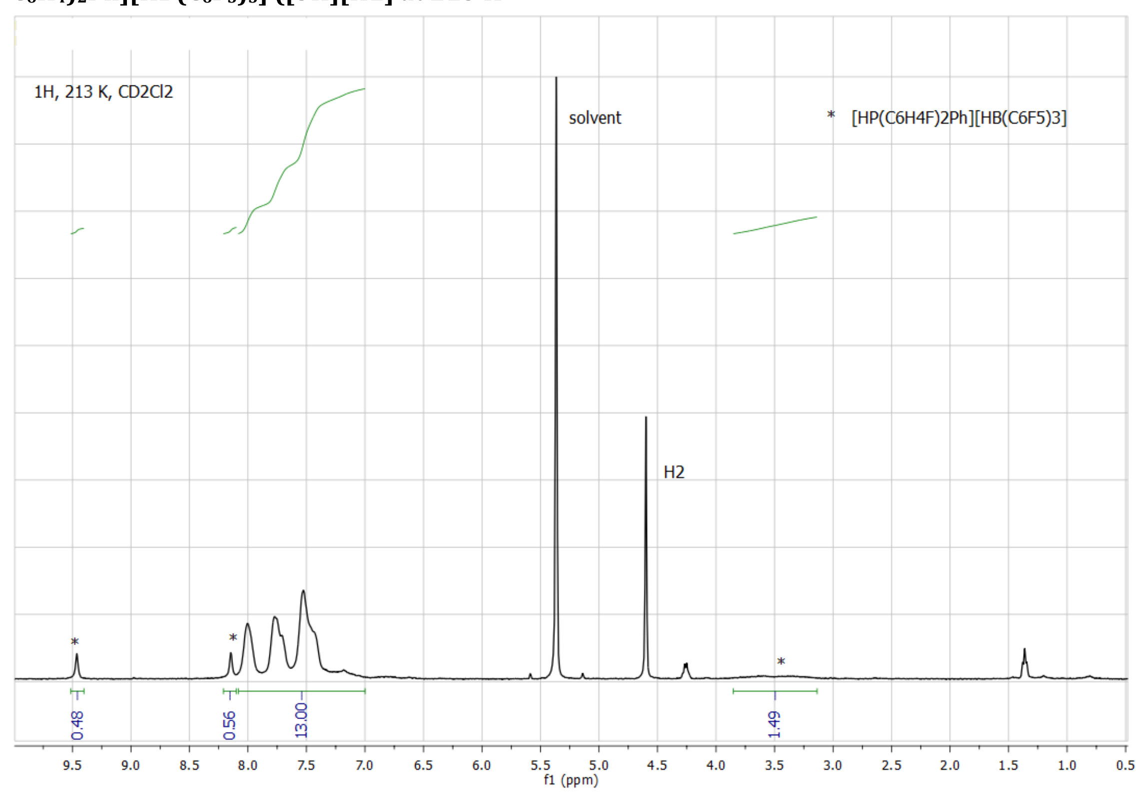


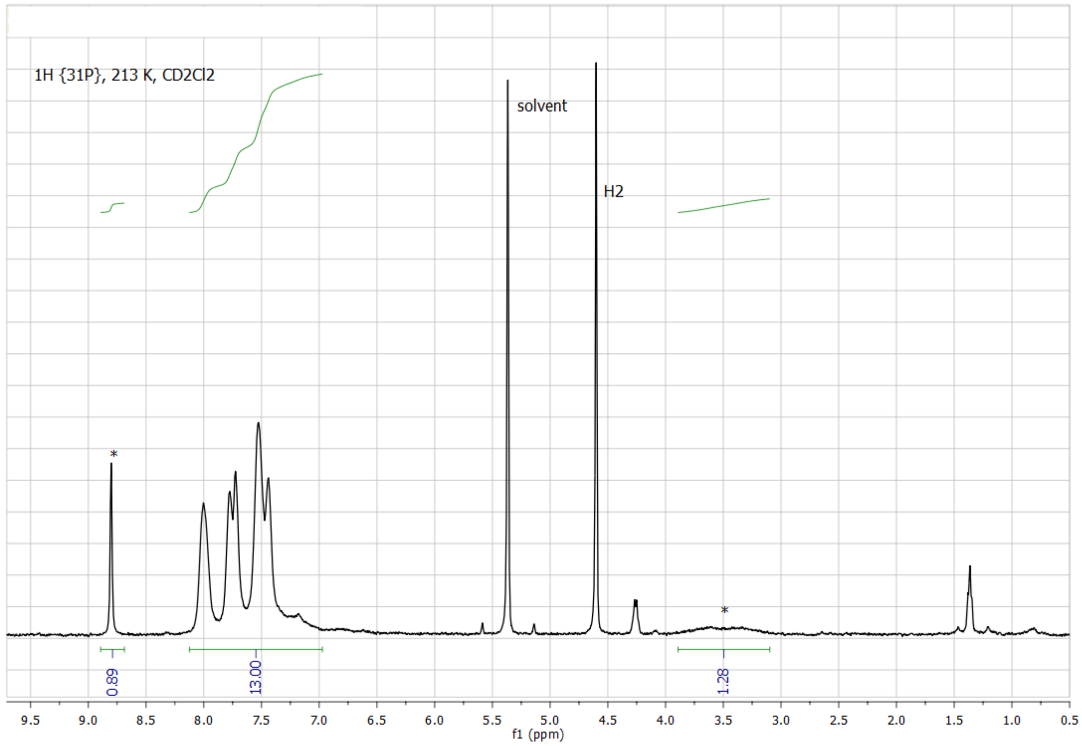

19F, 297 K, CD2Cl2
-103.88
-127.86
-143.71
-160.80
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
f1 (ppm)

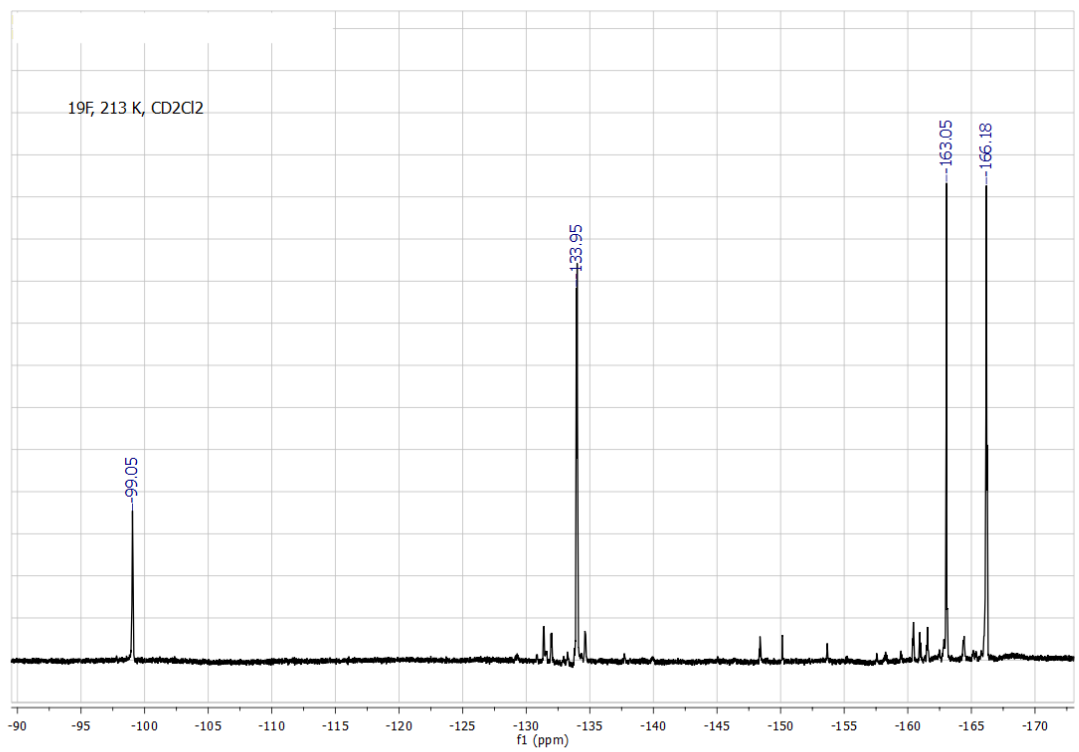

31P {1H}, 297 K, CD2Cl2
-29.14
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
f1 (ppm)

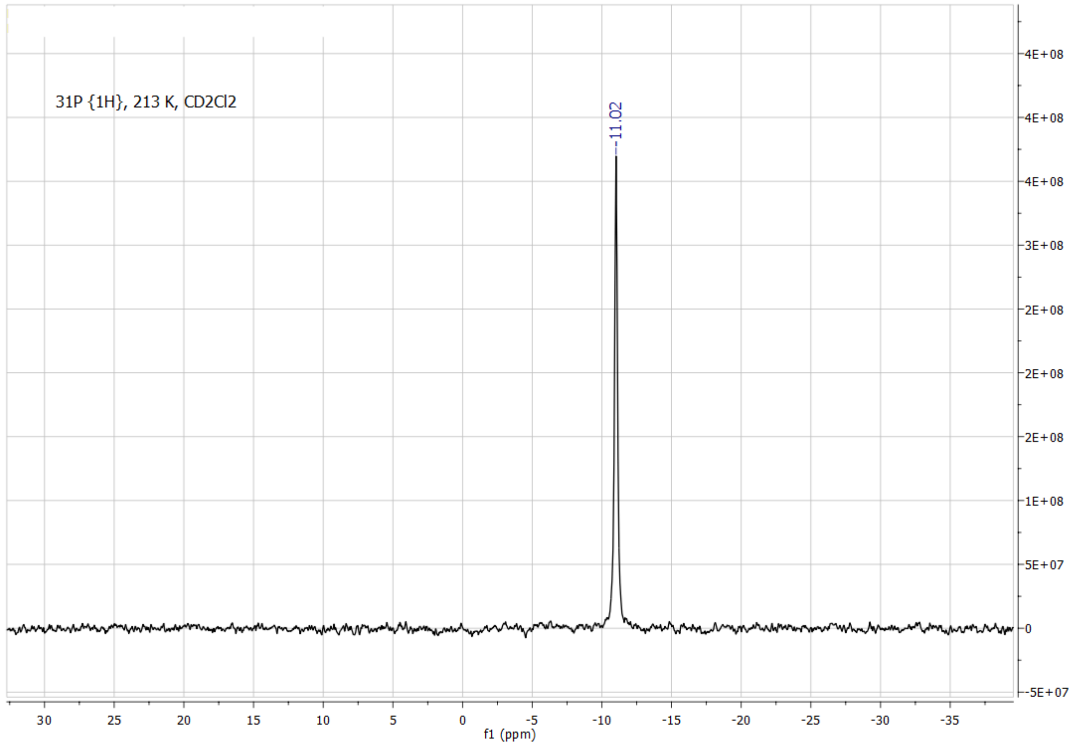


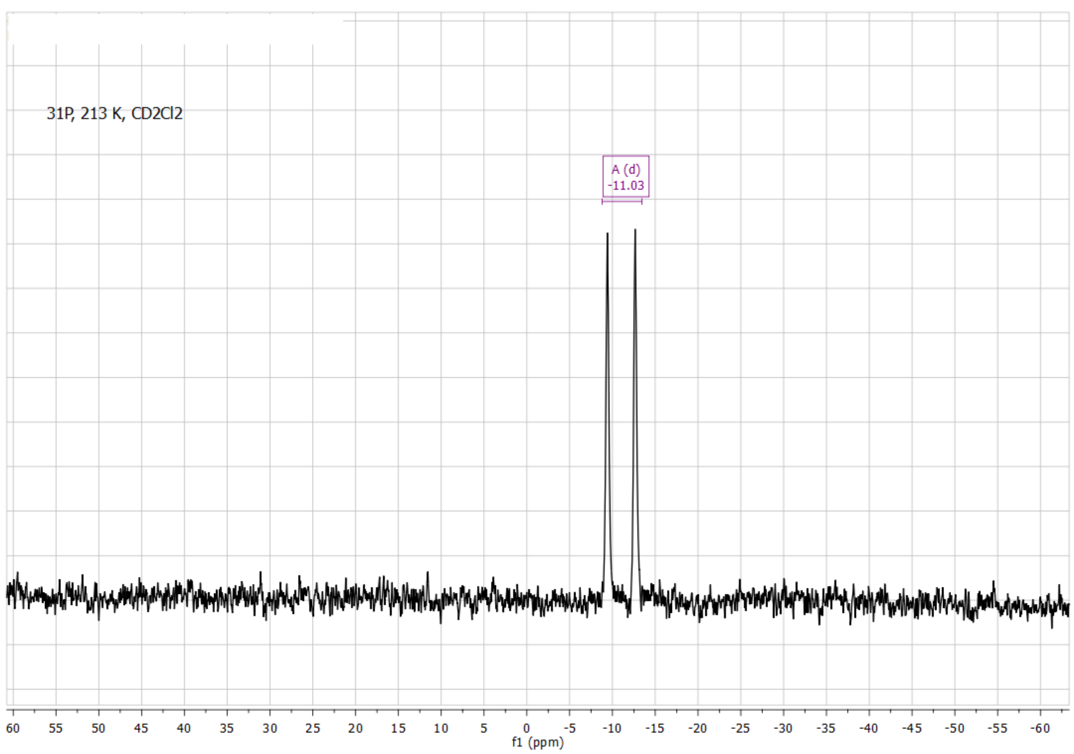

**[HP(2-F-$C_6H_4$)$_2$Ph][HB($C_6F_5$)$_3$] ([3H][H1] at 213 K**

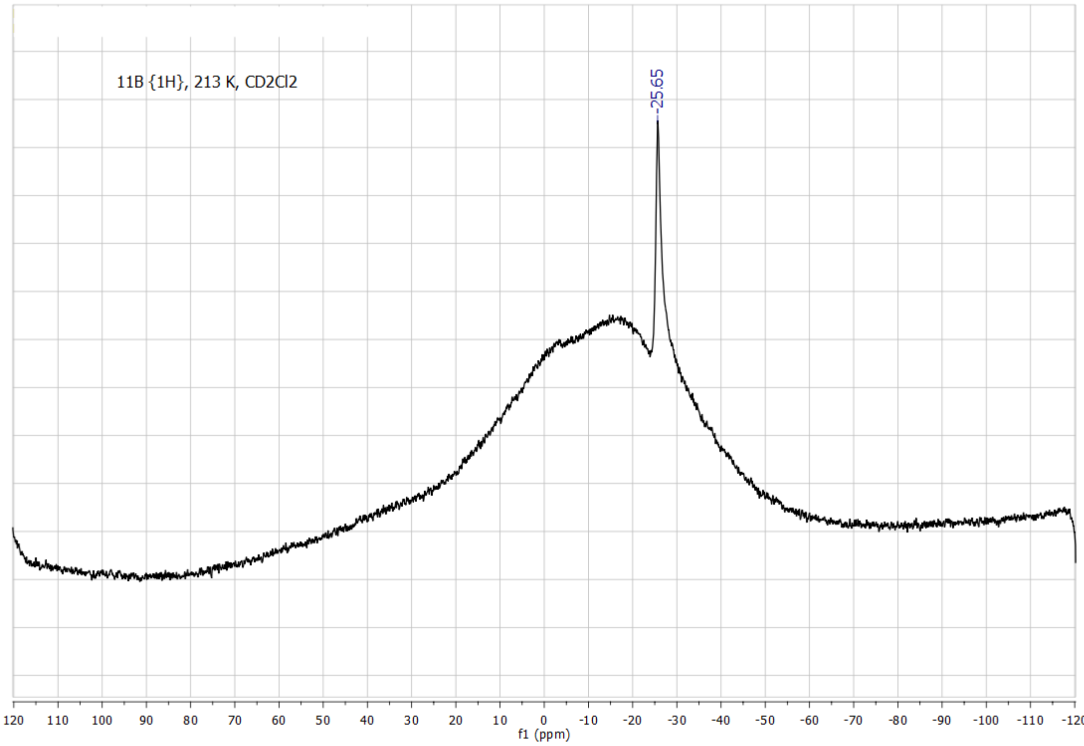


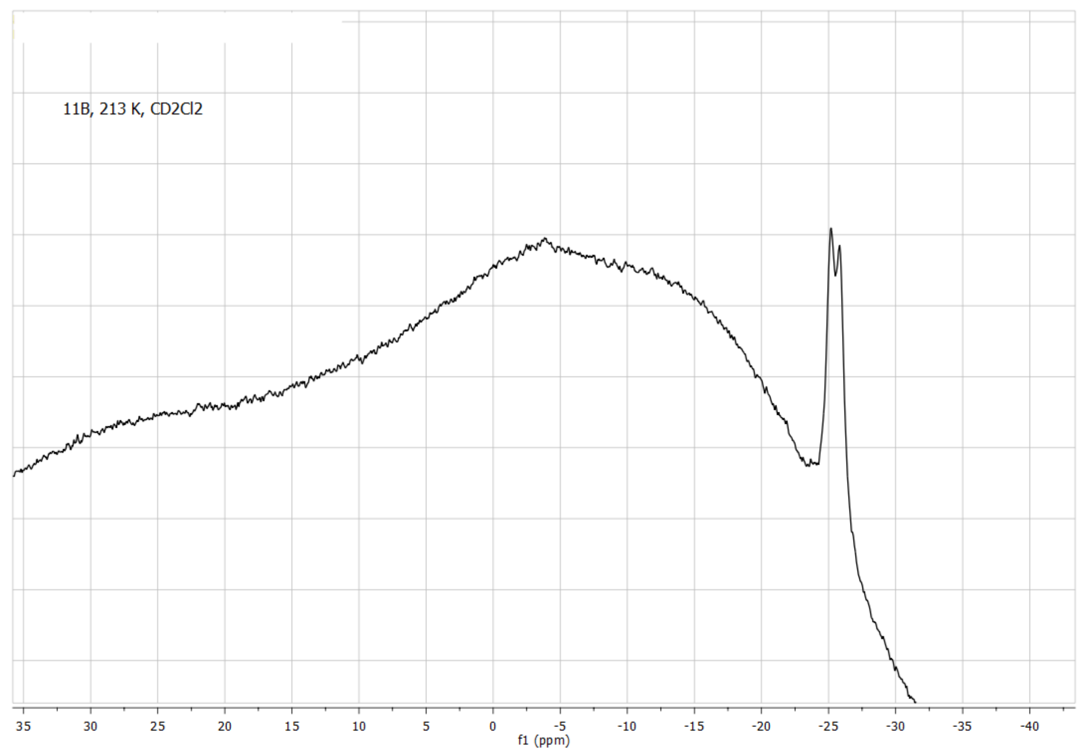

1H {31P}, 213 K, CD2Cl2
solvent
H2
*
*
0.89
13.00
1.28
f1 (ppm)


19F, 213 K, CD2Cl2
-99.05
-133.95
-163.05
-166.18
f1 (ppm)

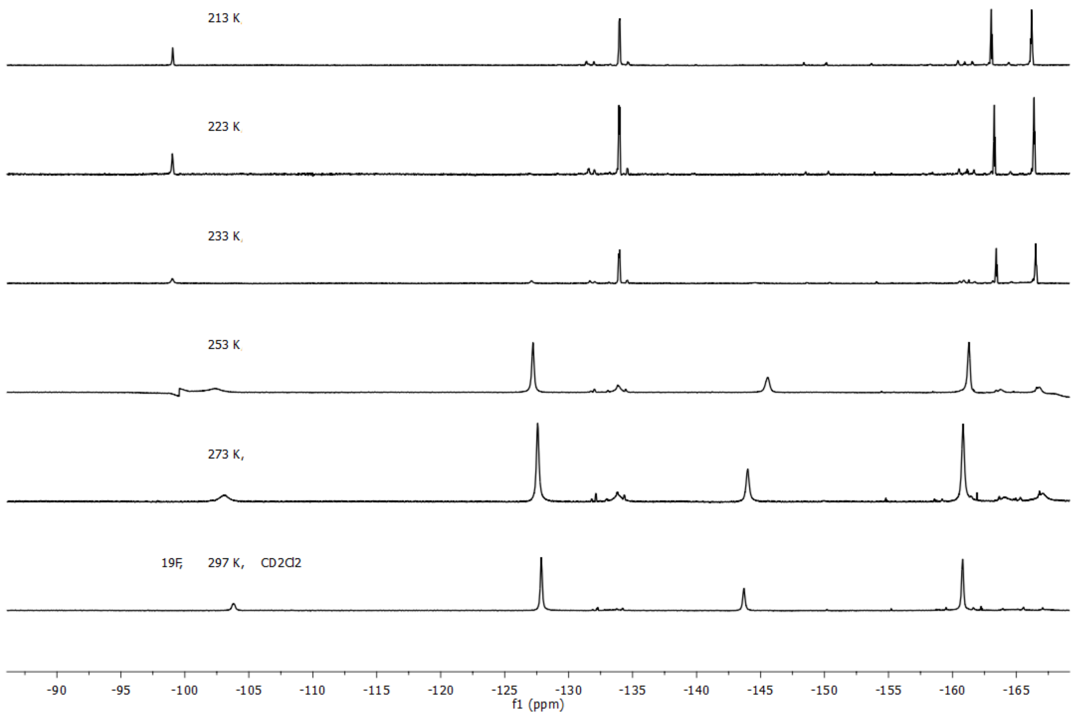

31P {1H}, 213 K, CD2Cl2
-11.02
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
f1 (ppm)

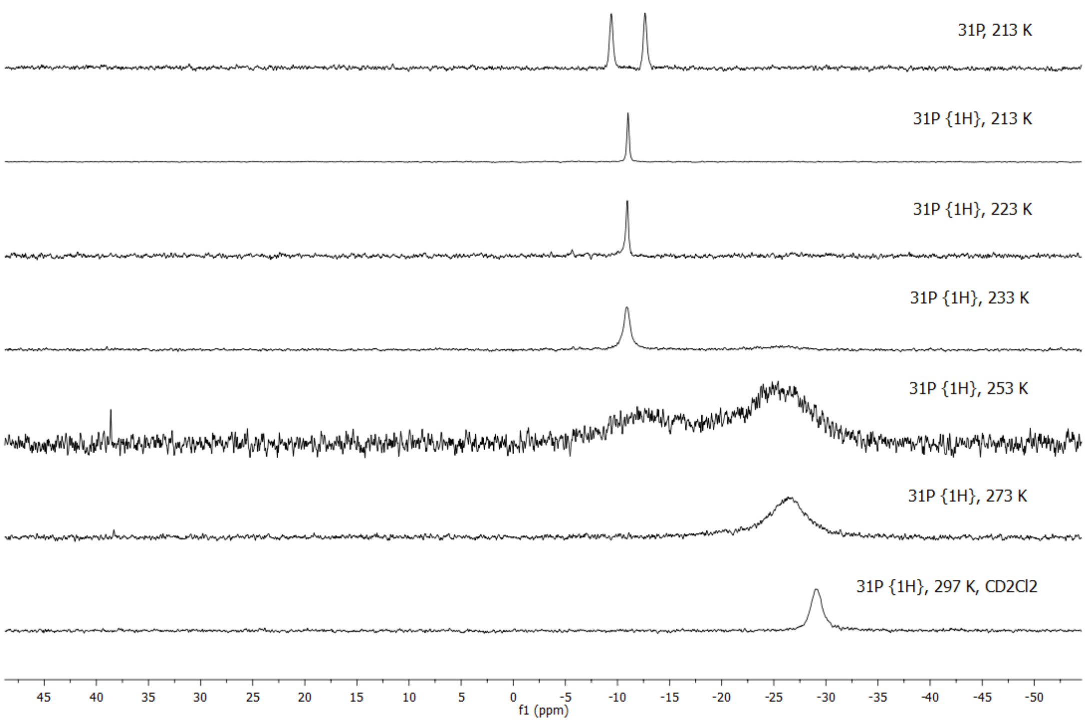

31P, 213 K, CD2Cl2
A (d)
-11.03
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
f1 (ppm)


11B {1H}, 213 K, CD2Cl2
-25.65
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120
f1 (ppm)

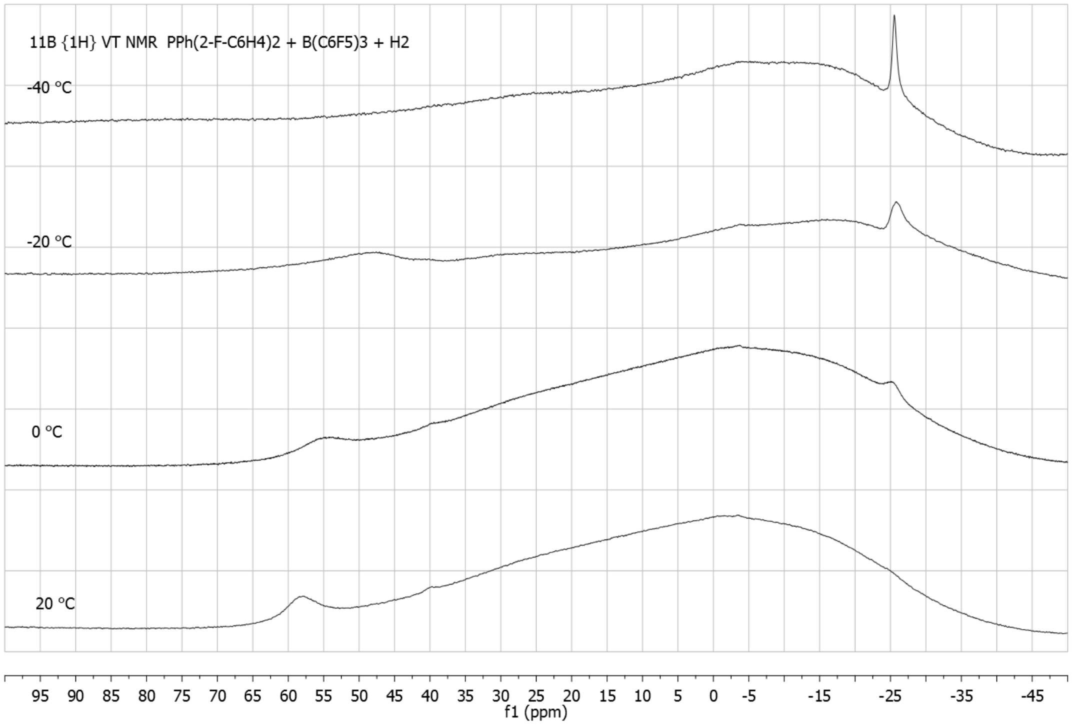

11B, 213 K, CD2Cl2
35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40
f1 (ppm)

**VT series for $P(2\text{-}F\text{-}C_6H_4)_2Ph$ (3) and $B(C_6F_5)_3$ (1)**



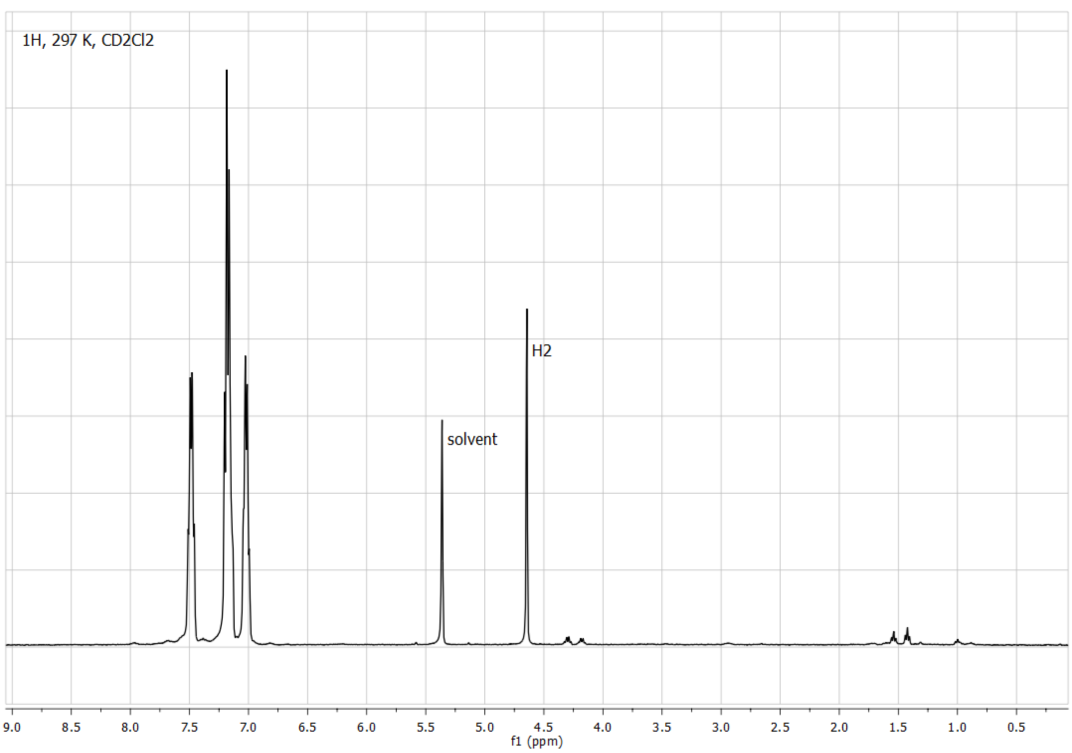



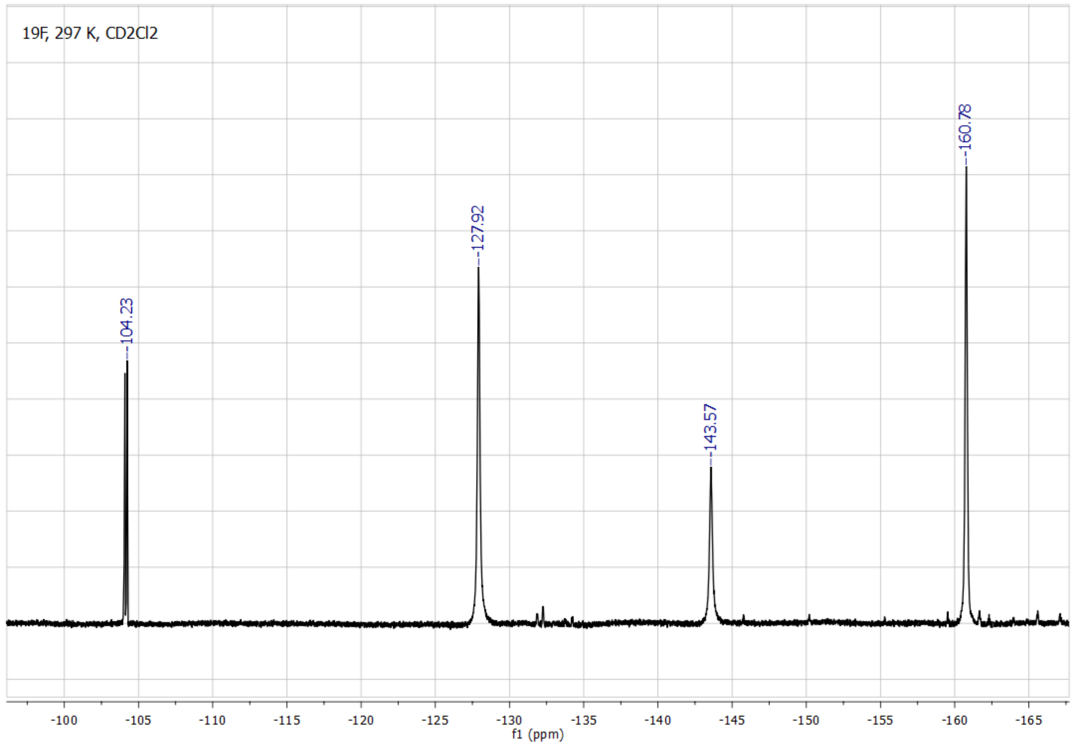
**$^{11}B$ NMR spectrum at highest measured temperature with detectable $HB(C_6F_5)_3$ species with 3 ("activation temperature")**

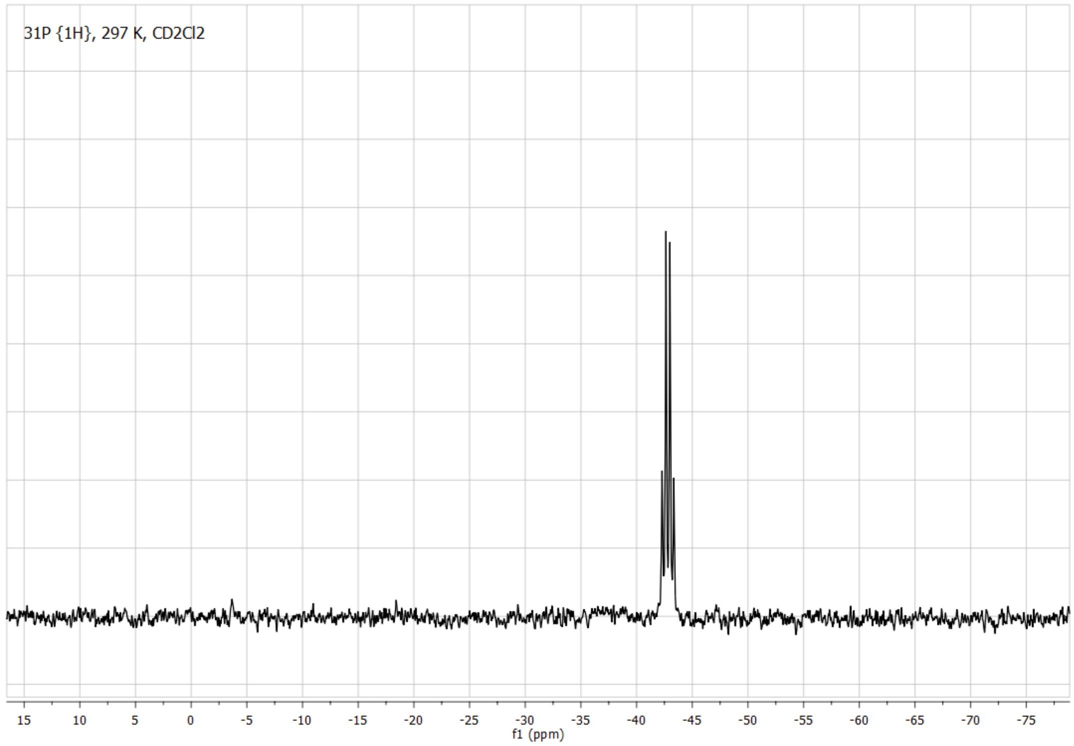


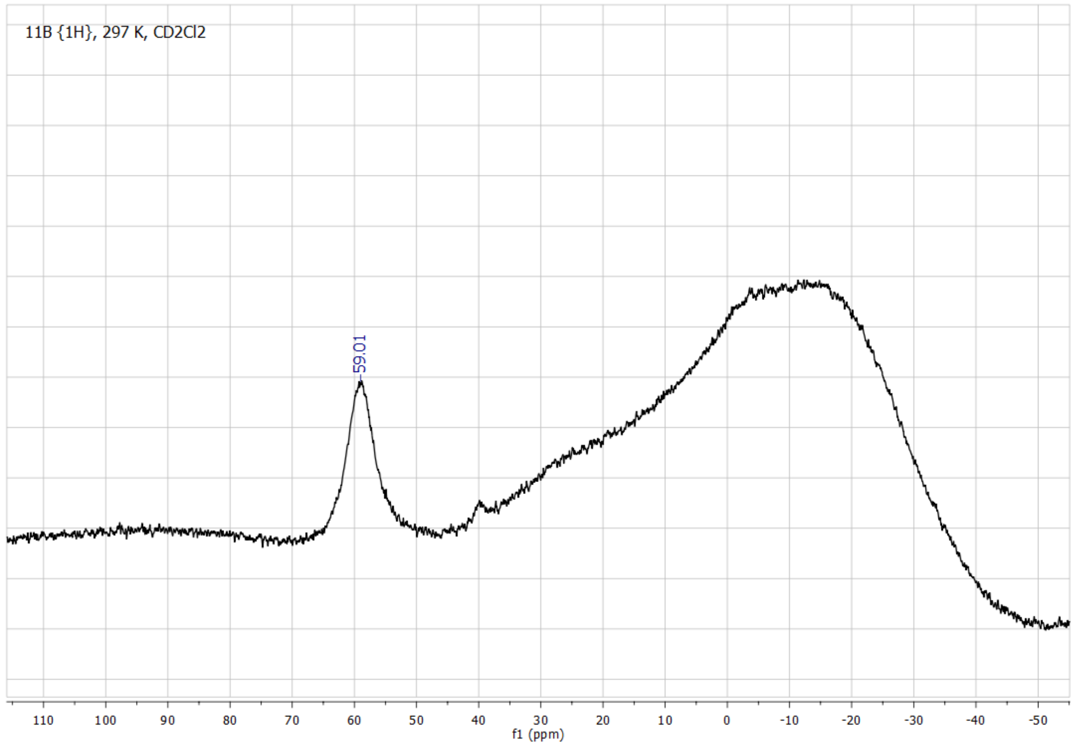

## $P(2\text{-}F\text{-}C_6H_4)_3$ (4) and $B(C_6F_5)_3$ (1)

**FLP + $H_2$ at rt**

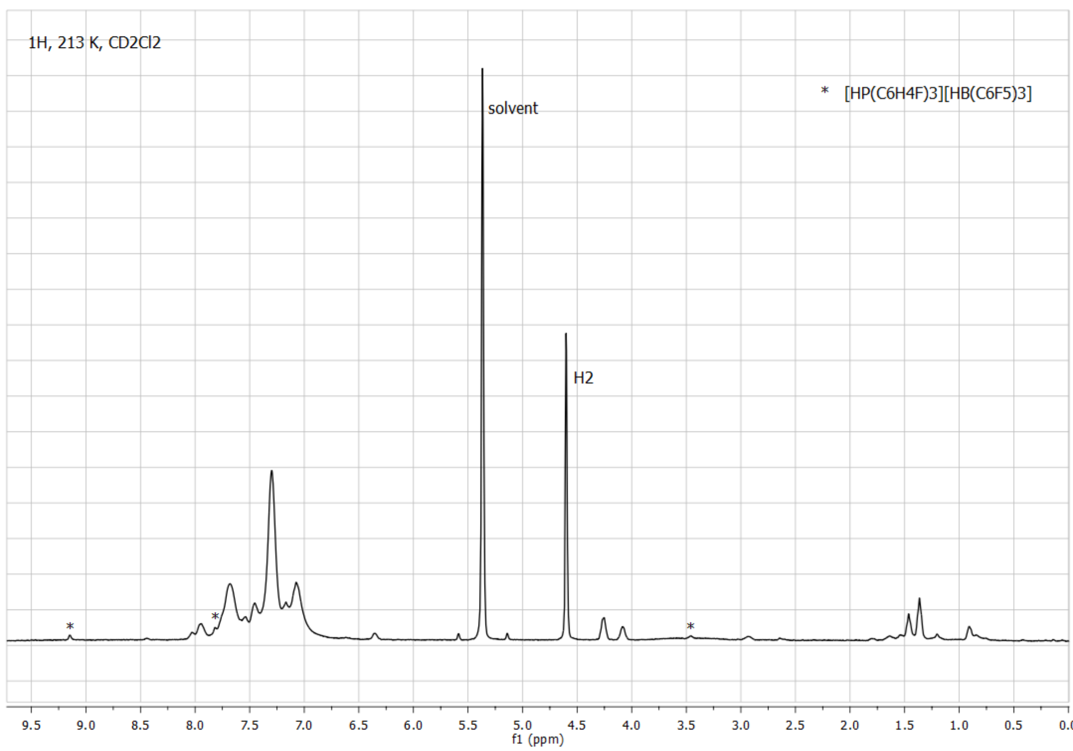


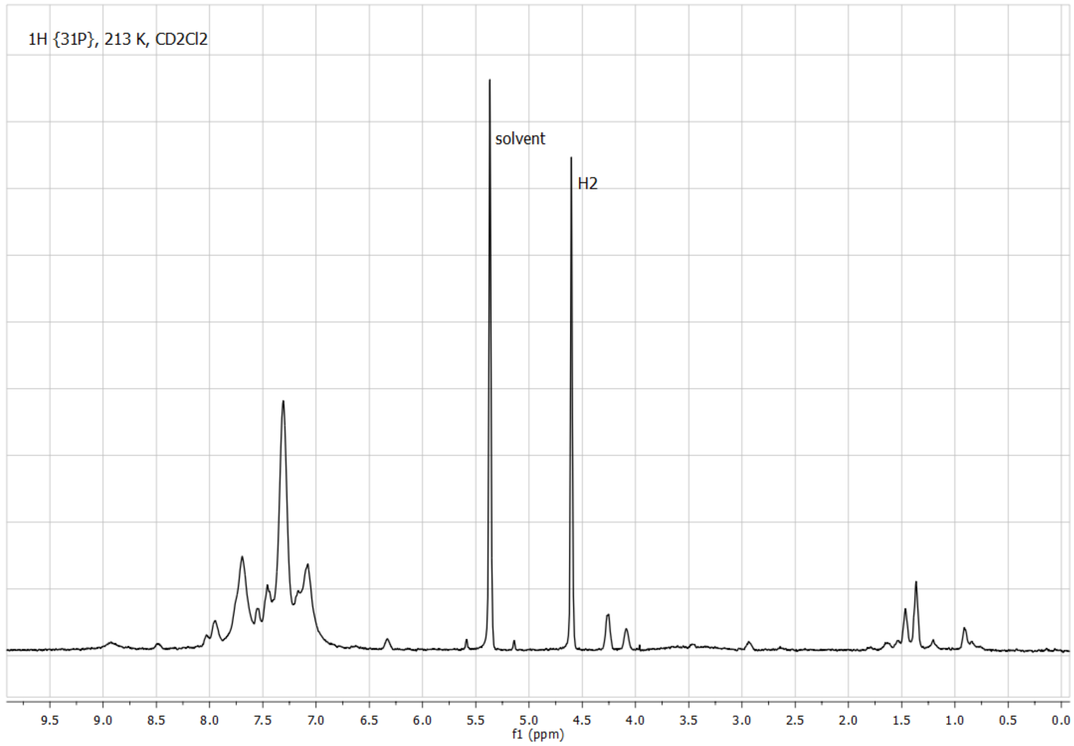

19F, 297 K, CD2Cl2
-104.23
-127.92
-143.57
-160.78
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
f1 (ppm)

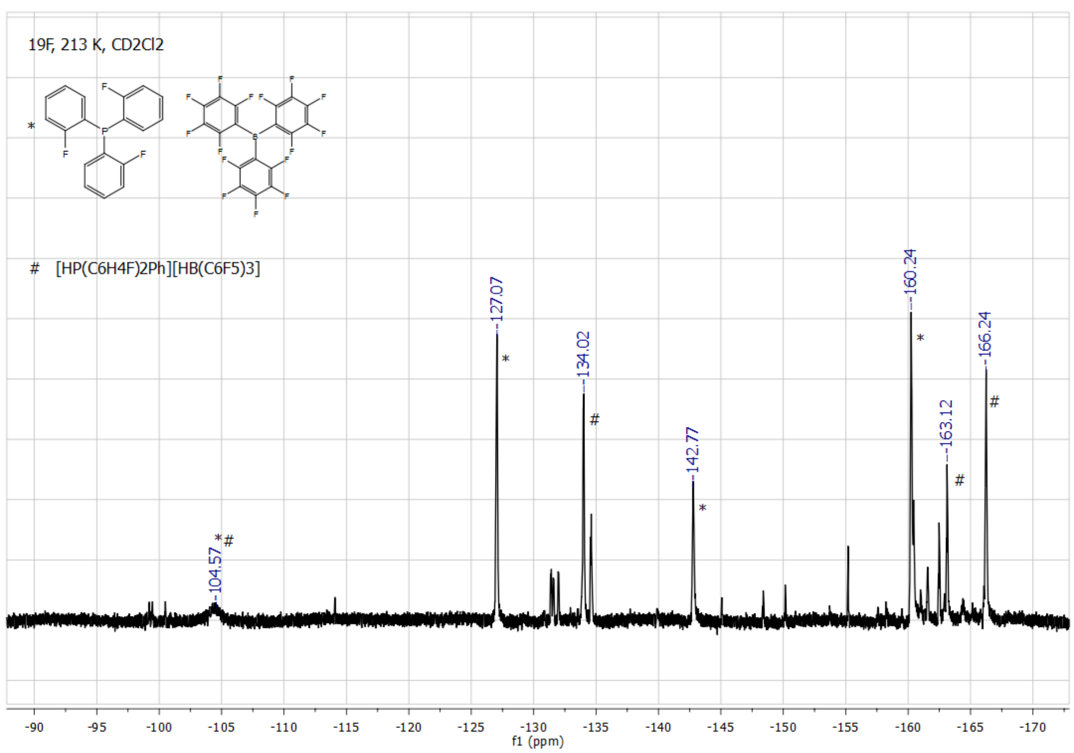

31P {1H}, 297 K, CD2Cl2
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
f1 (ppm)

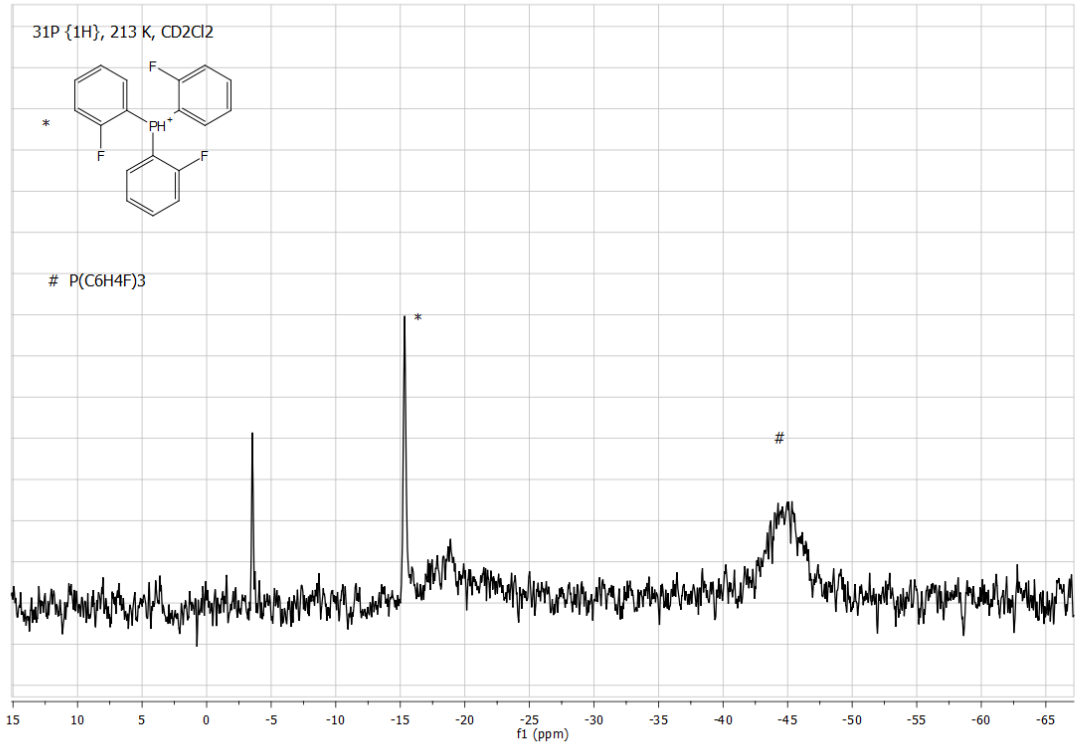


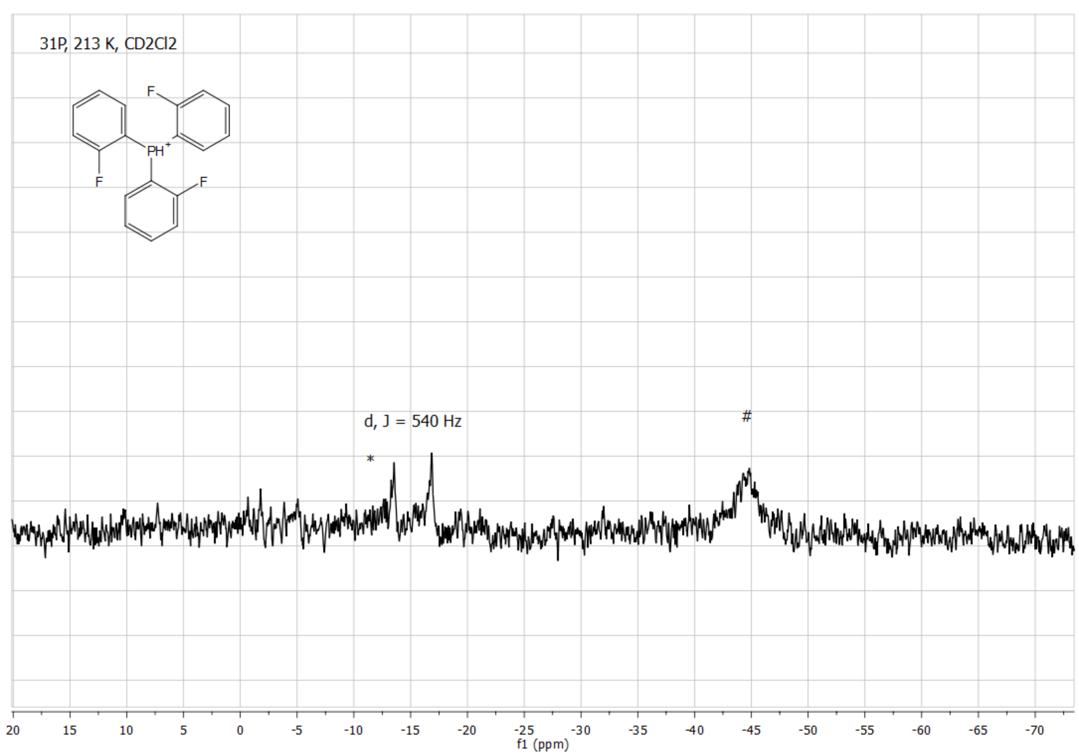

**[HP(2-F-$C_6H_4$)$_2$Ph][HB($C_6F_5$)$_3$] ([4H][H1])**

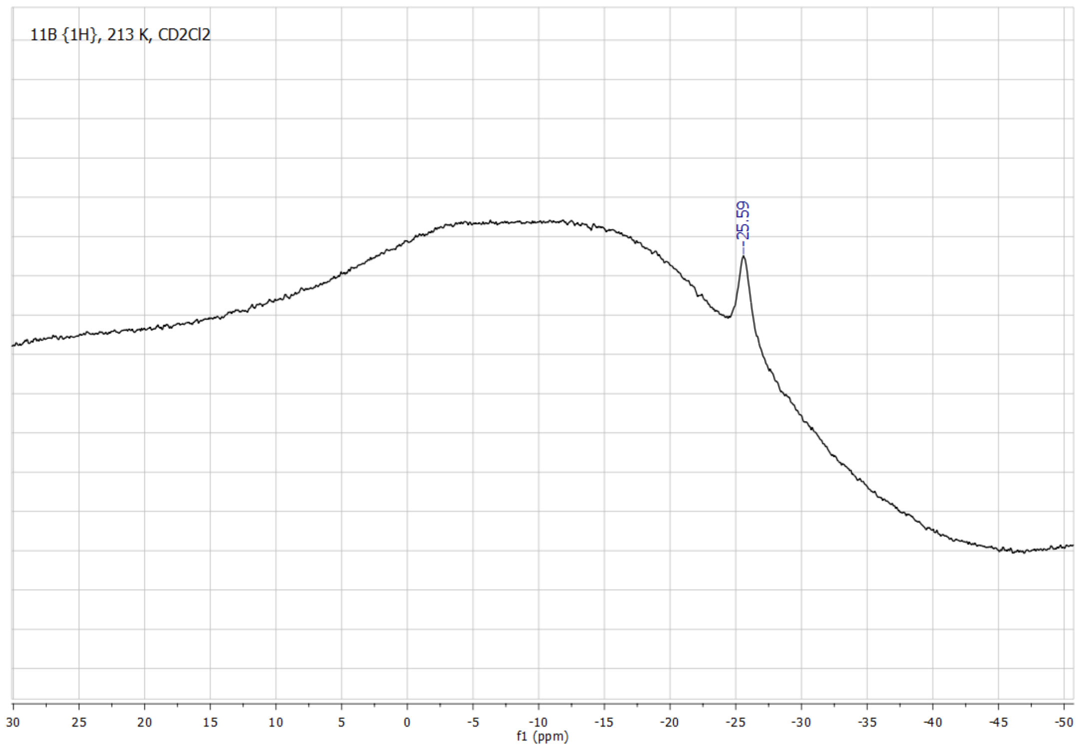



1H {31P}, 213 K, CD2Cl2
solvent
H2
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

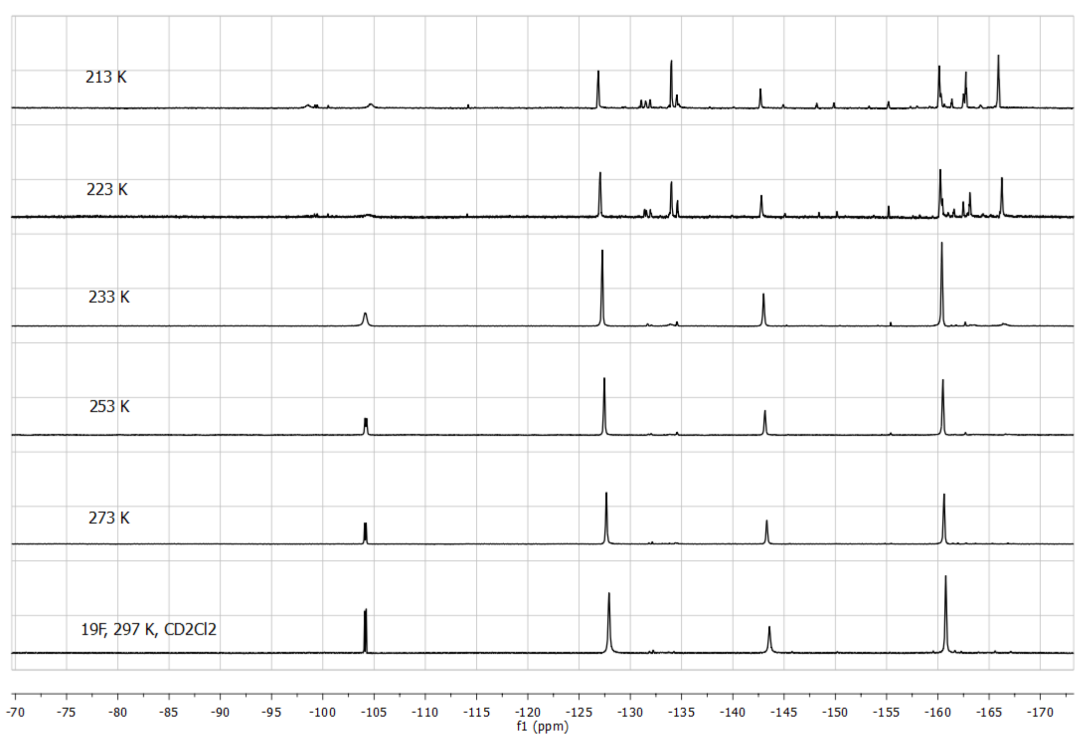

19F, 213 K, CD2Cl2
*
# [HP(C6H4F)2Ph][HB(C6F5)3]
-104.57 *#
-127.07 *
-134.02 #
-142.77 *
-160.24 *
-163.12 #
-166.24 #
-90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170
f1 (ppm)

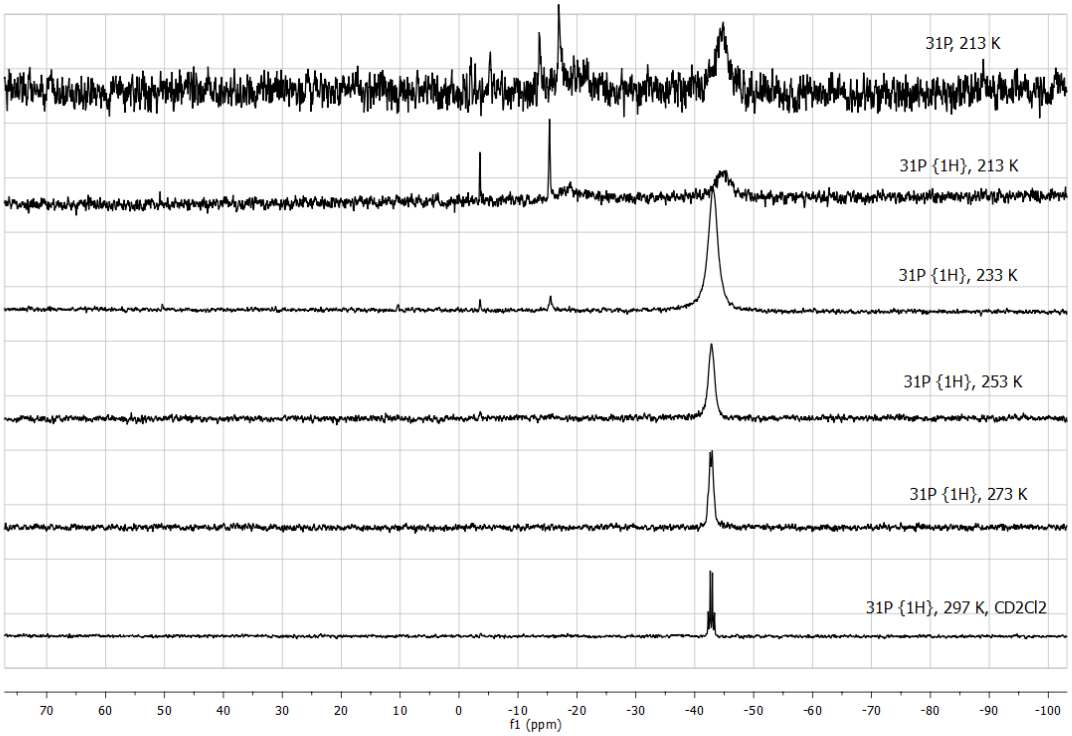

31P {1H}, 213 K, CD2Cl2
*
# P(C6H4F)3
f1 (ppm)


31P, 213 K, CD2Cl2
d, J = 540 Hz
*
#
f1 (ppm)

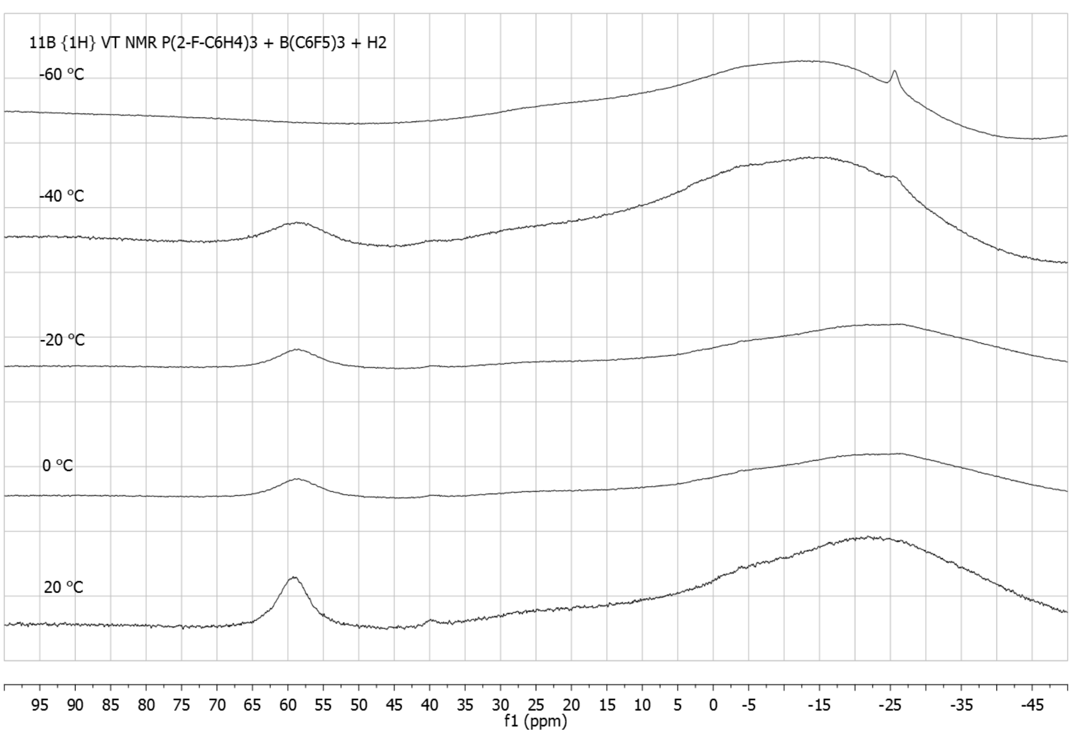



**VT series for P(2-F-$C_6H_4$)$_3$ (4) and B($C_6F_5$)$_3$ (1)**






**$^{11}B$ NMR spectrum at highest measured temperature with detectable $HB(C_6F_5)_3$ species with 4 ("activation temperature")**

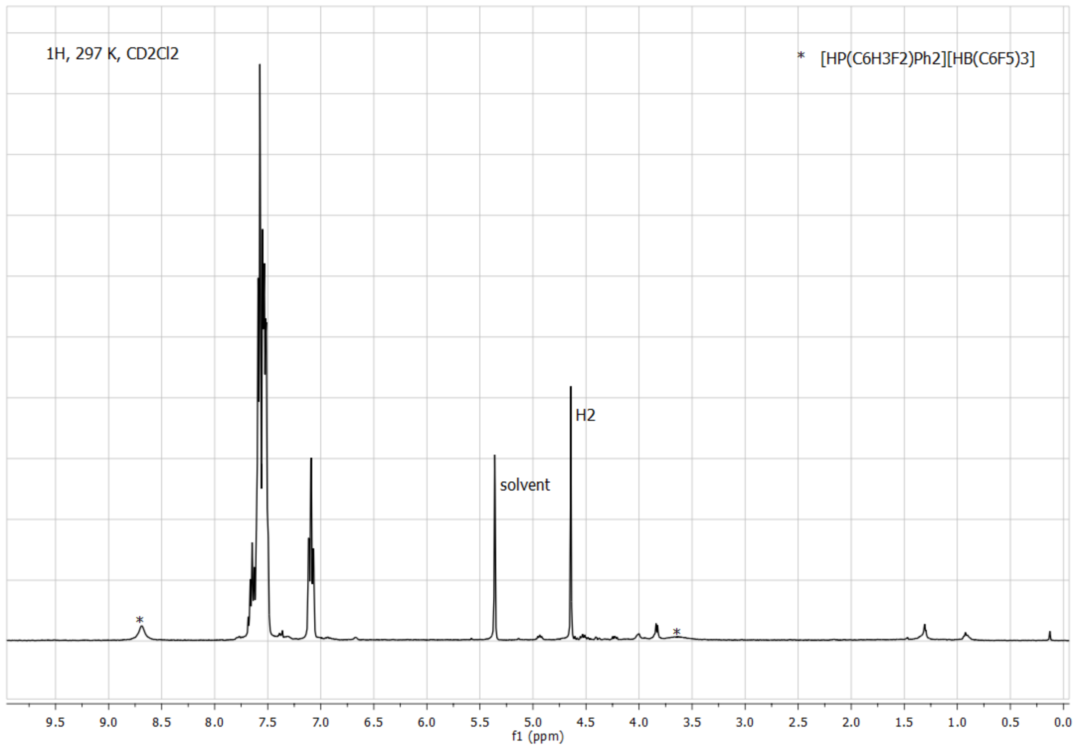


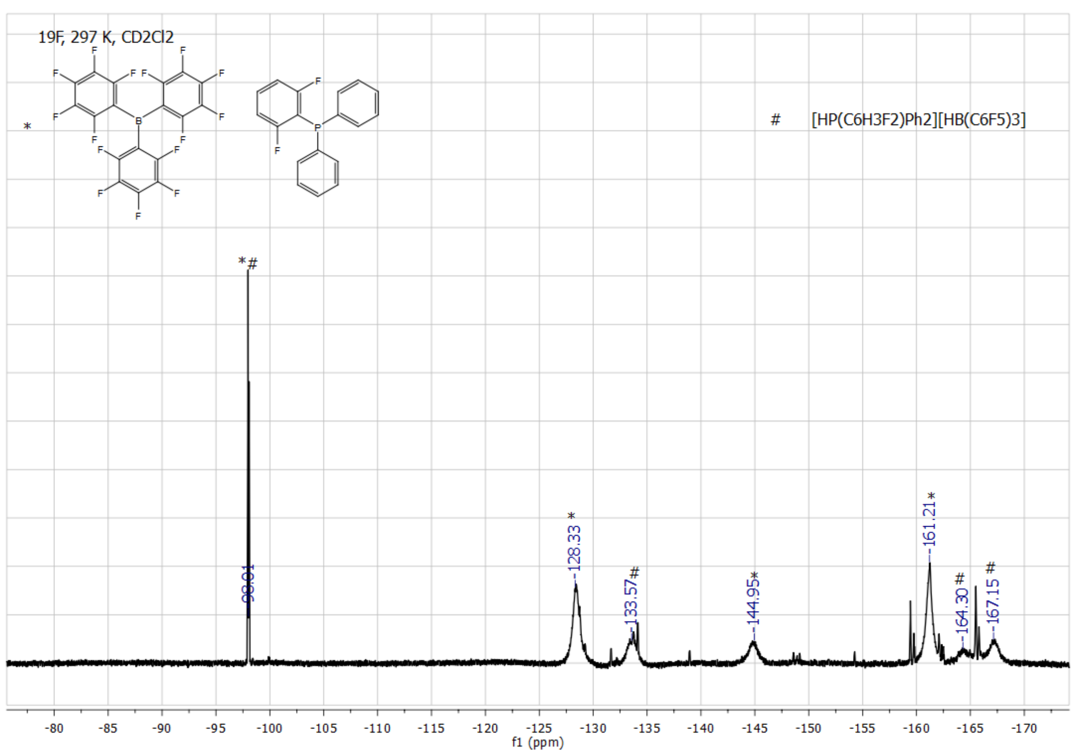
Electronic Supplementary Material (ESI) for Chemical Science
This journal is © The Royal Society of Chemistry 2013

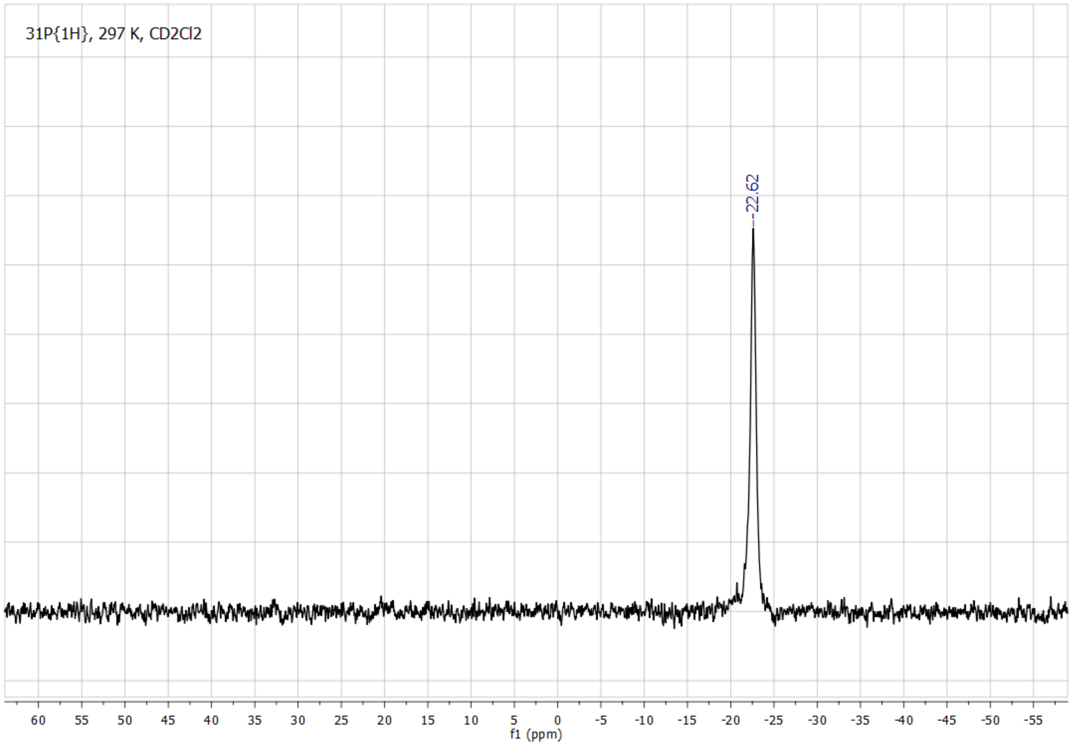


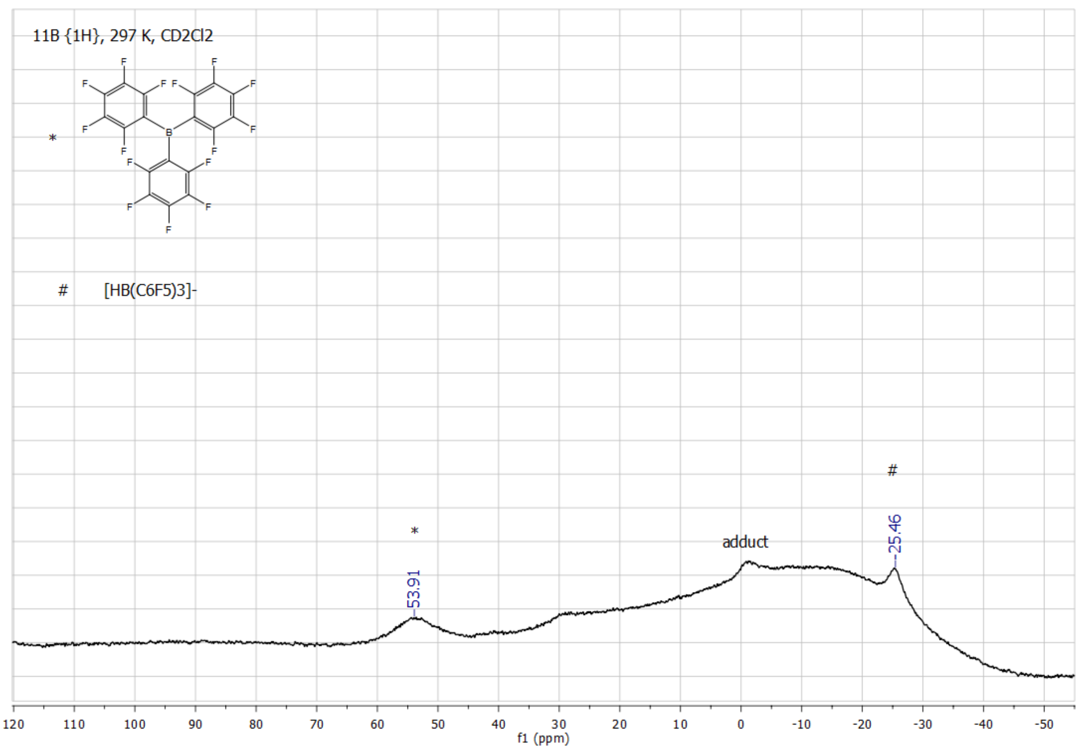
## $P(2,6\text{-}F_2\text{-}C_6H_3)Ph_2$ (5) and $B(C_6F_5)_3$ (1)

**FLP + $H_2$ at rt**

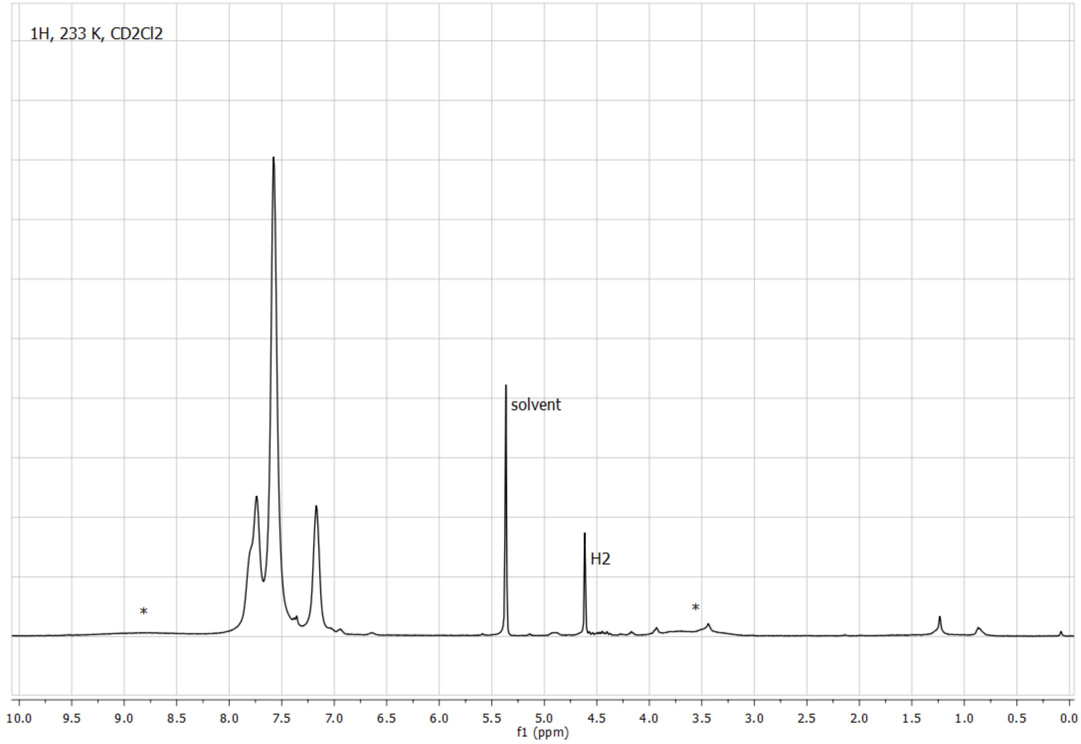


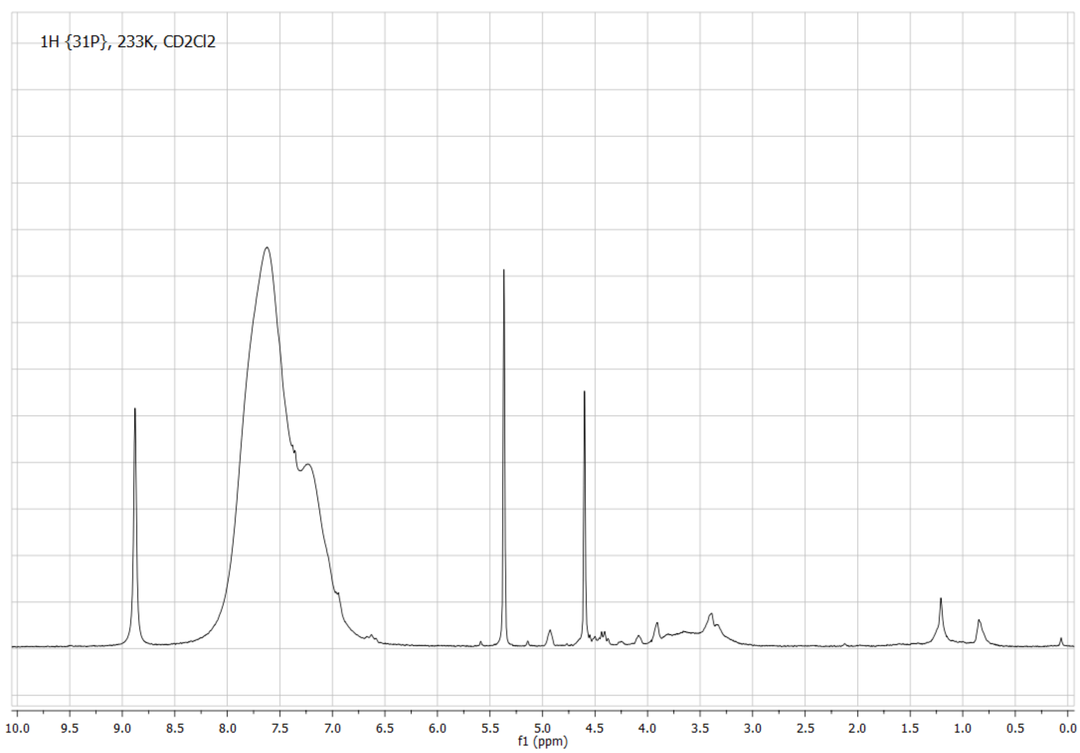



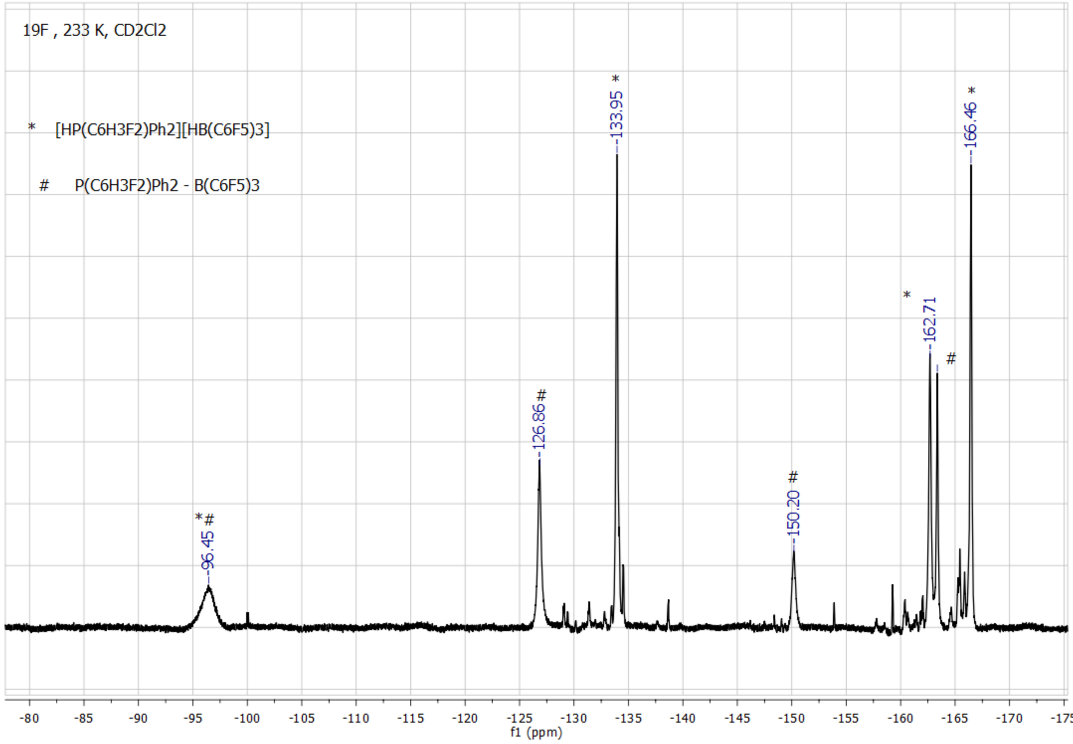

31P{1H}, 297 K, CD2Cl2
-22.62
60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55
f1 (ppm)

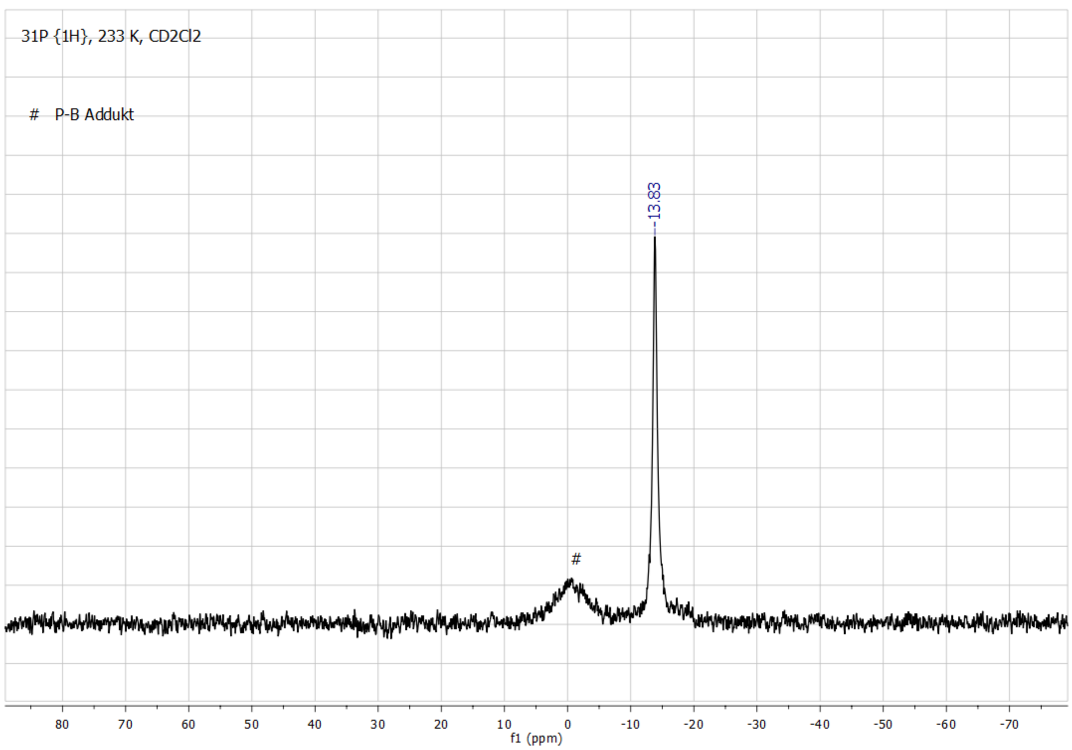

11B {1H}, 297 K, CD2Cl2
*
# [HB(C6F5)3]-
*
53.91
adduct
#
-25.46
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50
f1 (ppm)

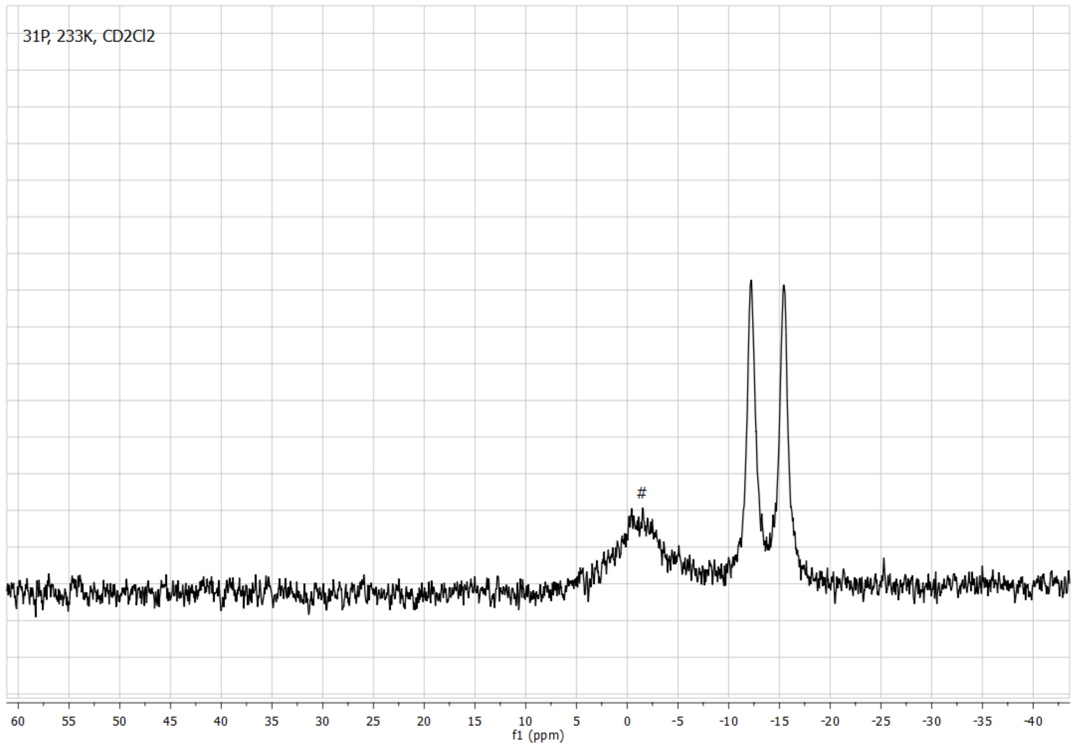
**$[HP(2,6\text{-}F_2C_6H_3)Ph_2][HB(C_6F_5)_3]$ ([5H][H1])**

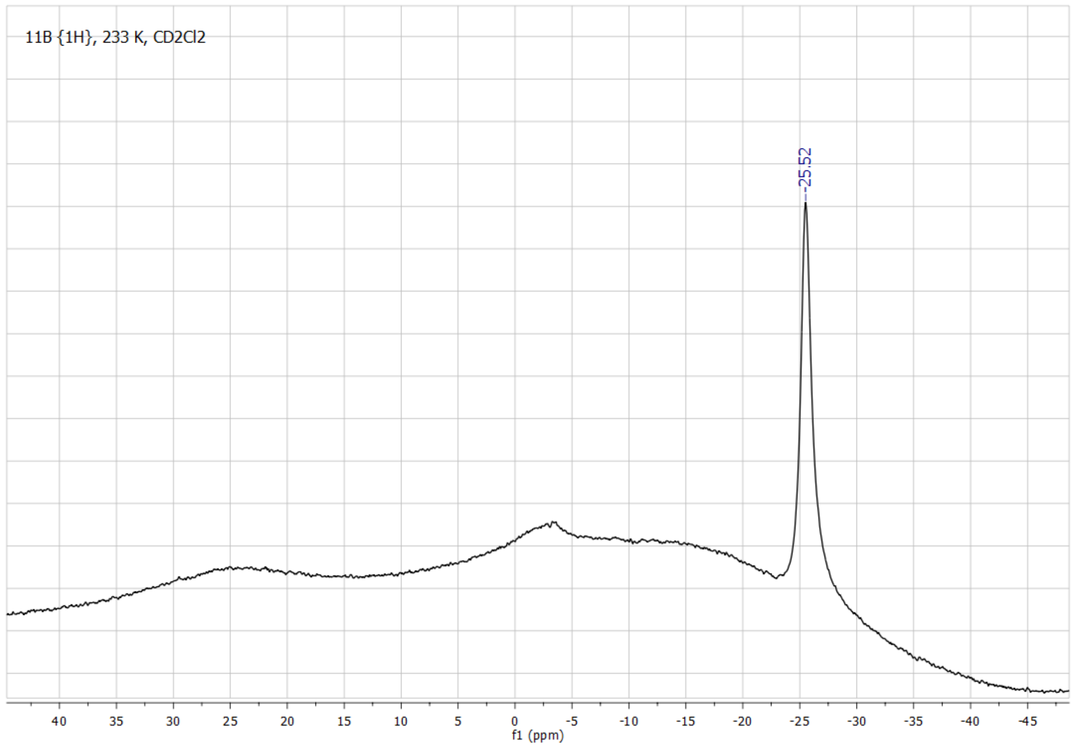


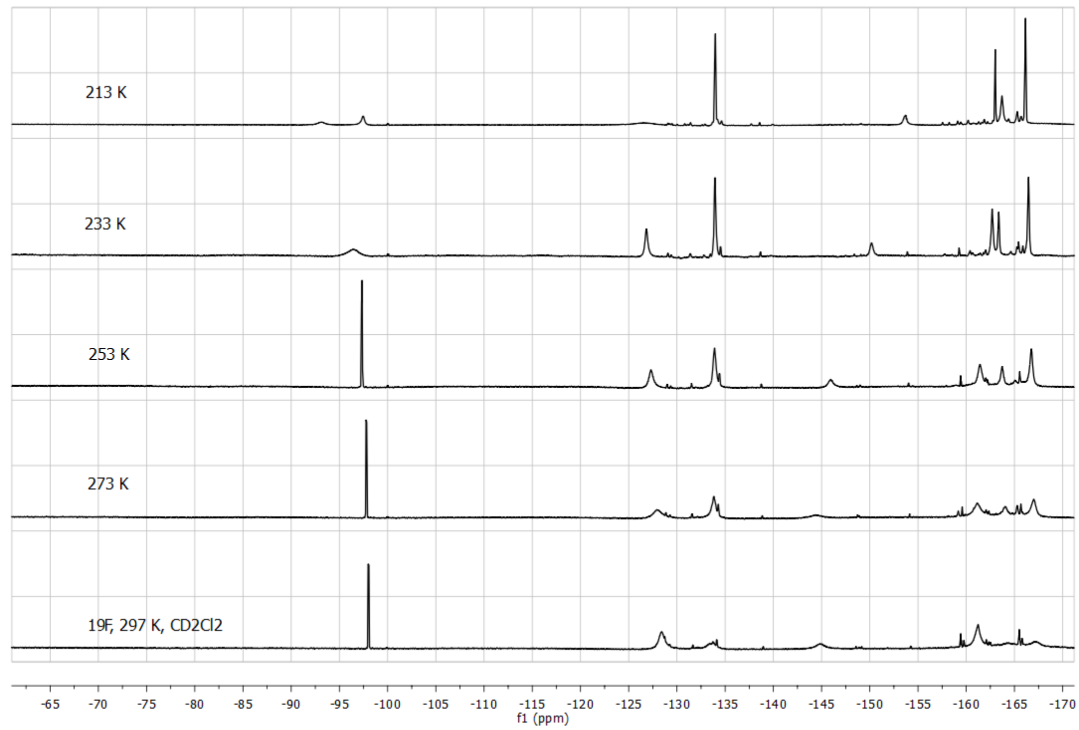

19F , 233 K, CD2Cl2
* [HP(C6H3F2)Ph2][HB(C6F5)3]
# P(C6H3F2)Ph2 - B(C6F5)3
-96.45
-126.86
-133.95
-150.20
-162.71
-166.46
f1 (ppm)

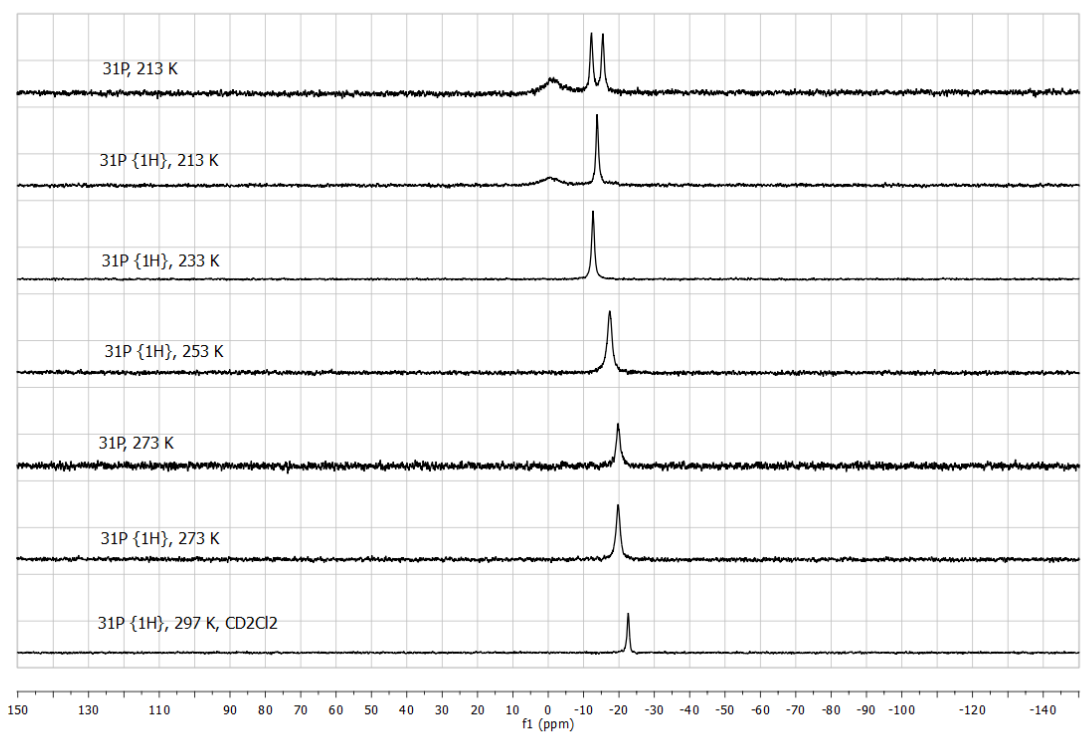

31P {1H}, 233 K, CD2Cl2
# P-B Addukt
-13.83
f1 (ppm)


31P, 233K, CD2Cl2
#
60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40
f1 (ppm)

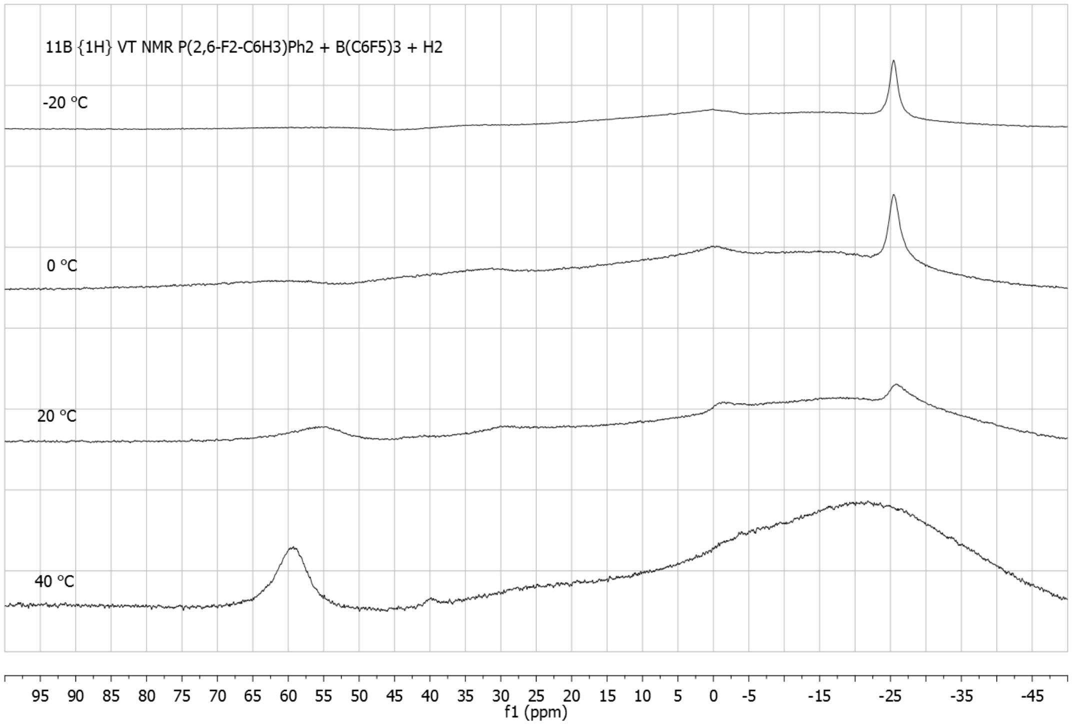

11B {1H}, 233 K, CD2Cl2
-25.52
40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45
f1 (ppm)

**VT series for $P(2,6\text{-}F_2\text{-}C_6H_3)Ph_2$ (5) and $B(C_6F_5)_3$ (1)**



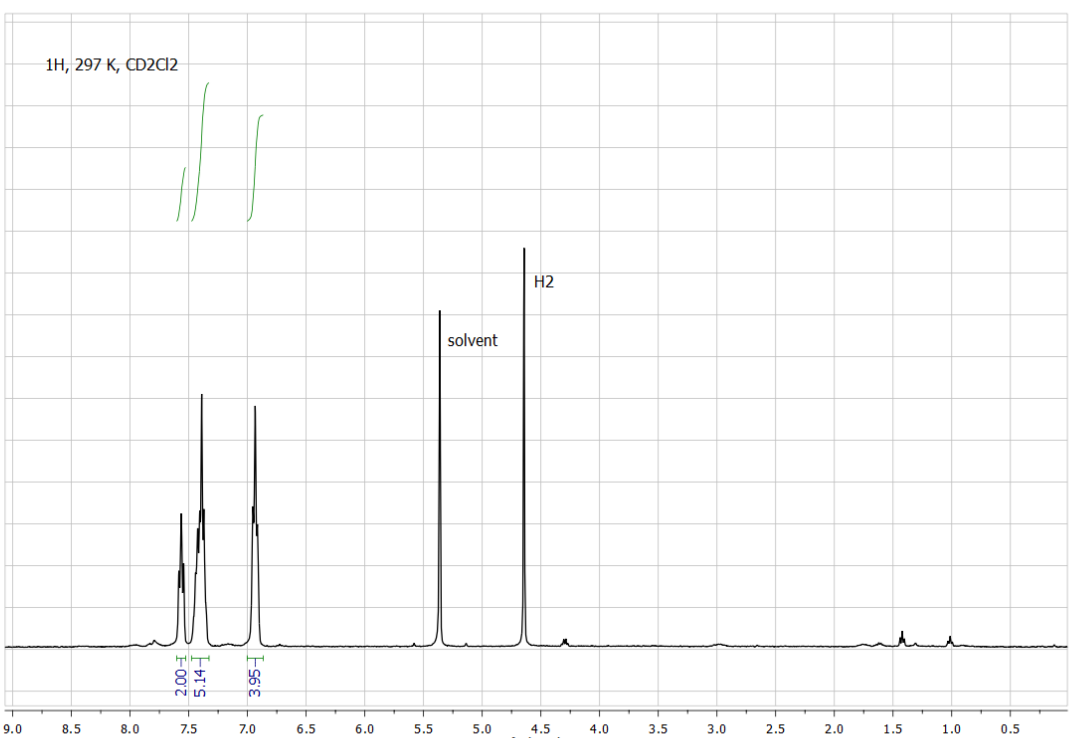



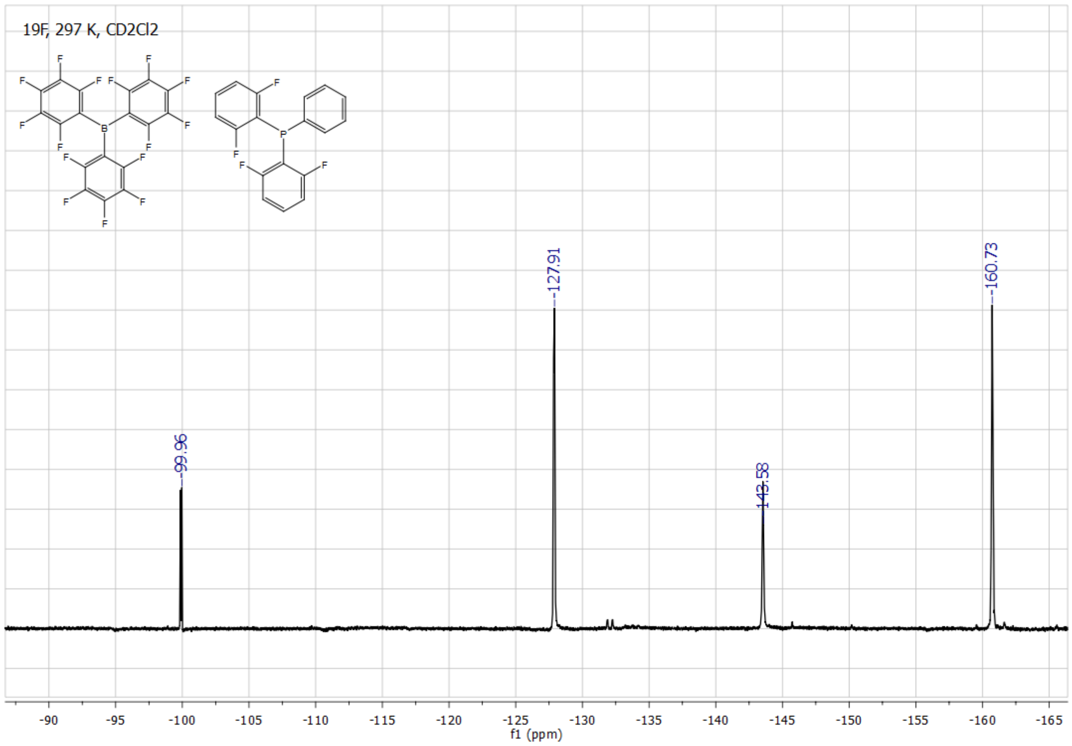
**$^{11}$B NMR spectrum at highest measured temperature with detectable $HB(C_6F_5)_3$ species with 5 ("activation temperature")**

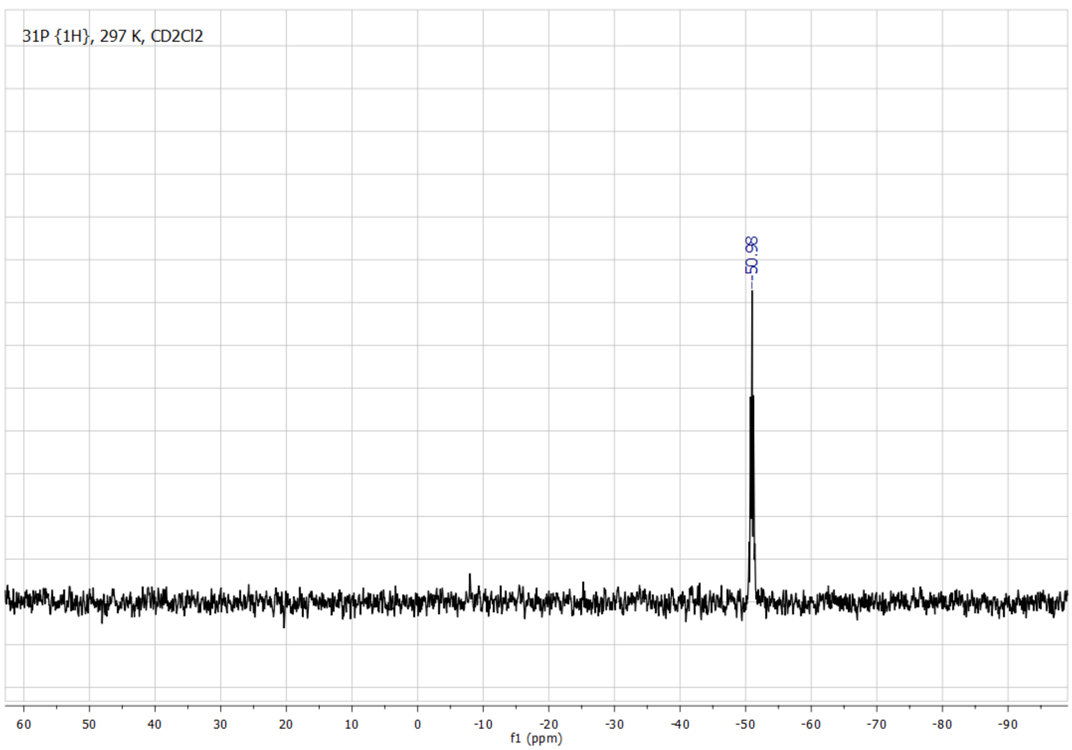



## $P(2,6\text{-}F_2C_6H_3)_2Ph$ (6) and $B(C_6F_5)_3$ (1)

**FLP + $H_2$ at rt**

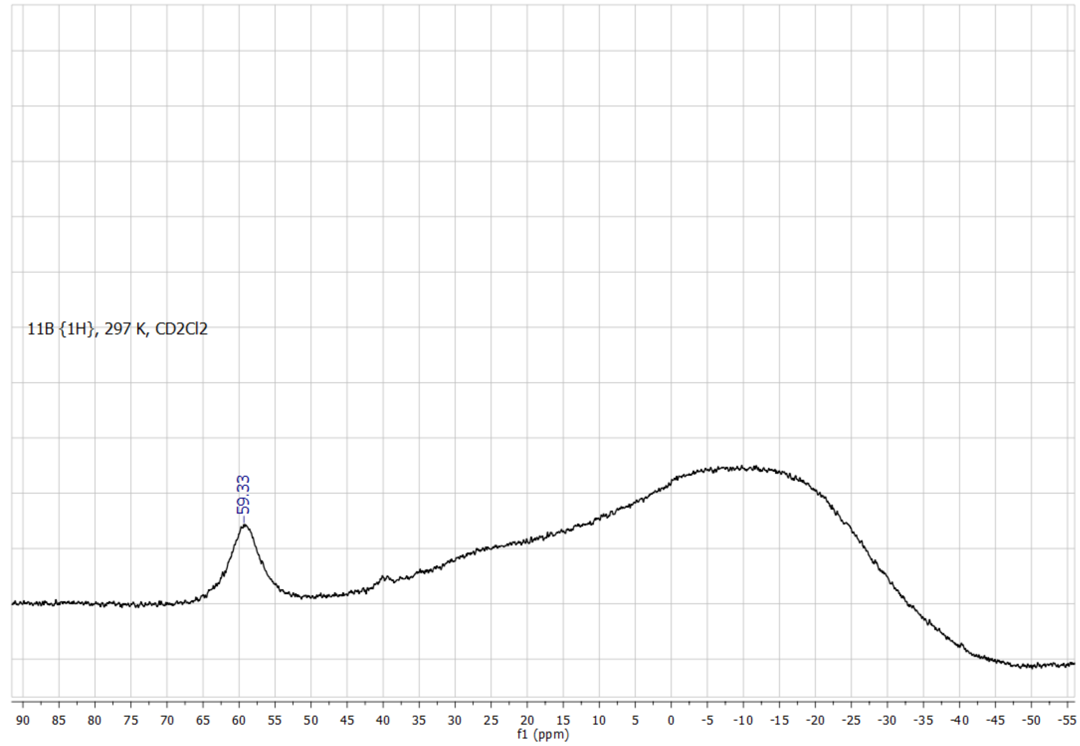



19F, 297 K, CD2Cl2
-99.96
-127.91
-143.58
-160.73
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
f1 (ppm)

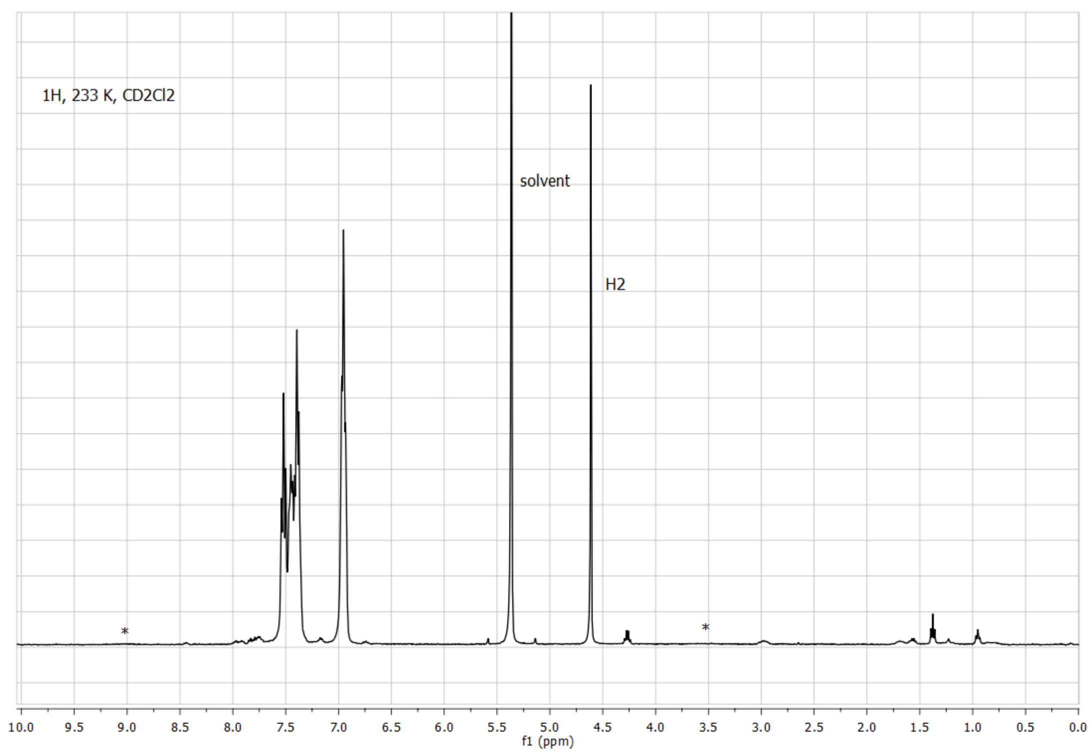

31P {1H}, 297 K, CD2Cl2
-50.98
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

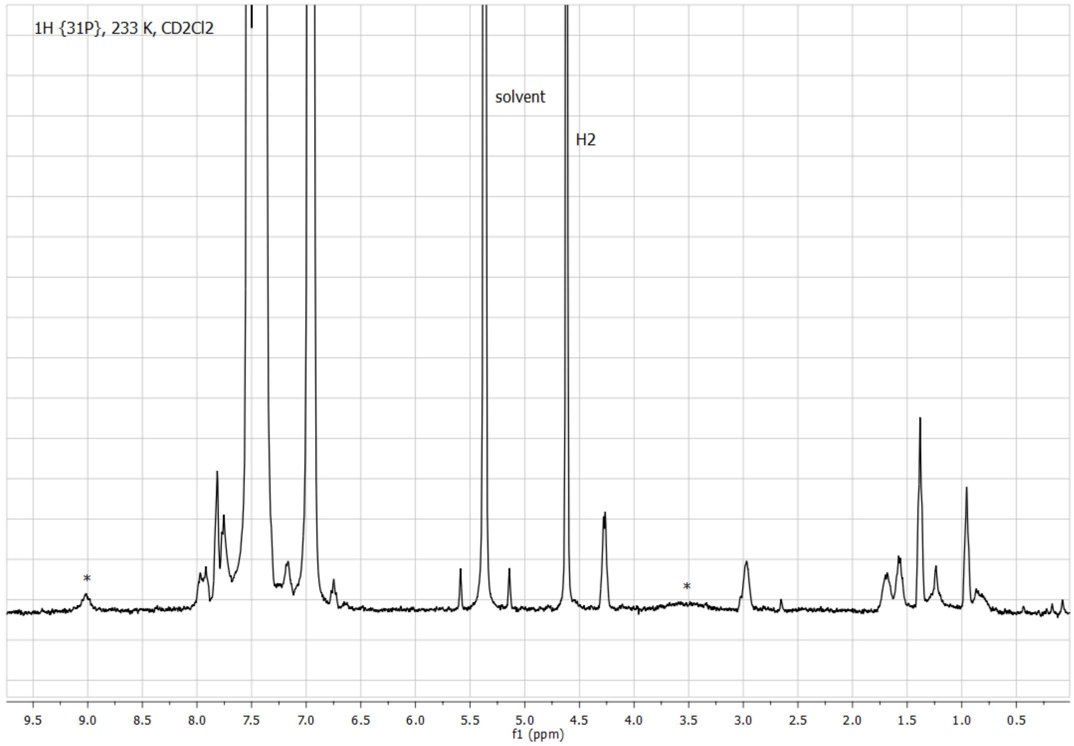
Electronic Supplementary Material (ESI) for Chemical Science
This journal is © The Royal Society of Chemistry 2013

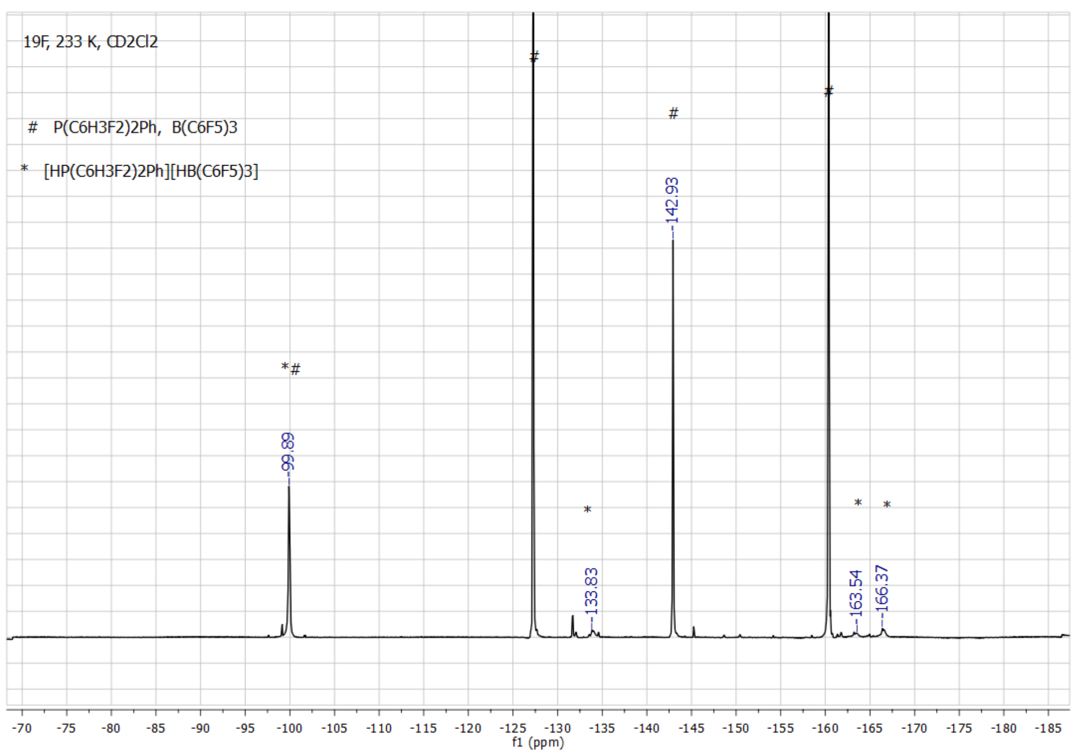


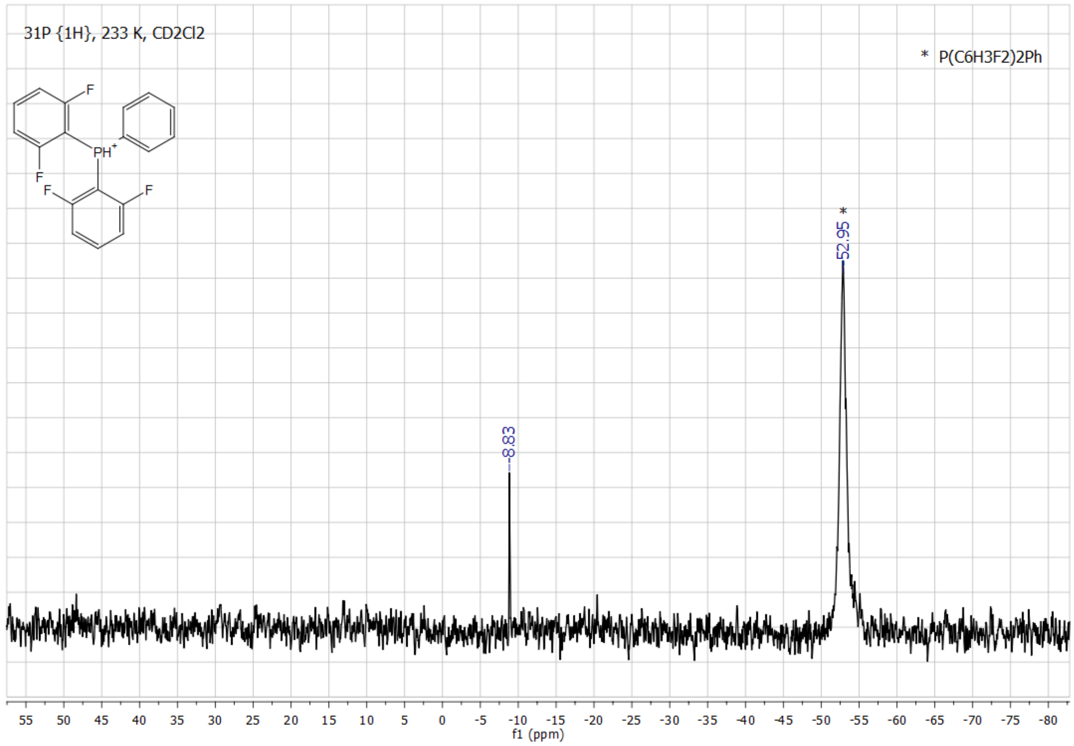


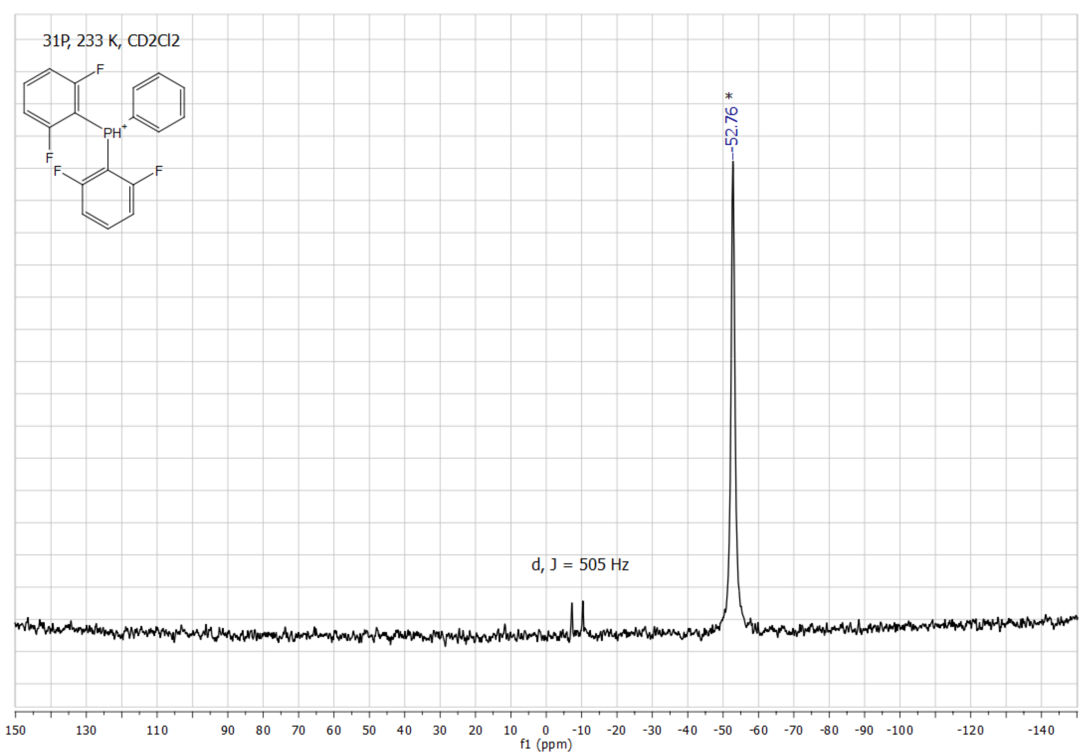

**[HP(2,6-$F_2C_6H_3)_2$Ph][HB($C_6F_5)_3$] ([6H][H1])**

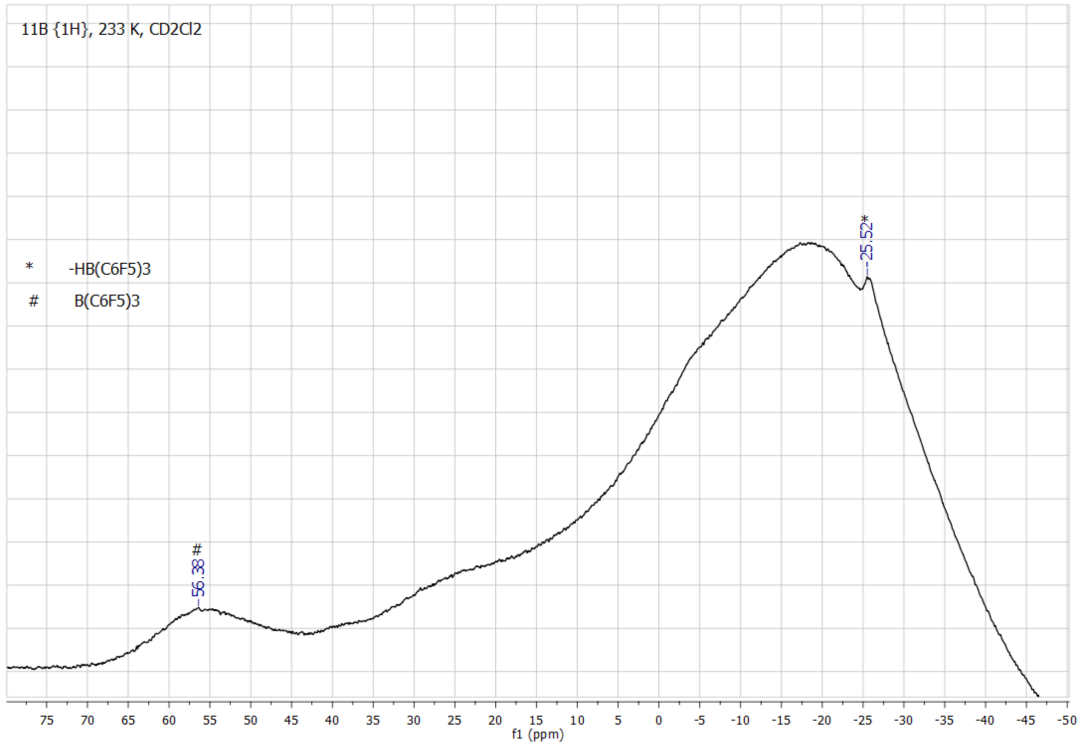


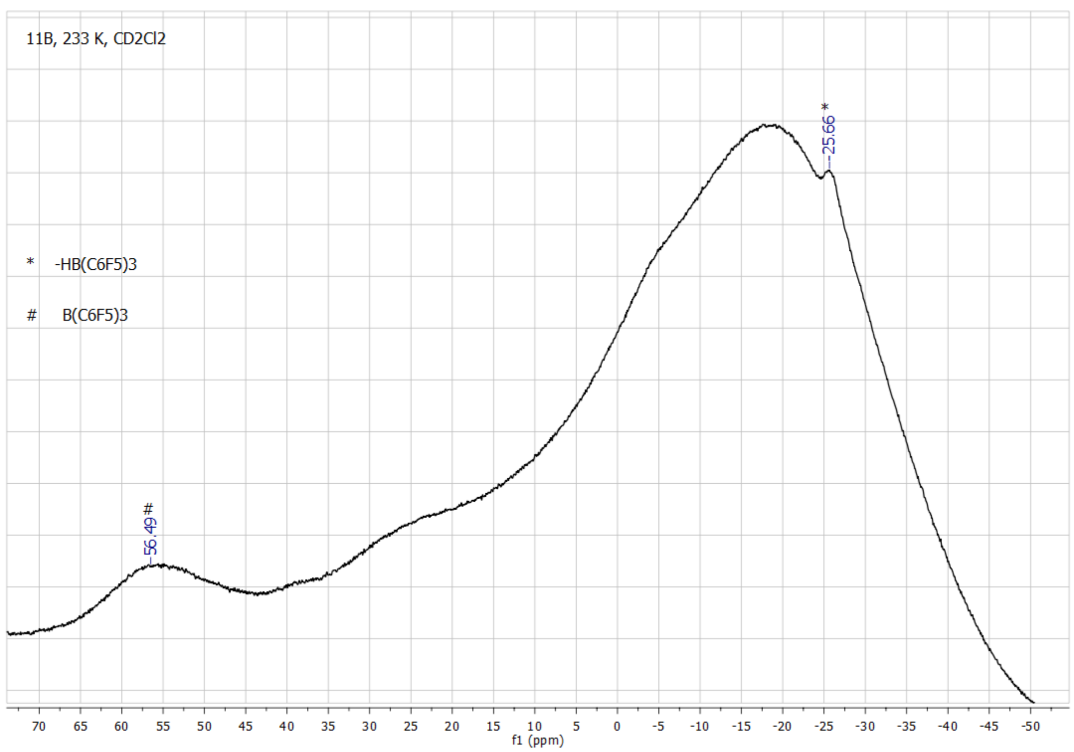

1H {31P}, 233 K, CD2Cl2
solvent
H2
*
*
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


19F, 233 K, CD2Cl2
# P(C6H3F2)2Ph, B(C6F5)3
* [HP(C6H3F2)2Ph][HB(C6F5)3]
*#
-99.89
#
*
-133.83
#
-142.93
#
* *
-163.54
-166.37
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
-175
-180
-185
f1 (ppm)

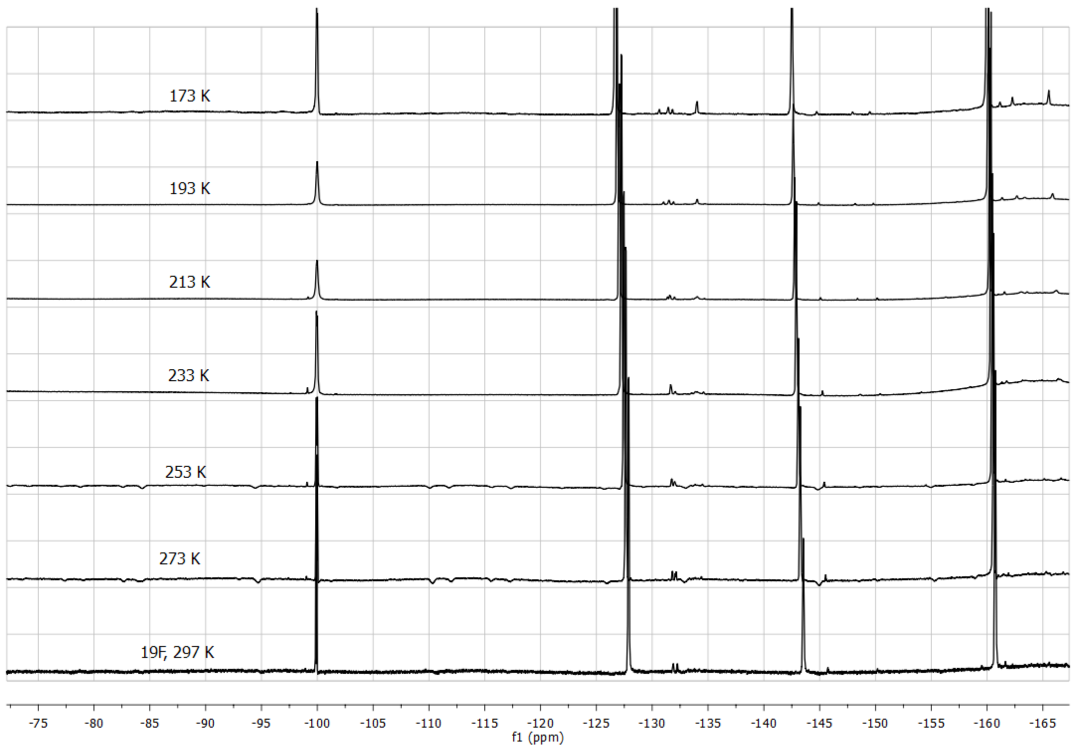

31P {1H}, 233 K, CD2Cl2
* P(C6H3F2)2Ph
-8.83
-52.95
f1 (ppm)

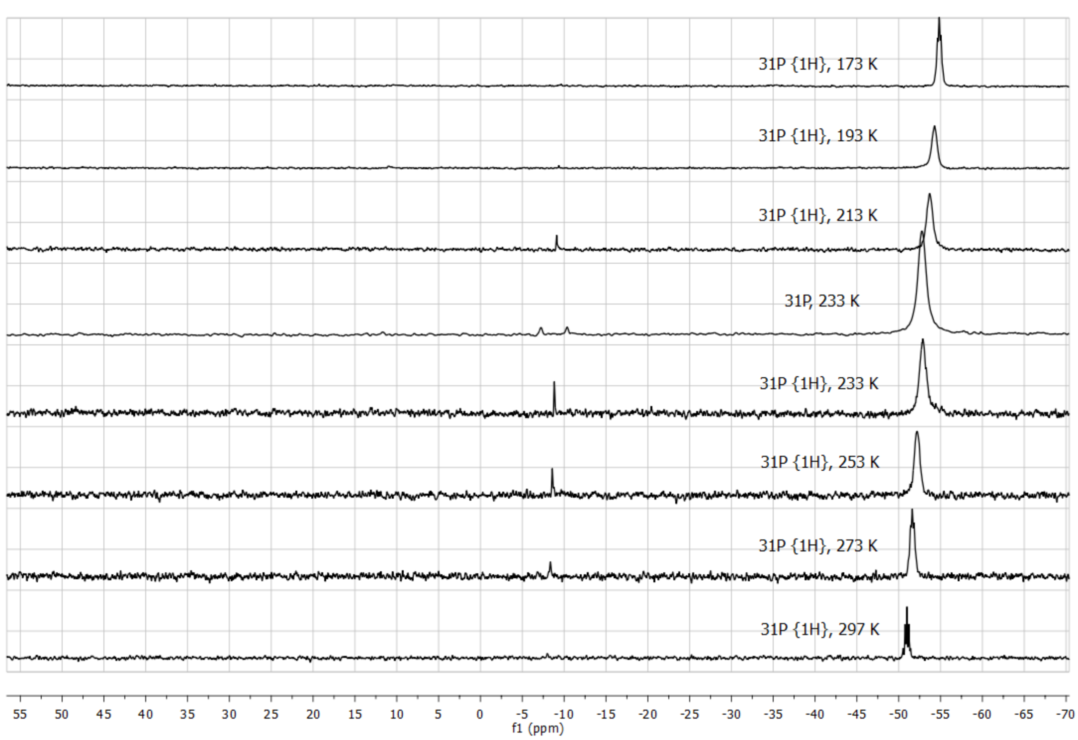

31P, 233 K, CD2Cl2
-52.76
d, J = 505 Hz
f1 (ppm)


11B {1H}, 233 K, CD2Cl2
* -HB(C6F5)3
# B(C6F5)3
56.38 #
-25.52 *
75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50
f1 (ppm)


11B, 233 K, CD2Cl2
* -HB(C6F5)3
# B(C6F5)3
56.49 #
-25.66 *
70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50
f1 (ppm)

**VT series for $P(2,6\text{-}F_2C_6H_3)_2Ph$ (6) and $B(C_6F_5)_3$ (1)**

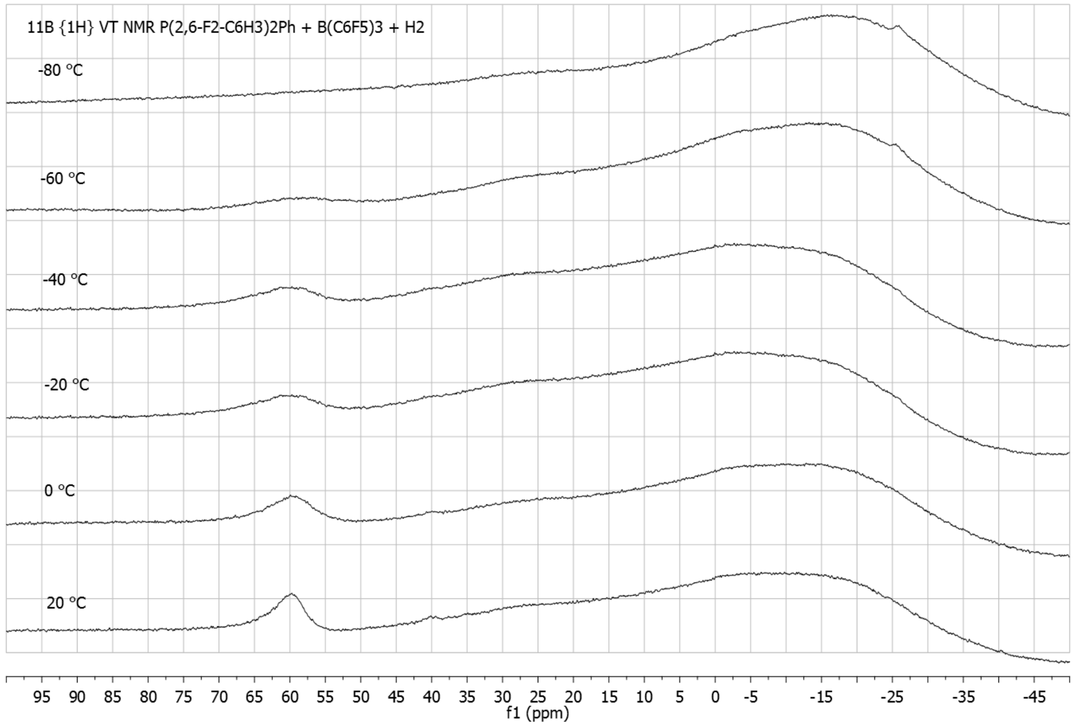


Electronic Supplementary Material (ESI) for Chemical Science
This journal is © The Royal Society of Chemistry 2013

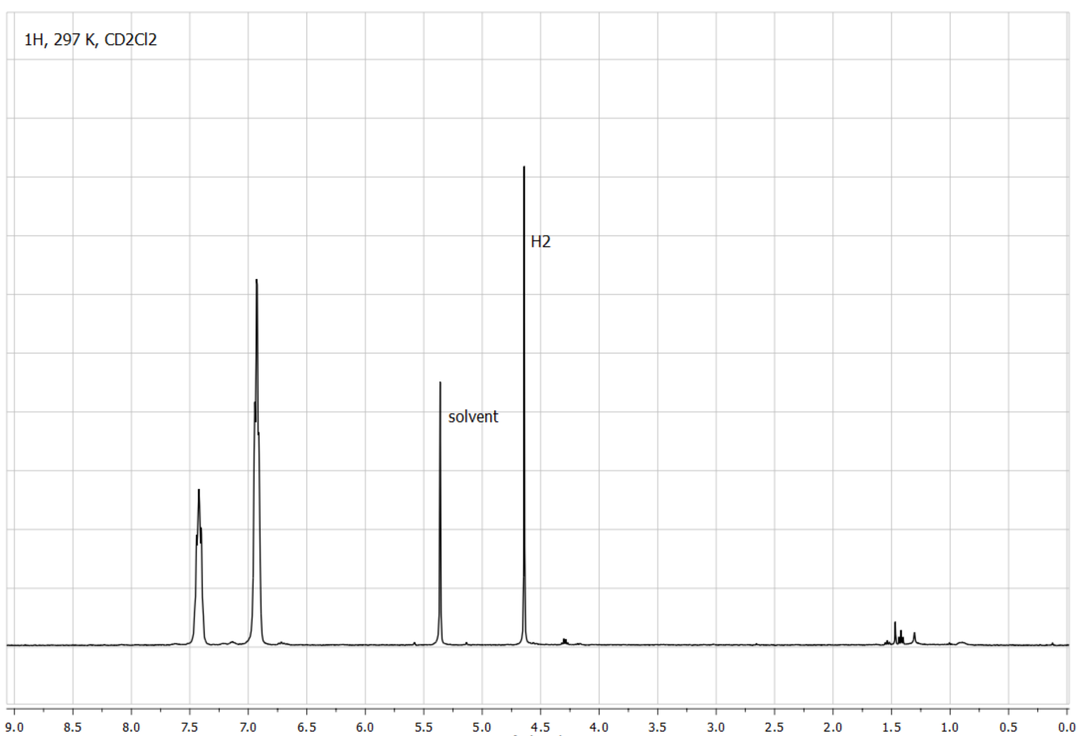


**$^{11}$B NMR spectrum at highest measured temperature with detectable $HB(C_6F_5)_3$ species with 6 ("activation temperature")**



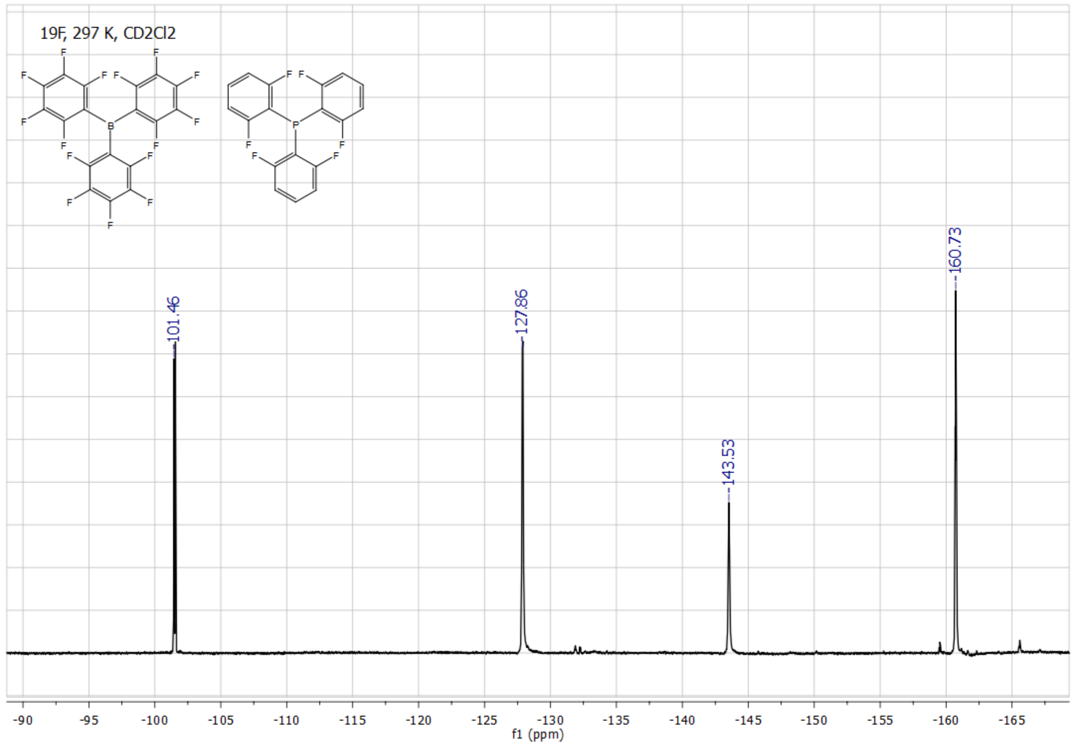

## $P(2,6\text{-}F_2C_6H_3)_3$ (7) and $B(C_6F_5)_3$ (1)

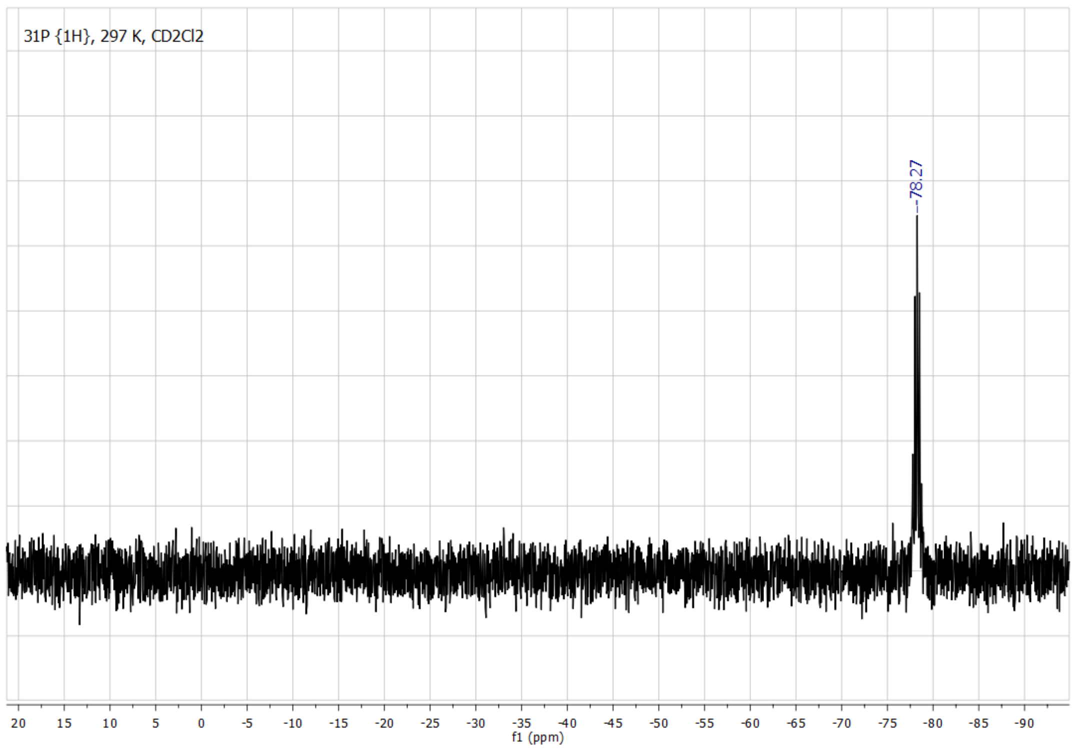
**FLP + $H_2$ at rt**

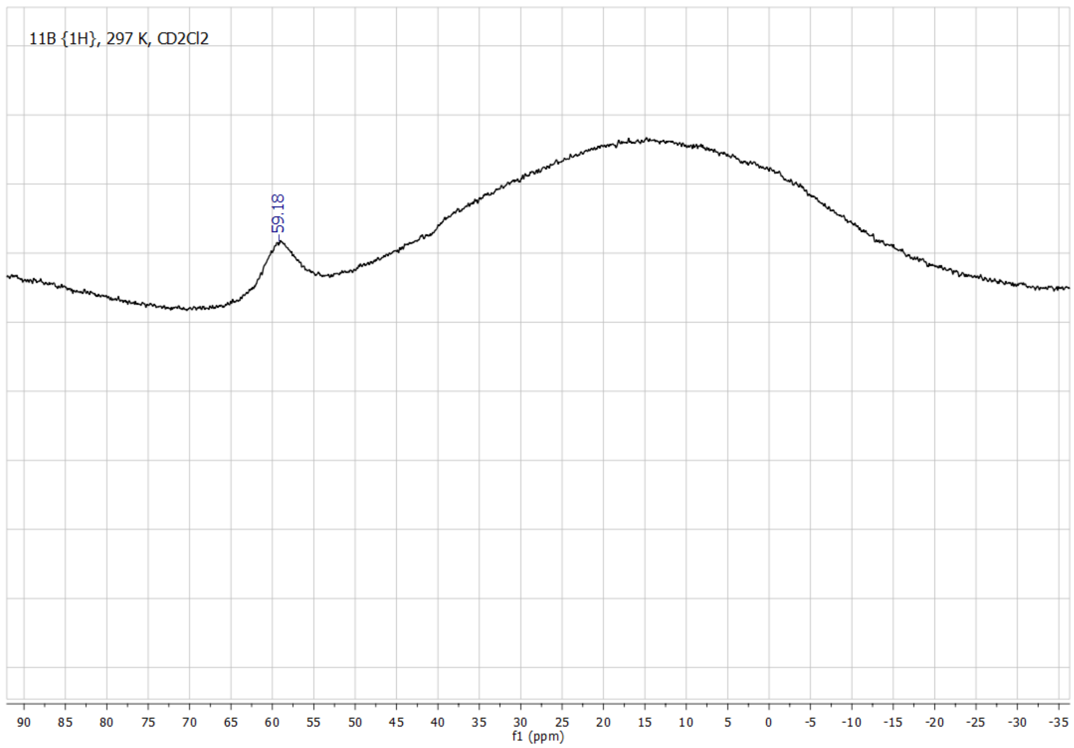


Electronic Supplementary Material (ESI) for Chemical Science







[1] a) H. B. Stegmann, H. M. Kühne, G. Wax, K. Scheffler, ***Phosphorous and Sulfur and the Related Elements*** **1982,** ***13*****, 331-336; b) J. A. S. Howell, N. Fey, J. D. Lovatt, P. C. Yates, P. McArdle, D. Cunningham, E. Sadeh, H. E. Gottlieb, Z. Goldschmidt, M. B. Hursthouse, M. E. Light,** ***Journal of the Chemical Society, Dalton Transactions*** **1999, 3015-3028; c) C. Corcoran, J. Fawcett, S. Friedrichs, J. H. Holloway, E. G. Hope, D. R. Russell, G. C. Saunders, A. M. Stuart,** ***Journal of the Chemical Society, Dalton Transactions*** **2000, 161-172; d) G. P. Schiemenz,** ***Phosphorus Sulfur*** **2000,** ***163*****, 185-202.**

[2] **K. Haav, J. Saame, A. Kütt, I. Leito,** ***European Journal of Organic Chemistry*** **2012,** ***2012*****, 2167-2172.**

[3] **I. Kaljurand, A. Kütt, L. Sooväli, T. Rodima, V. Mäemets, I. Leito, I. A. Koppel,** ***The Journal of Organic Chemistry*** **2005,** ***70*****, 1019-1028.**

[4] **A. A. Kolomeitsev, I. A. Koppel, T. Rodima, J. Barten, E. Lork, G.-V. Röschenthaler, I. Kaljurand, A. Kütt, I. Koppel, V. Mäemets, I. Leito,** ***Journal of the American Chemical Society*** **2005,** ***127*****, 17656-17666.**

[5] **A. Kütt, T. Rodima, J. Saame, E. Raamat, V. Mäemets, I. Kaljurand, I. A. Koppel, R. Y. Garlyauskayte, Y. L. Yagupolskii, L. M. Yagupolskii, E. Bernhardt, H. Willner, I. Leito,** ***The Journal of Organic Chemistry*** **2010,** ***76*****, 391-395.**

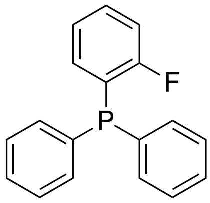
[6] **L. Greb, P. Oña-Burgos, B. Schirmer, S. Grimme, D. W. Stephan, J. Paradies,** ***Angewandte Chemie*** **2012,** ***124*****, 10311-10315.**

## Collection of calculated thermodynamical data

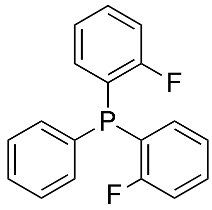
All calculations have been performed with the TURBOMOLE 6.3 suite of programs[1]. The structures have been optimized on TPSS-D3 level[2] applying the new D3-dispersion correction with Becke-Johnson damping[3,4]. Subsequent single point calculations have been carried out at B2PLYP-D3 level[5,6]. For both calculations the large Gaussian-AO basis set def2-TZVP[7] and the RI approximation[8,9] have been used. The final level of theory can therefore be abbreviated as B2PLYP-D3(BJ)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP and has an estimated accuracy of about 1-2 kcal/mol.
The thermodynamic corrections are based on harmonic vibrational frequencies calculated at TPSS-D3 level with very tight convergence criteria (energy: $10^{-9}$, gradient $10^{-6}$) and the big numerical quadrature grid *m5*. For these calculations the TURBOMOLE version 6.4[10] was used since recently the frequency calculation module of the earlier release was found out to contain a bug. Low-lying frequencies (effectively those below 100 $cm^{-1}$) are treated in a quasy-free-rotor approximation in order to avoid errors in the entropy calculation[11]. These (free) enthalpy values are denoted ΔH(G), ΔE marks electronic energies (i.e., not including ZPVE).
For a more detailed description of solvent effects and the accurate treatment of thermodynamic corrections in solvent - here (free) enthalpies of solvation - the COSMO-RS program in the parametrization for dichloromethane has been used[12,13,14,15,16].
All energy values are given in kcal/mol.

## References

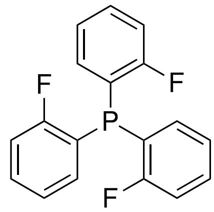
[1] TURBOMOLE, verison 6.3, R. Ahlrichs et. al., Universität Karlruhe 2008; see http://www.turbomole.com.
[2] J. Tao, J. P. Perdew, V. N. Staroverov and G. E. Scuseria, *Phys. Rev. Lett.*, 2003, **91**, 146401.
[3] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
[4] S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456–1465.
[5] S. Grimme, *J. Chem. Phys.*, 2006, **124**, 034108.
[6] T. Schwabe and S. Grimme, *Phys. Chem. Chem. Phys.*, 2006, **8**, 4398–4401.
[7] F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.
[8] K. Eichkorn, O. Treutler, H. Öhm, M. Häser and R. Ahlrichs, *Chem. Phys. Lett.*, 1995, **240**, 283–289.
[9] C. Hättig and F. Weigend, *J. Chem. Phys.*, 2000, **113**, 5154.
[10] TURBOMOLE, verison 6.4, R. Ahlrichs et. al., Universität Karlruhe 2012; see http://www.turbomole.com.
[11] S. Grimme, *Chem. Eur. J.*, 2012, **32**, 9955–9964.
[12] A. Klamt and G. Schüürmann, *J. Chem. Soc., Perkin Trans. 2*, 1993, 799–805.
[13] A. Klamt, *J. Phys. Chem.*, 1995, **99**, 2224–2235.
[14] F. Eckert and A. Klamt, *AIChE Journal*, 2002, **48**, 369–385.
[15] F. Eckert and A. Klamt, COSMOtherm, version C2.1, Release 01.11; COSMOlogic GmbH & Co. KG, Leverkusen, Germany.
[16] A. Klamt, *WIREs Comput. Mol. Sci.*, 2011, **1**, 699–709.



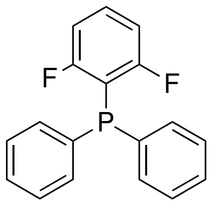

**2**



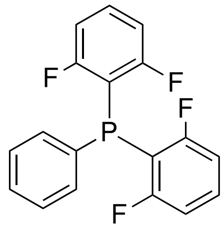

**3**



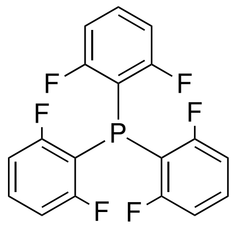

**4**



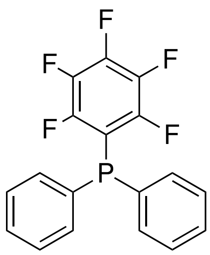

**5**




**6**




**7**




**8**

$B(C_6F_5)_3$
**1**

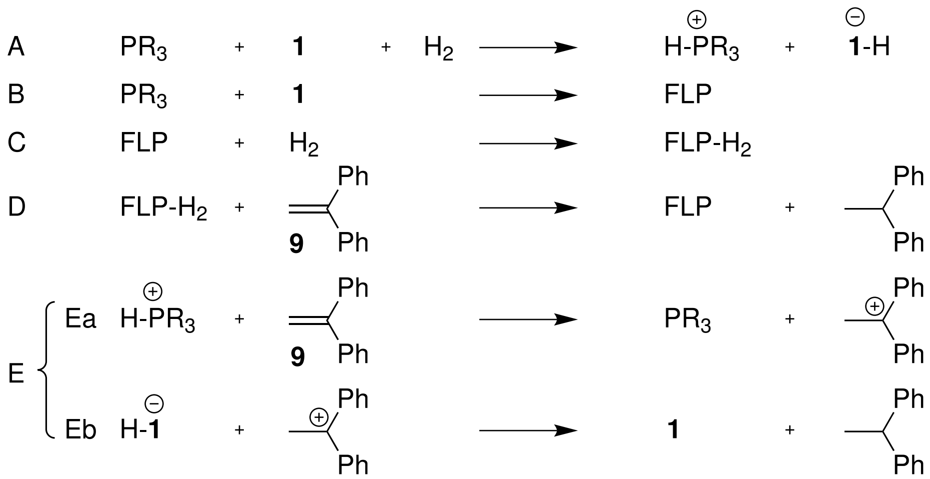



Figure 1: Computationally investigated reactions: formation of protonated phosphine and hydrated borane from separate reactants (**A**), association of the FLP (**B**), hydrogenation of the FLP (**C**), hydrogen transfer from the hydrogenated FLP to the olefine (**D**) and stepwise hydrogen transfer to the olefine (**E**). Reactions **B**, **C** and **D** include contributions for the association of the FLP and the ion pairs.

Tab. 1: Final free reaction enthalpies ΔG in solvation at two different temperatures based on B2PLYP-D3 electronic energies.

| reaction | phosphine | 298.15 K | 213.15 K |
|---|---|---|---|
| A | 2 | -3.66 | -4.09 |
| | 3 | -2.14 | -2.61 |
| | 4 | -0.56 | -1.10 |
| | 5 | -3.31 | -3.82 |
| | 6 | 0.10 | -0.41 |
| | 7 | 3.40 | 2.90 |
| | 8 | 1.03 | 0.36 |
| B | 2 | -2.92 | -6.01 |
| | 3 | 2.53 | -0.31 |
| | 4 | 0.33 | -3.26 |
| | 5 | -6.40 | -9.41 |
| | 6 | -1.20 | -3.98 |
| | 7 | 0.64 | -2.69 |
| | 8 | 2.06 | -1.15 |
| C | 2 | 1.47 | 0.94 |
| | 3 | -1.74 | -2.43 |
| | 4 | 3.49 | 3.63 |
| | 5 | 2.69 | 1.95 |
| | 6 | 0.90 | -0.15 |
| | 7 | 4.75 | 4.22 |
| | 8 | 0.40 | 0.53 |
| D | 2 | -22.89 | -22.61 |
| | 3 | -19.68 | -19.24 |
| | 4 | -24.91 | -25.31 |
| | 5 | -24.11 | -23.63 |
| | 6 | -22.32 | -21.52 |
| | 7 | -26.17 | -25.88 |
| | 8 | -21.82 | -22.19 |
| Ea | 2 | 12.86 | 12.62 |
| | 3 | 11.33 | 11.14 |
| | 4 | 9.75 | 9.63 |
| | 5 | 12.50 | 12.35 |
| | 6 | 9.11 | 8.94 |
| | 7 | 5.80 | 5.63 |
| | 8 | 8.18 | 8.16 |
| Eb | | -30.62 | -30.19 |
| E | 2 | -17.31 | -18.57 |
| | 3 | -19.28 | -20.05 |
| | 4 | -20.87 | -21.56 |
| | 5 | -18.11 | -18.84 |
| | 6 | -21.51 | -22.25 |
| | 7 | -24.81 | -25.56 |
| | 8 | -22.44 | -23.03 |

Table 2: Electronic reaction energies.

| reaction | phosphine | ΔE TPSS-D3 | ΔE B2PLYP-D3 |
|---|---|---|---|
| A | 2 | 49.55 | 50.04 |
| | 3 | 51.00 | 51.44 |
| | 4 | 52.26 | 52.57 |
| | 5 | 49.28 | 50.02 |
| | 6 | 52.37 | 53.43 |
| | 7 | 54.70 | 55.83 |
| | 8 | 56.40 | 57.89 |
| B | 2 | -17.28 | -20.90 |
| | 3 | -13.11 | -16.31 |
| | 4 | -16.26 | -19.96 |
| | 5 | -20.72 | -24.65 |
| | 6 | -14.61 | -17.90 |
| | 7 | -12.77 | -16.03 |
| | 8 | -12.25 | -15.79 |
| C | 2 | -1.42 | 1.88 |
| | 3 | -3.63 | -1.33 |
| | 4 | 1.50 | 4.94 |
| | 5 | 0.95 | 2.96 |
| | 6 | -0.67 | 2.04 |
| | 7 | 2.17 | 5.04 |
| | 8 | -2.24 | 0.70 |
| D | 2 | -26.73 | -32.46 |
| | 3 | -24.52 | -29.25 |
| | 4 | -29.65 | -35.52 |
| | 5 | -28.74 | -33.54 |
| | 6 | -27.48 | -32.62 |
| | 7 | -30.32 | -35.62 |
| | 8 | -25.91 | -31.28 |
| Ea | 2 | 13.83 | 16.63 |
| | 3 | 12.38 | 15.24 |
| | 4 | 11.12 | 14.11 |
| | 5 | 14.09 | 16.65 |
| | 6 | 11.00 | 13.24 |
| | 7 | 8.68 | 10.84 |
| | 8 | 6.98 | 9.08 |
| Eb | | -91.53 | -97.25 |
| E | 2 | -77.70 | -80.62 |
| | 3 | -79.15 | -82.02 |
| | 4 | -80.41 | -83.15 |
| | 5 | -77.43 | -80.60 |
| | 6 | -80.52 | -84.01 |
| | 7 | -82.85 | -86.41 |
| | 8 | -84.55 | -88.17 |

Table 3: Thermochemical and solvent correction terms at 298.15 K.

| reaction | phosphine | gas phase ΔH | gas phase ΔG | $CH_2Cl_2$ ΔH | $CH_2Cl_2$ ΔG |
|---|---|---|---|---|---|
| A | 2 | 3.83 | 11.25 | -59.79 | -64.95 |
| | 3 | 3.82 | 11.30 | -59.78 | -64.88 |
| | 4 | 3.82 | 11.49 | -59.56 | -64.61 |
| | 5 | 3.96 | 11.64 | -59.87 | -64.97 |
| | 6 | 3.96 | 11.33 | -59.70 | -64.67 |
| | 7 | 4.01 | 11.31 | -58.83 | -63.74 |
| | 8 | 3.97 | 11.55 | -63.40 | -68.11 |
| B | 2 | 1.71 | 19.57 | 5.49 | -1.58 |
| | 3 | 1.74 | 18.96 | 7.31 | -0.13 |
| | 4 | 1.65 | 19.63 | 7.95 | 0.66 |
| | 5 | 1.54 | 19.23 | 6.44 | -0.99 |
| | 6 | 1.48 | 17.30 | 6.40 | -0.60 |
| | 7 | 1.36 | 16.95 | 6.35 | -0.28 |
| | 8 | 1.47 | 19.39 | 5.54 | -1.54 |
| C | 2 | 3.30 | 9.39 | -3.98 | -9.80 |
| | 3 | 3.24 | 9.71 | -4.54 | -10.12 |
| | 4 | 3.27 | 8.42 | -4.24 | -9.88 |
| | 5 | 3.45 | 10.11 | -4.84 | -10.38 |
| | 6 | 3.24 | 11.27 | -6.99 | -12.42 |
| | 7 | 3.10 | 11.69 | -6.10 | -11.98 |
| | 8 | 3.38 | 9.47 | -3.69 | -9.77 |
| D | 2 | 3.05 | 5.16 | 4.98 | 4.41 |
| | 3 | 3.12 | 4.84 | 5.54 | 4.73 |
| | 4 | 3.08 | 6.13 | 5.24 | 4.48 |
| | 5 | 2.90 | 4.44 | 5.84 | 4.99 |
| | 6 | 3.11 | 3.28 | 7.99 | 7.02 |
| | 7 | 3.25 | 2.86 | 7.10 | 6.59 |
| | 8 | 2.97 | 5.08 | 4.70 | 4.38 |
| Ea | 2 | 0.87 | 0.62 | -4.99 | -4.40 |
| | 3 | 0.89 | 0.57 | -5.00 | -4.47 |
| | 4 | 0.88 | 0.38 | -5.22 | -4.74 |
| | 5 | 0.75 | 0.23 | -4.91 | -4.38 |
| | 6 | 0.74 | 0.55 | -5.08 | -4.68 |
| | 7 | 0.69 | 0.57 | -5.95 | -5.61 |
| | 8 | 0.84 | 0.33 | -1.37 | -1.23 |
| Eb | | 1.65 | 2.68 | 65.78 | 63.96 |
| E | 2 | 2.52 | 3.30 | 60.79 | 59.56 |
| | 3 | 2.54 | 3.25 | 60.78 | 59.48 |
| | 4 | 2.53 | 3.06 | 60.56 | 59.22 |
| | 5 | 2.40 | 2.91 | 60.87 | 59.58 |
| | 6 | 2.39 | 3.23 | 60.70 | 59.27 |
| | 7 | 2.34 | 3.25 | 59.83 | 58.35 |
| | 8 | 2.49 | 3.01 | 64.41 | 62.72 |

Tab. 4: Resulting B2PLYP-D3 (free) enthalpies in gas phase and in solvent ($CH_2Cl_2$) at 298.15 K.

| reaction | phosphine | gas phase ΔH | gas phase ΔG | $CH_2Cl_2$ ΔH | $CH_2Cl_2$ ΔH |
|---|---|---|---|---|---|
| A | 2 | 53.87 | 61.29 | -5.92 | -3.66 |
| | 3 | 55.26 | 62.74 | -4.52 | -2.14 |
| | 4 | 56.39 | 64.06 | -3.17 | -0.56 |
| | 5 | 53.98 | 61.66 | -5.88 | -3.31 |
| | 6 | 57.39 | 64.76 | -2.31 | 0.10 |
| | 7 | 59.84 | 67.14 | 1.01 | 3.40 |
| | 8 | 61.46 | 69.14 | -1.94 | 1.03 |
| B | 2 | -19.19 | -1.33 | -13.61 | -2.92 |
| | 3 | -14.57 | 2.65 | -7.26 | 2.53 |
| | 4 | -18.31 | -0.33 | -10.36 | 0.33 |
| | 5 | -23.11 | -5.42 | -16.67 | -6.40 |
| | 6 | -16.42 | -0.60 | -10.02 | -1.20 |
| | 7 | -14.67 | 0.92 | -8.32 | 0.64 |
| | 8 | -14.32 | 3.60 | -8.78 | 2.06 |
| C | 2 | 5.18 | 11.27 | 1.20 | 1.47 |
| | 3 | 1.91 | 8.38 | -2.63 | -1.74 |
| | 4 | 8.21 | 13.36 | 3.97 | 3.49 |
| | 5 | 6.41 | 13.07 | 1.57 | 2.69 |
| | 6 | 5.28 | 13.31 | -1.71 | 0.90 |
| | 7 | 8.14 | 16.73 | 2.03 | 4.75 |
| | 8 | 4.08 | 10.17 | 0.39 | 0.40 |
| D | 2 | -29.41 | -27.30 | -24.43 | -22.89 |
| | 3 | -26.13 | -24.41 | -20.59 | -19.68 |
| | 4 | -32.44 | -29.39 | -27.20 | -24.91 |
| | 5 | -30.64 | -29.10 | -24.80 | -24.11 |
| | 6 | -29.51 | -29.34 | -21.52 | -22.32 |
| | 7 | -32.37 | -32.76 | -25.26 | -26.17 |
| | 8 | -28.31 | -26.20 | -23.61 | -21.89 |
| Ea | 2 | 17.50 | 17.25 | 12.51 | 12.86 |
| | 3 | 16.13 | 15.81 | 11.13 | 11.33 |
| | 4 | 14.98 | 14.48 | 9.77 | 9.75 |
| | 5 | 17.40 | 16.88 | 12.49 | 12.50 |
| | 6 | 13.98 | 13.79 | 8.91 | 9.11 |
| | 7 | 11.53 | 11.41 | 5.58 | 5.80 |
| | 8 | 9.92 | 9.41 | 8.55 | 8.18 |
| Eb | | -95.60 | -94.57 | -29.82 | -30.62 |
| E | 2 | -78.10 | -77.32 | -17.31 | -17.76 |
| | 3 | -79.47 | -78.76 | -18.69 | -19.28 |
| | 4 | -80.62 | -80.09 | -20.05 | -20.87 |
| | 5 | -78.20 | -77.69 | -17.33 | -18.11 |
| | 6 | -81.62 | -80.78 | -20.92 | -21.51 |
| | 7 | -84.07 | -83.16 | -24.24 | -24.81 |
| | 8 | -85.68 | -85.16 | -21.27 | -22.44 |

Table 5: Thermochemical and solvent correction terms at 213.15 K.

| reaction | phosphine | gas phase ΔH | gas phase ΔG | $CH_2Cl_2$ ΔH | $CH_2Cl_2$ ΔG |
|---|---|---|---|---|---|
| A | 2 | 4.24 | 9.17 | -60.08 | -63.30 |
| | 3 | 4.23 | 9.20 | -60.12 | -63.25 |
| | 4 | 4.24 | 9.34 | -59.97 | -63.01 |
| | 5 | 1.38 | 9.49 | -60.18 | -63.34 |
| | 6 | 4.39 | 9.25 | -60.13 | -63.09 |
| | 7 | 4.44 | 9.26 | -59.36 | -62.19 |
| | 8 | 4.29 | 9.39 | -63.86 | -66.62 |
| B | 2 | 1.49 | 14.31 | 6.37 | 0.59 |
| | 3 | 1.51 | 13.86 | 8.17 | 2.13 |
| | 4 | 1.42 | 14.29 | 8.38 | 2.41 |
| | 5 | 1.30 | 13.97 | 7.28 | 1.27 |
| | 6 | 1.19 | 12.42 | 7.05 | 1.50 |
| | 7 | 1.06 | 12.10 | 6.55 | 1.25 |
| | 8 | 1.22 | 14.04 | 6.28 | 0.60 |
| C | 2 | 3.67 | 7.49 | -4.48 | -8.44 |
| | 3 | 3.62 | 7.72 | -5.10 | -8.82 |
| | 4 | 3.64 | 6.80 | -4.44 | -8.11 |
| | 5 | 3.85 | 8.09 | -5.41 | -9.10 |
| | 6 | 3.68 | 8.99 | -7.60 | -11.18 |
| | 7 | 3.56 | 9.30 | -6.21 | -10.12 |
| | 8 | 3.79 | 7.65 | -3.76 | -7.82 |
| D | 2 | 3.11 | 4.76 | 5.48 | 5.09 |
| | 3 | 3.16 | 4.53 | 6.10 | 5.47 |
| | 4 | 3.14 | 5.45 | 5.44 | 4.76 |
| | 5 | 2.94 | 4.16 | 6.41 | 5.75 |
| | 6 | 3.11 | 3.27 | 8.60 | 7.83 |
| | 7 | 3.23 | 2.96 | 7.21 | 6.77 |
| | 8 | 3.00 | 4.61 | 4.77 | 4.48 |
| Ea | 2 | 0.79 | 0.69 | -5.38 | -4.71 |
| | 3 | 0.80 | 0.66 | -5.35 | -4.76 |
| | 4 | 0.79 | 0.52 | -5.50 | -5.00 |
| | 5 | 0.65 | 0.37 | -5.29 | -4.67 |
| | 6 | 0.65 | 0.61 | -5.34 | -4.92 |
| | 7 | 0.59 | 0.60 | -6.10 | -5.81 |
| | 8 | 0.74 | 0.48 | -1.61 | -1.39 |
| Eb | | 1.75 | 2.40 | 66.47 | 64.66 |
| E | 2 | 2.53 | 2.09 | 61.08 | 59.95 |
| | 3 | 2.54 | 2.06 | 61.12 | 59.90 |
| | 4 | 2.53 | 1.92 | 60.97 | 59.66 |
| | 5 | 2.39 | 1.77 | 61.18 | 59.99 |
| | 6 | 2.39 | 2.01 | 61.13 | 59.74 |
| | 7 | 2.33 | 2.00 | 50.37 | 58.85 |
| | 8 | 2.48 | 1.87 | 64.86 | 63.27 |

Tab. 6: Resulting B2PLYP-D3 (free) enthalpies in gas phase and in solvent ($CH_2Cl_2$) at 213.15 K.

| reaction | phosphine | gas phase ΔH | gas phase ΔG | $CH_2Cl_2$ ΔH | $CH_2Cl_2$ ΔH |
|---|---|---|---|---|---|
| A | 2 | 54.28 | 59.21 | -5.80 | -4.09 |
| | 3 | 55.67 | 60.64 | -4.45 | -2.61 |
| | 4 | 56.81 | 61.91 | -3.16 | -1.10 |
| | 5 | 51.40 | 59.51 | -8.77 | -3.82 |
| | 6 | 57.82 | 62.68 | -2.31 | 0.41 |
| | 7 | 60.27 | 65.09 | 0.91 | 2.90 |
| | 8 | 61.88 | 66.98 | -1.98 | 0.36 |
| B | 2 | -19.41 | -6.59 | -13.05 | -6.01 |
| | 3 | -14.80 | -2.45 | -6.62 | -0.31 |
| | 4 | -18.54 | -5.67 | -10.16 | -3.26 |
| | 5 | -23.35 | -10.68 | -16.07 | -9.41 |
| | 6 | -16.71 | -5.48 | -9.66 | -3.98 |
| | 7 | -14.97 | -3.93 | -8.42 | -2.69 |
| | 8 | -14.57 | -1.75 | -8.29 | -1.15 |
| C | 2 | 5.55 | 9.37 | 1.07 | 0.94 |
| | 3 | 2.29 | 6.39 | -2.81 | -2.43 |
| | 4 | 8.58 | 11.74 | 4.14 | 3.63 |
| | 5 | 6.81 | 11.05 | 1.40 | 1.95 |
| | 6 | 5.72 | 11.03 | -1.88 | -0.15 |
| | 7 | 8.60 | 14.34 | 2.38 | 4.22 |
| | 8 | 4.49 | 8.35 | 0.73 | 0.53 |
| D | 2 | -29.35 | -27.70 | -23.87 | -22.61 |
| | 3 | -26.09 | -24.72 | -19.99 | -19.24 |
| | 4 | -32.38 | -30.07 | -26.94 | -25.31 |
| | 5 | -30.60 | -29.38 | -24.19 | -23.63 |
| | 6 | -29.51 | -29.35 | -20.91 | -21.52 |
| | 7 | -32.39 | -32.66 | -25.17 | -25.88 |
| | 8 | -28.28 | -26.67 | -23.51 | -22.19 |
| Ea | 2 | 17.42 | 17.32 | 12.04 | 12.62 |
| | 3 | 16.04 | 15.90 | 10.69 | 11.14 |
| | 4 | 14.89 | 14.62 | 9.40 | 9.63 |
| | 5 | 17.30 | 17.02 | 12.01 | 12.35 |
| | 6 | 13.89 | 13.85 | 8.55 | 8.94 |
| | 7 | 11.43 | 11.44 | 5.33 | 5.63 |
| | 8 | 9.82 | 9.55 | 8.21 | 8.16 |
| Eb | | -95.50 | -94.85 | -29.03 | -30.19 |
| E | 2 | -78.09 | -78.53 | -17.01 | -18.57 |
| | 3 | -79.48 | -79.95 | -18.36 | -20.05 |
| | 4 | -80.62 | -81.22 | -19.65 | -21.56 |
| | 5 | -78.21 | -78.83 | -17.03 | -18.84 |
| | 6 | -81.62 | -82.00 | -20.49 | -22.25 |
| | 7 | -84.08 | -84.41 | -23.71 | -25.56 |
| | 8 | -85.69 | -86.30 | -20.84 | -23.03 |

## Coordinates of all structures (TPSS-D3(BJ)/def2-TZVP) in bohrs

**1**

-4.23249240776686 2.06215889597757 1.39899612432370 c
-2.94823329880599 0.20612471456784 0.00613091574228 c
-4.48800941605508 -1.44218064026580 -1.38898675935114 c
-7.10713533376698 -1.26316729855424 -1.43599637499515 c
-8.29317461867255 0.60240636889926 -0.00117505128396 c
-6.84914243443467 2.27243581618083 1.43824822691958 c
-0.00258062382489 -0.00421192230071 0.00130677167984 b
1.29029208904593 -2.66007946587504 -0.00295121660290 c
3.48208918598846 -3.16439711315246 -1.40815267518948 c
4.64844961597692 -5.51610036818445 -1.45172429715037 c
3.64346694193502 -7.47496557579630 -0.00296521589537 c
1.47993997871087 -7.06482179296155 1.44500002586572 c
0.34080055497439 -4.69955583317529 1.40133617009343 c
4.51415784098651 -1.34173182944171 -2.86082609254523 f
6.71644914464817 -5.92397909159164 -2.85816270039375 f
4.75270818601668 -9.74210521716244 -0.00219740712813 f
0.53141755767817 -8.94728898334228 2.85140950147362 f
-1.73093374361264 -4.39371079670237 2.85435742287120 f
-3.43433472492424 -3.26102293646080 -2.83049434583431 f
-8.50125661149016 -2.85179840134628 -2.83371689221195 f
-10.81010989488059 0.78962339858502 -0.00556974469566 f
-7.99734265538399 4.05077800015779 2.83108309119742 f
-2.92533115713911 3.70647890340557 2.84272505981949 f
4.68157927065500 0.67485302162055 2.82872318537294 f
3.90307131588927 2.62924493834478 1.38988275725971 c
1.65233270627211 2.44159719603071 -0.00044340284147 c
0.98782678924624 4.59996951210376 -1.39087957114483 c
2.44426951051501 6.78383351763382 -1.43325942931426 c
4.65329550971487 6.88259495413628 0.00086714677941 c
5.38586773451011 4.79558026448144 1.43379977052018 c
-1.11584372811583 4.59365902600095 -2.83022982739915 f
1.75631712993141 8.78642754992634 -2.82485491792865 f
6.06585930562720 8.97417794947575 0.00205853756793 f
7.50017624755118 4.90420498778507 2.82626869741926 f

**2**

5.96569025732868 -2.13433208292382 1.37974399189357 c
6.53198705933009 -2.18349404897956 3.95508749243940 c
4.59760837995868 -1.90737850272006 5.72718412370753 c
2.10944468711366 -1.59148770261115 4.92163037006893 c
1.52474764047666 -1.50580108572856 2.33603426962604 c
3.48005238089044 -1.79037931107801 0.57253607781495 c
-1.81410737615022 -1.05014449911602 1.47774120988078 p
-1.92301091221841 2.41591845304490 1.21708973219181 c
-4.20333644240788 3.56324106491185 0.53548155100831 c
-4.53616072225550 6.15817370351094 0.39660215302698 c
-2.49436280672364 7.71936535667085 0.98911526321446 c
-0.18612684201622 6.65775554153221 1.69179369453279 c
0.09207373890221 4.03857498951890 1.79842230562200 c
-1.80363365588564 -1.99223838800627 -1.86527142351450 c

-1.40578812586461 -0.32117748941264 -3.88002470080654 c
-1.41425672671644 -1.19898681460634 -6.36579158344982 c
-1.80326575532548 -3.75765292524828 -6.86853309889695 c
-2.20309188753573 -5.43773867533183 -4.87409159801054 c
-2.22173172915012 -4.55699139904729 -2.39275170407053 c
1.89592014804170 3.22476229512653 2.33791996045807 h
-2.56519335481616 -5.86296241250250 -0.84329915357216 h
0.59853338207923 -1.40716309003975 6.30277795381255 h
-6.20073514193323 2.04975541703419 -0.05170970990835 f
-1.08528290223138 1.67069055173894 -3.50142336340157 h
3.05219893580664 -1.74727768656913 -1.43391637272181 h
7.46386543040079 -2.35859113847708 -0.00684079682059 h
8.46974475202368 -2.44949688697862 4.57893939570622 h
5.02314452933807 -1.96044690571393 7.73514286877455 h
-6.35797916754036 6.91619734570245 -0.16111687482144 h
-2.71658588330230 9.75737193010912 0.89839528710872 h
1.40701303758240 7.86732593872663 2.15002710215585 h
-1.10898030762491 0.11858011322031 -7.91113809099564 h
-1.80747642779917 -4.43842690742746 -8.80533527725978 h
-2.52181619177551 -7.43031874832965 -5.25330605479331 h

**3**
9.73386605865075 -0.31915463225089 2.99698950678394 c
10.23435277268100 -2.54192285848196 4.32680135844704 c
8.28378215537410 -4.24952391188010 4.80988311862201 c
5.84029402788544 -3.72876771012114 3.97233698438482 c
5.32428915487845 -1.51369997906385 2.61249491465268 c
7.29595087415886 0.18981844371840 2.13706879465703 c
2.05152297030002 -1.02562576230033 1.55375586461051 p
2.03121592049444 2.41114170995188 1.03063377124638 c
1.87264099015607 3.98658668928272 3.14479598370289 c
1.75610559767455 6.59961509952753 2.99759266377519 c
1.77996949936611 7.72443792385219 0.61241242461511 c
1.93018669105313 6.22467132898587 -1.55024480138160 c
2.05959921155146 3.60096853485708 -1.33685701962627 c
2.25968568446626 -2.17565887279665 -1.72198775810285 c
0.07312586198247 -2.18390906648068 -3.20499347731068 c
-0.02688021911652 -3.15360238259932 -5.63715589397059 c
2.16642327612397 -4.20118640363932 -6.66040596323519 c
4.38923769433556 -4.24714384332020 -5.24376778191630 c
4.43160731875001 -3.24165256832086 -2.80781425221130 c
2.19460388742799 2.44744471256817 -3.02799201558506 h
6.16806495635052 -3.27998574273155 -1.71709584204978 h
4.31225244068800 -5.04191934029991 4.37639557641687 h
1.86177147925208 2.89855609880294 5.47654497702624 f
-2.07133649716491 -1.15756414247880 -2.21823911219571 f
11.24613593869966 1.01926557419434 2.62465810321572 h
12.13524106847193 -2.93493019421433 4.99529708809688 h
8.65974072318880 -5.97519254398472 5.85671830419285 h
1.64709313297518 7.70637187106697 4.72028618229064 h
1.68300490715144 9.76811111263764 0.45450577300651 h
1.95415305297430 7.09505899818475 -3.40828800550604 h
-1.78890257559570 -3.08267071055219 -6.68347651939530 h

2.12812080537568 -4.97765379661772 -8.55948326097043 h
6.09859764427301 -5.06042618276251 -6.03579948774258 h
6.91677252593451 1.91605886055066 1.09327774526566 h

**4**
9.66273420272497 -0.08584108448494 3.60194965322130 c
10.28040516690711 -2.51049960790349 4.43334766907346 c
8.47707469352591 -4.43240522113786 4.35322856256688 c
6.08577515169562 -3.86108161855177 3.44551635712782 c
5.38563874695997 -1.46220781637426 2.59000728044474 c
7.24531244066104 0.42407054866501 2.68630548827620 c
2.09114979562809 -0.95885902638118 1.60006302039864 p
2.12867751947763 2.46361828208983 0.99329289660607 c
1.87643844153789 4.10256058573383 3.04931315061104 c
1.74770160633319 6.70939321124619 2.81443762598092 c
1.85982123369149 7.75794576145169 0.39777209628338 c
2.10819681643057 6.19275508106370 -1.70925585081105 c
2.24736900203517 3.57880833599931 -1.40817214977388 c
2.21200232704698 -2.18574030040884 -1.65024649391679 c
-0.03171242935549 -2.27664977610152 -3.04130269636809 c
-0.19924425223399 -3.28618976907380 -5.45370439745311 c
1.98215206104917 -4.28131659083794 -6.55103576185397 c
4.26301025657504 -4.23388895729491 -5.22957912208689 c
4.37178341420425 -3.19130215436370 -2.81208174635049 c
2.45280323856468 2.37138237146827 -3.05394752276337 h
6.15469388206825 -3.14869243827340 -1.79848068509114 h
4.34008284375704 -5.74781043960507 3.35246946905230 f
1.78629837166512 3.09042787772168 5.41247271842862 f
-2.16109003783455 -1.29098755548201 -1.98698293539524 f
11.06472624777142 1.41128647116300 3.65871263650597 h
12.16205251602765 -2.91600631274139 5.14454031135259 h
8.89276440859917 -6.34039614912518 4.97840264405347 h
1.56150066443238 7.86870393071786 4.49535434258932 h
1.75383020435233 9.79470749010667 0.17128510113212 h
2.20064292583002 7.00525594425805 -3.59113225222705 h
-2.00347210855556 -3.28506869446076 -6.42781935311660 h
1.89050072391594 -5.08873060123254 -8.43529191926983 h
5.96380421604473 -5.00263385839248 -6.08190690193552 h
6.77886362167053 2.31130908724420 2.03131670851803 h

**5**
6.09732096094926 -3.12436311352049 1.65988930370789 c
6.85068094950223 -2.12502091039016 3.97831392458292 c
5.10258873254548 -0.81645843269998 5.46054261594432 c
2.62498641962824 -0.51498206145455 4.62783106523701 c
1.85817812990325 -1.47617461331213 2.27302924540787 c
3.62248020352391 -2.80101260924659 0.81090098600696 c
-1.49428903297628 -1.21012580845798 1.44936811677791 p
-2.03110488973276 2.22897530661156 1.33291930326643 c
-4.56493530307906 3.00152103031464 1.19882701866965 c
-5.18817536376704 5.55950837781906 1.13169237983320 c
-3.28585943976420 7.38197557846959 1.25312736715133 c
-0.76330857371689 6.63035013745067 1.42389982267718 c

-0.13552792878188 4.07206192362551 1.45166733232932 c
-1.48696047509602 -1.99190910005483 -1.94936716470817 c
-0.13139459148351 -0.71589796906518 -3.83528500690247 c
-0.26542760748168 -1.30411796006247 -6.38756054244493 c
-1.82797393537310 -3.28877756274260 -7.13873660368222 c
-3.21591360324017 -4.64728554654953 -5.36198408938195 c
-3.01048988690054 -3.96910182640191 -2.83328111117448 c
1.83205398479793 3.50309432861128 1.54856552928677 h
-4.37484774320596 -5.31825874991701 -1.13631523756475 f
1.27284556355930 0.48695607297846 5.80729512678784 h
-6.05155987266782 1.58242029478307 1.15051006941604 h
1.42515127550762 1.19375066123746 -3.14696727002956 f
3.06615577885656 -3.58191103891803 -1.00360256015704 h
7.44122880286455 -4.15105227873959 0.49522508003024 h
8.78104067025651 -2.36920207659042 4.63195131861117 h
5.66613765503877 -0.04037437581086 7.27610209969179 h
-7.15750877529568 6.12827308832733 1.01304539198922 h
-3.76697973098214 9.37760946794191 1.22487845168791 h
0.72586642425722 8.04153814718835 1.51633648269029 h
0.84087078125319 -0.22388108593536 -7.73240021601873 h
-1.96003580277227 -3.78155581826062 -9.12556968379205 h
-4.43900277612688 -6.20209247722886 -5.89528454592691 h

**6**

5.67549790861145 -2.24505142050023 2.13175257155403 c
5.78957176675001 -2.27244785385934 4.76706387419717 c
3.58770932196106 -1.93184635379055 6.17606330728271 c
1.28337319348927 -1.57597071219308 4.95026099603431 c
1.16115997939950 -1.51285472735858 2.30358622570244 c
3.37850388248998 -1.85802087016089 0.90407700122778 c
-2.01211250927242 -0.96551846348795 0.97477005392746 p
-1.94585876855312 2.51957891243718 0.91067368861105 c
-3.76250523557659 3.85642502682833 2.29210634600637 c
-3.79492637952851 6.47259033154391 2.51938189748291 c
-1.91548427175608 7.85753340193608 1.30567699052720 c
-0.05191719813035 6.64004394470228 -0.10698502496683 c
-0.11640334954597 4.02674620977646 -0.26540664893611 c
-1.64264539776810 -1.90800796614237 -2.35027962599097 c
-2.35338817857500 -0.53354416622503 -4.49828504086599 c
-2.21415323311039 -1.46700432218192 -6.94674065479902 c
-1.36505267899457 -3.92931022958014 -7.32580101713307 c
-0.70320947045178 -5.43060054425808 -5.26463029224316 c
-0.88947985386100 -4.39854727038379 -2.86474842759778 c
1.68453494895922 2.87796694963107 -1.67812123152944 f
-0.32261398957473 -5.90923092874616 -0.86523244415746 f
-0.43877310582101 -1.34744899564490 6.04890234547975 h
-5.60663612087467 2.54216614239588 3.49395097083256 f
-3.26599187020432 1.84843772868316 -4.21512874253843 f
3.31172587322899 -1.81410037016802 -1.14501178664009 h
7.38420704634037 -2.51578768720420 1.02553702304522 h
7.58514893317276 -2.56945334474037 5.71686108281000 h
3.65722832061188 -1.96730864589101 8.22762952005021 h
-5.26726338656934 7.37182283820994 3.62447947035410 h

-1.90225627516683 9.90320354311534 1.45550727767065 h
1.42233459811753 7.67658527505851 -1.08211155820542 h
-2.77921561327970 -0.26135846315057 -8.50438298984604 h
-1.24335114732833 -4.68839104306455 -9.22679541068274 h
-0.07529173918908 -7.36887392558636 -5.48138374666348 h

**7**
5.91564016627331 -2.47807046282293 2.24369190271632 c
5.96543473139044 -2.27902290329869 4.86700387087117 c
3.77757678159116 -1.65426075403024 6.19585005120215 c
1.57684069741263 -1.26497112570004 4.83210831514863 c
1.39006380306942 -1.44349198158349 2.19434223221646 c
3.65852494470803 -2.04619916614307 0.97300041048674 c
-1.81665589972032 -0.98268371777993 0.89964152936779 p
-1.88969091883028 2.49127124431927 0.91628138502250 c
-3.92685730793035 3.71991430471079 2.07181435571608 c
-4.08280844194608 6.32548934376325 2.35549852626147 c
-2.10778796868672 7.80433441597648 1.43975297989660 c
-0.02910740373744 6.69401135703568 0.25718330534988 c
0.02294687457218 4.08588747096931 0.02271333789056 c
-1.56419481992614 -1.89254136502859 -2.43851184422556 c
-2.20333412930786 -0.46491226451468 -4.57015159493898 c
-2.25607902754364 -1.43921546391748 -7.00808621763729 c
-1.67387651403004 -3.97712600882381 -7.38352926669126 c
-1.06644353872686 -5.51634887399387 -5.33114842189185 c
-1.05225880854192 -4.44167496096449 -2.94812069018531 c
2.02439962539043 3.03176435231609 -1.17138230695824 f
-0.48316186310188 -5.94427915792641 -0.93919667030746 f
-0.54970723754748 -0.63389836568979 6.13042476833066 f
-5.86667244989431 2.30701795796920 2.96013517339050 f
-2.83142762985213 2.00812586859925 -4.29596498326660 f
3.71925148596824 -2.21065686676371 -1.57850877973749 f
7.59250454850731 -2.94018651189288 1.16010223111173 h
7.71842003170980 -2.60221310235033 5.88119035985662 h
3.75228805942997 -1.46783062449318 8.23593265403052 h
-5.72071431885067 7.14537392939428 3.27314582646124 h
-2.18971847266850 9.84411868832881 1.64034078658618 h
1.51943123968682 7.80912161267767 -0.48907840176097 h
-2.75244502069901 -0.19910743513990 -8.56205503712559 h
-1.70316349174624 -4.76262223949193 -9.27746451099744 h
-0.61474972642184 -7.50269219371058 -5.54971827618954 h

**8**
-7.90527535988007 -3.40727156794141 -3.72632332164925 c
-5.73336006682289 -4.87163923248428 -4.00920118305427 c
-3.45420628586484 -4.09150075031294 -2.93976977075597 c
-3.31261893946413 -1.83163405613686 -1.56856648441922 c
-5.52187777619965 -0.39066883431316 -1.25742481672833 c
-7.79056244391881 -1.16221910175260 -2.34455683634322 c
-9.67637222914262 -4.01179308170981 -4.56884494924708 h
-5.80399184033270 -6.62460306357738 -5.07572445017248 h
-1.77776163286728 -5.25091120635274 -3.18158689813689 h
-5.45883236504492 1.35183648424731 -0.17037431880446 h

-9.47426138679535 -0.01227359756371 -2.10385142884818 h
1.24004471853669 7.36903460440530 -2.44571593534894 c
-0.50404522218554 5.95676570619666 -3.83236052671360 c
-1.05896681710597 3.47695624838105 -3.13965334060264 c
0.11313402104153 2.38652830573338 -1.03120818454848 c
1.83514952418231 3.83262744536855 0.37546528289213 c
2.41578622477052 6.29951388427069 -0.34178694109801 c
1.67221732409235 9.29872086990544 -2.99678468626757 h
-1.42416597399411 6.78244195614177 -5.47180403275087 h
-2.39562979669549 2.38169579723778 -4.24295366309557 h
2.71642000707683 3.01417265201271 2.04253751913318 h
3.76242229948573 7.39272482856582 0.75641282115236 h
6.09057746503860 -5.30047351729681 -3.71151938393118 c
4.51840799356594 -3.80750650862275 -5.20872780103904 c
2.53075489370365 -2.50021248271312 -4.08985455084752 c
2.03689711486459 -2.61117899055172 -1.49222683519934 c
3.65247651661872 -4.13619037250674 -0.05770991099955 c
5.65707794376027 -5.47157920276805 -1.12192989867147 c
8.00857912802467 -6.57114800290199 -4.76470385377535 f
4.93396577406274 -3.65874453428422 -7.70880845111563 f
1.05362676456833 -1.11198486628015 -5.62227998603630 f
3.31350364931887 -4.36552759189343 2.45329208810495 f
7.16791277621093 -6.91564650505371 0.31739246894280 f
-0.48402600260877 -0.83031171544906 0.15615225997495 p

**9**

-7.39909294368645 0.30959420299212 -2.87975263173787 c
-5.23898180485715 -0.54473373434089 -4.12934149165766 c
-3.02949436020637 -1.02239666699347 -2.78099575147880 c
-2.94120462429409 -0.67908943466132 -0.15054655711111 c
-5.12191617058228 0.19773352680438 1.07912598379477 c
-7.32963214581064 0.68387665398172 -0.26992386684922 c
6.57879704265084 0.62196365281971 -1.98780998436649 c
4.50511249634010 2.21929528563142 -2.31345973780633 c
2.16855759402701 1.58514472180308 -1.28079617814925 c
1.86285807989734 -0.64831926815769 0.12033059685520 c
3.95959029690891 -2.24554608316257 0.41804420401957 c
6.29483171846578 -1.61619979853853 -0.62174689135544 c
-0.60891616938505 -1.27416587003012 1.29079991351204 c
-0.73144284877798 -2.35100727680027 3.59292390721888 c
-9.11768120838077 0.69633645310253 -3.93373568395048 h
-5.27578004274102 -0.84213610007432 -6.16062613066870 h
-1.35428695578796 -1.69043538116766 -3.76097836543125 h
-5.05834985145446 0.53810867378297 3.10276194363969 h
-8.99250975092543 1.37823624722044 0.71441141503826 h
8.39729357430763 1.10947881112576 -2.80601582839483 h
4.70883909857966 3.96595299324489 -3.37343851835862 h
0.56112941311546 2.83573579250968 -1.53592707187721 h
3.73133164808379 -4.01276915230430 1.43772916105229 h
7.89061470360817 -2.88647454647827 -0.38507468633659 h
-2.52579957790132 -2.90084477544789 4.42112557689132 h
0.96013278880640 -2.70533892686138 4.69791667350790 h

**1**-H anion
-2.15966524388772 1.88812559414274 1.02056619261237 c
-0.44022097491906 -0.03362152660559 0.48029773553655 c
-1.50783069640697 -2.13229111721241 -0.71800645628480 c
-4.05267261454437 -2.34381422537652 -1.34064125668623 c
-5.68408634076611 -0.36372820275761 -0.76491349541268 c
-4.72503812002176 1.77070363721389 0.42472101490029 c
2.61120868396007 -0.02310167834144 0.99699895744949 b
3.49473614953216 -2.17023131505879 3.05389413404784 c
5.98796921489147 -3.03604928656125 3.01257639728827 c
6.92942034828325 -4.89063334390761 4.62396701538976 c
5.33055135243712 -5.97854624245818 6.40400167889154 c
2.83342990226449 -5.17499401947049 6.53763198237663 c
1.98353119075936 -3.30286982856925 4.89153054098760 c
7.65660171808987 -2.04813714054986 1.33313477894494 f
9.36883879459442 -5.65546608527416 4.48626284186611 f
6.19684364634317 -7.78834699163432 7.98750755326474 f
1.27129787585111 -6.20762608161962 8.28251683059884 f
-0.46321654335892 -2.58807658996425 5.19322823596608 f
-0.02611460229425 -4.13877422974593 -1.32086802896185 f
-4.96849005443977 -4.43605661908729 -2.49674942866107 f
-8.16633798314049 -0.51649692695218 -1.35517925329635 f
-6.30020616981255 3.70465266020977 1.00018119154987 f
-1.40646165880096 4.03524005646312 2.21271508730105 f
3.06184193834535 2.29395210881431 6.18033802205301 f
3.99375707517009 3.65620871688369 4.21515656673152 c
3.77380589719430 2.74490188320591 1.75098104774412 c
4.72418267374652 4.36616846714733 -0.09956643996611 c
5.83624304289155 6.69516868752750 0.42497003124948 c
6.02903152215079 7.50000287729262 2.91828056688445 c
5.09463881163980 5.96413958333103 4.83546892284784 c
4.58262994026510 3.72922132679669 -2.57916954349191 f
6.73435679260109 8.18719334185063 -1.45195180861522 f
7.10261961715028 9.75212724355413 3.47206407785872 f
5.25206950751779 6.74874390292279 7.26639788097399 f
3.57272630671376 -0.62638263620927 -0.98533957393879 h

**2**-H cation
6.15370665817906 -2.57295748030144 1.68621679984757 c
6.50499640751468 -2.49812849598972 4.29899319906177 c
4.49327265803554 -1.91328479964075 5.90747186287948 c
2.11809821934131 -1.39344906635925 4.90808818745450 c
1.77029507282967 -1.46862910851053 2.27693631957784 c
3.78411639592442 -2.06170691762373 0.65921397840086 c
-1.25236223867164 -0.71119880598487 0.98161059217202 p
-1.78906934928669 2.61704156463643 1.11895757539445 c
-4.23296807133226 3.55461097924442 0.73918549881236 c
-4.77340634743934 6.11268660178083 0.78982320228803 c
-2.78474812409763 7.79160503288746 1.22669380083046 c
-0.32187282050491 6.91691453795190 1.60887748949308 c
0.18364859793485 4.33773427396986 1.56185502087907 c
-1.62642978151886 -1.90759724327069 -2.14794019113585 c
-1.42063900008516 -0.27374539890151 -4.22358205148926 c

-1.63338635973618 -1.25168483144164 -6.65824363837183 c
-2.05195036443520 -3.83118348527341 -7.01305558294824 c
-2.26048590143905 -5.45430886968415 -4.94015251302510 c
-2.04606974428382 -4.50496835657047 -2.49846646997888 c
2.08655300580754 3.63830698497313 1.87414919563038 h
-2.20913909522135 -5.76692460707035 -0.88659071701930 h
0.55340317539978 -0.93935783470451 6.15850457407335 h
-6.10496554981190 1.86200013924494 0.31471876970339 f
-1.11180098448780 1.73441133873516 -3.93588257226181 h
3.49279870972915 -2.13733825028165 -1.37047287136326 h
7.71984697853049 -3.03900330563330 0.44715013296395 h
8.35267748600319 -2.90783960299451 5.09048134115721 h
4.77419478668133 -1.87201048486433 7.93844727660884 h
-6.69662198106086 6.75731795539011 0.49630637168770 h
-3.17131303597707 9.80536001357925 1.27290061701600 h
1.19975638235828 8.24629051337020 1.95215174289888 h
-1.48278244519659 0.00167163420437 -8.27429281624720 h
-2.22694637672921 -4.58262333328998 -8.91379340799154 h
-2.59935130953369 -7.45633397259060 -5.22707704983863 h
-3.07745865342033 -1.87599931898668 2.51186533283960 h

**3**-H cation
9.96601025760821 -0.37775898146378 3.42577413480673 c
10.25998179566012 -2.68137157057188 4.67731124002353 c
8.23751158958678 -4.36686884886436 4.87964841065275 c
5.90668193959425 -3.75867145090984 3.82595859382754 c
5.61821817019644 -1.44075255165269 2.56658556606022 c
7.64274547810026 0.25818027587859 2.36549365608400 c
2.66406390231055 -0.69930752899560 1.12674228820084 p
2.19239691213492 2.62498495381267 0.84420714955979 c
1.77708022369033 4.05227429923880 3.03145595541519 c
1.42162608700478 6.64182201927709 2.96411108310100 c
1.50021477835314 7.84272441727336 0.61574109394921 c
1.91709727152297 6.47179794216715 -1.60331951202320 c
2.25820542919785 3.86782302188980 -1.49983334621629 c
2.39171249638698 -2.18652274829415 -1.88880492729730 c
0.02748236725636 -2.32135698998553 -3.06704767665815 c
-0.30799439734083 -3.44261862571261 -5.40561370807972 c
1.81024117793450 -4.45734844117705 -6.60896191048714 c
4.19772008163809 -4.35280660884980 -5.48371563106762 c
4.49693750255426 -3.22737061230669 -3.12716084010212 c
2.56744281056872 2.78580478737392 -3.21520218841204 h
6.33856098166168 -3.15775843390954 -2.22623434551546 h
4.33046696223216 -5.06451963915104 3.99137963301918 h
1.72563793363885 2.81141364060000 5.26886711634211 f
-1.97575007899958 -1.30861757250214 -1.83653716608495 f
11.54043033895894 0.92859743701653 3.28484268662708 h
12.07083283616186 -3.16207303171685 5.51276236248949 h
8.47310905252963 -6.14782698518991 5.86848765720737 h
1.08916763696428 7.67337712503128 4.70359271870995 h
1.22795838996666 9.87354913482888 0.52432243723652 h
1.96610620087663 7.43367699290990 -3.41233262233573 h
-2.17584047422808 -3.51463875808654 -6.24615493681821 h

1.58516216600248 -5.34434468246034 -8.44454920936598 h
5.82135969457332 -5.15896890711170 -6.43994306243639 h
7.39558181708375 2.05801704810595 1.41059766886833 h
0.75446866987839 -1.67454343946966 2.68031589647755 h

**4**-H cation
9.88398503128347 -0.23054461192653 3.79728560405543 c
10.24237572601091 -2.66155075709065 4.76691841101859 c
8.33083857125672 -4.47587038794214 4.63638981911598 c
6.06863567912608 -3.79828631776366 3.51317367302778 c
5.64826184107881 -1.37876666300251 2.53176860476997 c
7.59393035484351 0.42015150193373 2.68431052548363 c
2.67333382412244 -0.67025705907751 1.11911532280806 p
2.25524889429091 2.65884260625587 0.81638743319516 c
1.80881215100143 4.10583568663183 2.98458510525000 c
1.46489621875529 6.69622791028300 2.88861387136650 c
1.58516009502476 7.87594198793010 0.53132119041968 c
2.03490549454061 6.48461412530643 -1.66869789531863 c
2.36619041278239 3.88076639124157 -1.53717933215164 c
2.37747059886099 -2.19026531867119 -1.87269395517930 c
-0.01294073301829 -2.40425083047305 -2.98351726780669 c
-0.37775822538691 -3.56125639333904 -5.30013457181004 c
1.73607208974714 -4.52667495531585 -6.55015976652598 c
4.14998132291730 -4.33645544028774 -5.49406928003743 c
4.47943097032507 -3.17648181419350 -3.15901260999863 c
2.69840736166698 2.78173845087991 -3.23733750575747 h
6.34398806564725 -3.03615427549674 -2.31500235341376 h
4.16747468598199 -5.50188289340198 3.33600804860134 f
1.71886337316672 2.88540665276826 5.23184231420896 f
-2.00855300648672 -1.43119939791208 -1.71118053430565 f
11.38677796095561 1.15747352734433 3.92019915231801 h
12.02945899664609 -3.15705803231196 5.64289955653920 h
8.57373694432766 -6.36822933808245 5.38482988981254 h
1.11103405645356 7.74493462959825 4.61354016420073 h
1.31847273224390 9.90634528253842 0.41757373927828 h
2.11609194048648 7.43053118805345 -3.48489250117450 h
-2.26467861852466 -3.69843686100729 -6.08815383556953 h
1.48754053031391 -5.44232555576710 -8.36848694832435 h
5.77042643493676 -5.10242156944976 -6.48783352795574 h
7.29109174722241 2.30897753115913 1.94311682712458 h
0.76942808403640 -1.59875258746124 2.70422488717151 h

**5**-H cation
5.91427059016760 -3.69510887466277 2.09945446881856 c
6.66655798032479 -2.42094467710854 4.28365488488062 c
5.08531939183067 -0.62571504139859 5.39882948962502 c
2.74170291810330 -0.08990524426059 4.33369895520206 c
1.99128399978705 -1.37422488667014 2.13463687000435 c
3.57366756838654 -3.18219306849463 1.01472335541769 c
-1.07127651378425 -0.76963092790916 0.85443775202349 p
-2.01554864320111 2.43978701245893 1.26782704473385 c
-4.53994780086561 2.93788075713403 1.92052144368637 c
-5.33408242284521 5.43039180743191 2.19438204937139 c

-3.62610604160827 7.40604986496572 1.81979584170002 c
-1.11545800368783 6.90483770493478 1.17432572008995 c
-0.29377202857521 4.42352415244145 0.89140825292448 c
-1.28286602530002 -1.86995739762970 -2.33520133819238 c
0.24123362545350 -0.84003955476043 -4.24518142339625 c
0.11058509244559 -1.60416924049327 -6.73928973888955 c
-1.63129609302097 -3.48552576289192 -7.36999813215238 c
-3.20130789711001 -4.57568340756628 -5.55368169595736 c
-3.00302824409322 -3.74934969831673 -3.07810529642356 c
1.65532474515063 4.02808249305681 0.39323813728133 h
-4.51138303090584 -4.78508079730778 -1.29822971306998 f
1.51501463676574 1.31400989667691 5.19081779636989 h
-5.86508095009473 1.39805154318295 2.22067943244295 h
1.90335391048618 0.97837182428791 -3.56371732338160 f
2.98558972422040 -4.16815391299528 -0.68572251619365 h
7.15130440858944 -5.08471828681097 1.23709752162251 h
8.49597243258376 -2.82481245706763 5.11928947615381 h
5.67940499708905 0.36140486437923 7.09528005718840 h
-7.27846091256083 5.82798451417148 2.71027199383475 h
-4.25181175503840 9.34715528438581 2.04104608381833 h
0.20395611254054 8.44928442941895 0.89271480896550 h
1.33469553612005 -0.74418863081398 -8.13832179142969 h
-1.76776545072324 -4.11184246127624 -9.31756267402035 h
-4.55696465808832 -6.03601714680591 -6.02860506533523 h
-2.90635919854164 -2.19862767368644 2.11516727228666 h

**6**-H cation
6.15010221605966 -3.19555146047779 1.83832886798705 c
6.66340590455157 -2.46276335853248 4.31782725782268 c
4.84885628549933 -1.17213323178764 5.73920784928548 c
2.51214700786302 -0.60153477894803 4.68388902898266 c
2.00632612753274 -1.34272824211989 2.18590726380841 c
3.81527688189202 -2.64211350369389 0.75611635248446 c
-1.01821010339095 -0.65374250070296 0.87367821617827 p
-1.82667863124761 2.61839073611821 1.05513838485337 c
-4.38361606299675 3.30171389686799 1.29188355161233 c
-5.18251190191075 5.78025721113700 1.48916200939415 c
-3.35140173944515 7.67986044424085 1.42780339765674 c
-0.78871962214858 7.11578400368862 1.17081627163259 c
-0.06739311491893 4.60707121575419 0.97862705255937 c
-1.39512313389661 -1.91623026088567 -2.23028077101212 c
-0.37707503378395 -0.71900623512017 -4.36617772575428 c
-0.70618820811620 -1.63424085212813 -6.79162811815994 c
-2.11045237381885 -3.84731240966292 -7.10603789232893 c
-3.15848907480674 -5.12346589985735 -5.04926473099507 c
-2.78017286539408 -4.14123220811760 -2.65448090186011 c
2.39605957796548 4.04834375801983 0.70688709639434 f
-3.75807112386552 -5.35048310423805 -0.63434063583978 f
1.10532929048371 0.41206992045256 5.78443425273345 h
-6.10825281195854 1.41505853505269 1.31544266155935 f
0.98353763503631 1.40557264936836 -3.98626087454082 f
3.40609101274356 -3.21394165685793 -1.17053461051040 h
7.56475488846378 -4.19726987692018 0.74299229714534 h

8.48601229653566 -2.89830809977859 5.15219294623894 h
5.25689904644026 -0.61109490508141 7.66885583563673 h
-7.17919024521234 6.19716936742697 1.67545663146763 h
-3.93624920494753 9.63961952575504 1.57380819576230 h
0.64088638781165 8.58148468962303 1.10657661397467 h
0.11949449160506 -0.63721745405034 -8.37897229798808 h
-2.38897544417788 -4.59545821006203 -8.99462558987988 h
-4.24358134699873 -6.84551594419732 -5.27933949329528 h
-2.88078600744817 -1.86838476028492 2.29824660699442 h

**7**-H cation
6.49640910754056 -2.28266687266889 1.93526336409195 c
6.51645190510008 -2.67958812122888 4.54337504310792 c
4.33870015281549 -2.38404653178004 6.00382308956943 c
2.13200290322025 -1.68487939921360 4.79256310696543 c
1.99893116735873 -1.28179200373447 2.17138946385079 c
4.24789435245942 -1.58492150161050 0.79832329192461 c
-0.96647994583083 -0.50341810245337 0.77860411789305 p
-1.67888695408045 2.78657265045238 0.88097398868669 c
-4.20438558962843 3.54436955374201 1.19305049922599 c
-4.91595497635880 6.05068551506509 1.38090704048048 c
-3.02893720095363 7.88956571744115 1.23351069902893 c
-0.49288264468809 7.24418061827241 0.90028789270751 c
0.13727495404538 4.71268064748754 0.72128899840913 c
-1.41274083646071 -1.86725929580832 -2.26772450710153 c
-0.95007998374041 -0.59253644793077 -4.54708852518633 c
-1.40664044670613 -1.68720352808644 -6.87727353873147 c
-2.34549283395185 -4.15161257685043 -6.94701614824035 c
-2.82070293394322 -5.51361198707041 -4.73734102519775 c
-2.33795906356855 -4.34942108470276 -2.44915408450592 c
2.56867573370445 4.05134819315991 0.36545954061118 f
-2.75414557517925 -5.61408483034262 -0.26899663693640 f
-0.00897550961579 -1.35869288473479 6.14685845586988 f
-5.97811584885878 1.70879058127241 1.30266906842766 f
-0.01577189479043 1.77224818503319 -4.43624343406527 f
4.19223981055040 -1.16077374818779 -1.71037433768557 f
8.18437140086020 -2.49406413598613 0.79436869594330 h
8.26873575558447 -3.22228466416301 5.45925361364399 h
4.33959576126764 -2.67820897713714 8.03083565406989 h
-6.89076148360103 6.53467529200948 1.62817311598422 h
-3.54778073318567 9.86831587110289 1.37178539242414 h
0.97734515118725 8.66416226931697 0.76700047716736 h
-1.01968775095358 -0.62693067638010 -8.58655199485714 h
-2.70685768870559 -5.03346097504535 -8.76239043540799 h
-3.54065197876931 -7.43081729470583 -4.77429881788133 h
-2.77091728212375 -1.65033345453386 2.31878387571343 h

**8**-H cation
-8.02819037953059 -3.52335723167682 -3.29670288397625 c
-5.94175874772652 -5.12909935232804 -3.46977099792469 c
-3.56806333887948 -4.29056559871175 -2.70911191135666 c
-3.29964475947991 -1.82238225922398 -1.77782840475462 c
-5.39596384549654 -0.20148610255350 -1.59937058407871 c

-7.75760800550940 -1.06920733167485 -2.36288882755129 c
-9.87455922013607 -4.18559343610433 -3.89689333984774 h
-6.16108542794945 -7.03221403637471 -4.20087739670738 h
-1.94353877068719 -5.53655631357258 -2.84258474546441 h
-5.17979258173237 1.70929765394590 -0.88369039549470 h
-9.38506077552887 0.17166680186978 -2.23438324800504 h
1.04292321162563 7.66931670644035 -1.96517710565227 c
-0.17338008646210 6.25358703378676 -3.83296902002757 c
-0.62420207122863 3.69020437740847 -3.46367194318967 c
0.15390204835600 2.55491336055521 -1.19387953645315 c
1.37412695299004 3.97442176816432 0.68976957349400 c
1.81239978952962 6.53650330521548 0.29039961986600 c
1.38473945835725 9.66947776425140 -2.26628520276749 h
-0.77219065267052 7.14828122541052 -5.57825609308139 h
-1.57259234017649 2.58717672739874 -4.90877136079658 h
1.96286023965220 3.09263803049995 2.44848487472769 h
2.74225590617877 7.64789897560308 1.74114164182207 h
6.15920698326892 -5.60597421147224 -3.83742890154202 c
4.61674176670551 -4.22603208819935 -5.48456545021193 c
2.66173968240104 -2.78638173826092 -4.48977361710195 c
2.18920785696055 -2.68042217652958 -1.88529902042469 c
3.76798774410613 -4.08078010857431 -0.28078780493815 c
5.73930316158454 -5.53898925861952 -1.22966778771481 c
8.03252104226306 -6.98875378634790 -4.75856389547467 f
5.03121432693829 -4.30386564178065 -7.96418600648339 f
1.17947813641051 -1.46131814508331 -6.06945852581382 f
3.39236711048789 -4.04107440261359 2.22799430929632 f
7.21518615800871 -6.86316668443714 0.31707980106882 f
-0.30800170859634 -0.73811075958264 -0.66787073381658 p
-0.08542386403410 -1.07300506682824 1.94776992037676 h

**9**-H cation, $[Ph_2C\text{-}CH_3]^+$
-6.95340872223401 0.71255249358922 -2.21436607575831 c
-4.78135837065385 0.04600655971284 -3.56751527860048 c
-2.57874909574668 -0.55114447995149 -2.28789403115664 c
-2.51517484545315 -0.54585068327949 0.40186623654006 c
-4.76543317682309 0.06901649174195 1.73307529585631 c
-6.93414799418607 0.73478624059737 0.43348818403428 c
6.98352356676806 0.30832208447753 -1.36425578866930 c
4.92825623096537 1.82933438193351 -2.03408732278526 c
2.55530810694189 1.32103298267375 -1.05270390981606 c
2.19369478928534 -0.72429620962082 0.65460947407381 c
4.32691849539658 -2.19173285737966 1.36852834252343 c
6.67573809951470 -1.70352302524058 0.33410725429848 c
-0.24561469032176 -1.22850021443787 1.71687445866510 c
-0.41445907210467 -2.56282042788614 4.19647679533724 c
-8.67420722782741 1.19472367557129 -3.22275637064123 h
-4.82928315726170 -0.03235962222238 -5.61586830841200 h
-0.92470944035242 -1.17411194886524 -3.32502067887085 h
-4.75413977060592 0.14774666154703 3.78049170768276 h
-8.62101168786280 1.27352870884938 1.46692383809902 h
8.84082604400104 0.70601928229363 -2.14079676798892 h
5.19714481187227 3.42630962017994 -3.29152857709882 h

0.98297808801736 2.56615562745572 -1.47323488206889 h
4.09393535851169 -3.76808530451834 2.65783211764822 h
8.28227034329820 -2.87358128937843 0.83799698144113 h
-0.16037682677470 -4.59845294894518 3.84352354260529 h
-2.27033357756275 -2.36575395518511 5.06716355016702 h
1.06333972119837 -1.96972684371222 5.50829221289469 h

activation product originating from 9, $Ph_2CH$-$CH_3$
-6.72479696496953 0.14362062972245 -2.43980914141664 c
-4.64480819944740 -1.31311364823598 -3.15679144971718 c
-2.54923806541820 -1.50116247119437 -1.57333767452459 c
-2.49904096108209 -0.24743737265755 0.75594841651046 c
-4.58970666838972 1.21033958619470 1.45370674567131 c
-6.69019348162198 1.40920754715698 -0.12877022601096 c
6.74373377877530 0.55503813214611 -1.60721230448474 c
5.03112541928431 2.53935998080404 -1.28724425712133 c
2.80467407516097 2.15462980471320 0.05789326597070 c
2.23747223053787 -0.20611140357301 1.12084992758379 c
3.96729085624080 -2.17446719294639 0.79202633540771 c
6.20311629657104 -1.79963087090344 -0.56365986536410 c
-0.25024355207472 -0.52347218752988 2.53529983031336 c
-0.45812988563614 -3.01139368536843 4.02530292448220 c
-8.35362352803596 0.29945046649529 -3.67956193080740 h
-4.65122436341850 -2.29468944468787 -4.96058128843621 h
-0.91929751468677 -2.60751951038835 -2.15686983721364 h
-4.56754578129970 2.20346165125503 3.25424681042219 h
-8.29352694464377 2.55879308746071 0.44119291958998 h
8.48236267451259 0.84827370277083 -2.65851286509366 h
5.43386265578295 4.38594273800910 -2.09025043028525 h
1.46527929923060 3.69802984029687 0.28029129567697 h
3.58380038951917 -4.02213844119088 1.59689597220663 h
7.52155068380323 -3.35671572263270 -0.79714657826185 h
-0.37252641528161 1.03340602922271 3.90277746984135 h
-0.46512166743283 -4.64274616585655 2.75209054611979 h
-2.23012015495327 -3.04194369067008 5.08924359607442 h
1.11387578897333 -3.21801138841248 5.35598179286671 h

FLP 1·**2**
-2.27096598797756 3.26832815672846 2.23201922193983 c
-1.21727280722353 0.97095198550887 1.44321818360789 c
-3.01341199957750 -0.89643610047140 0.87089471980157 c
-5.61248121230828 -0.54032434658241 1.02348792961391 c
-6.55409353755019 1.78945504252903 1.80609970828718 c
-4.86348585654075 3.69963739341493 2.43005563081993 c
1.80977516860305 0.51828755235451 1.06779367935622 b
2.83614454750979 -2.23437918737897 2.02986839490309 c
5.26883505306773 -3.06253689688688 1.43384274674203 c
6.34695056940773 -5.29851323274438 2.29588945796210 c
4.97504747036010 -6.83261321901980 3.92661141816593 c
2.58330298422578 -6.05143310762074 4.68716604272835 c
1.59126277266021 -3.79130303337668 3.77642180547336 c
6.75177723256101 -1.62596637340332 -0.07963684268579 f
8.68583371219970 -5.98002196520481 1.56564950553738 f

5.95607408170357 -9.00614127260016 4.78788729757172 f
1.27305338196019 -7.45490064118278 6.35459512094030 f
-0.63413766239729 -3.09710632427249 4.82343145314913 f
-2.27013292110142 -3.22079751733614 0.11620043100568 f
-7.21854215437946 -2.41708686540412 0.43052265654389 f
-9.05278202741868 2.18210415513706 1.95056328443998 f
-5.74150119282361 5.96631029056309 3.16568217134688 f
-0.80249621315813 5.27311241015685 2.81143200866371 f
3.55170387617662 0.58271826755779 6.31638170585772 f
4.39179682834664 2.49385850116728 4.84301233099750 c
3.60959118777291 2.70862490396846 2.31962538200944 c
4.47592590665497 4.90170840030503 1.14274118139650 c
6.07325475826876 6.67129619294652 2.24861462044224 c
6.85415451227551 6.32041226104914 4.73263508277906 c
5.98063118865114 4.21764059453948 6.04390500696297 c
3.70640883207571 5.45798845353699 -1.24381538308376 f
6.84085665900829 8.71692652341014 0.94676721200780 f
8.39140815869236 7.99571654687370 5.85140724698519 f
6.65756208918585 3.87427949144635 8.46764289802706 f
1.91563507621115 0.66836129045570 -3.03198002936544 p
0.05556557490560 3.29525817524636 -4.33852000092277 c
4.85671146093879 0.83181016990783 -4.84842581870110 c
0.38887316365263 -2.13100556870093 -4.39006959342192 c
-2.49705739986219 3.66863316900128 -3.71598384936621 c
-3.83633476402209 5.70902669880159 -4.70435535282989 c
-2.65730541158735 7.41154953576661 -6.33079333111501 c
-0.12697779201307 7.05202132172484 -6.97017495749404 c
1.21994030314700 5.01647159004040 -5.98546761209450 c
1.59563887692097 -4.48269762201209 -4.34373514395525 c
0.51112021763803 -6.67296481640659 -5.28557042197794 c
-1.89370054037312 -6.54101438509981 -6.34916665924718 c
-3.13918227308864 -4.22403717063458 -6.48891467547971 c
-2.00297454267268 -2.05178089662447 -5.53367215888992 c
4.81510781739423 -0.01552935047139 -7.36186040568956 c
6.95686002081780 0.20154102677730 -8.87436347937889 c
9.16152956719175 1.26909334304384 -7.89874597438677 c
9.21291532619997 2.11298468206575 -5.40352124783230 c
7.07415691535312 1.90004154554819 -3.88249786856976 c
-3.46820299394672 2.36135825240231 -2.48084048823112 h
-5.80750815110547 5.95763917746116 -4.18978739071359 h
-3.70109674741460 9.00608844943941 -7.09210250797813 h
0.81810295796877 8.36611113229620 -8.23172092769815 h
3.19383307591500 4.78905066393485 -6.47832962560611 h
3.96833547028173 -4.65262503812850 -3.39797318959395 f
1.56043874754701 -8.43052977737913 -5.17783804191762 h
-2.77495629453549 -8.24247225114780 -7.08146725971079 h
-4.99774981208533 -4.09674790531597 -7.34631264883198 h
-2.98179631000969 -0.26198809828394 -5.69050212649058 h
3.10299138386070 -0.83549865776829 -8.13904657188430 h
6.89959522517198 -0.46567993344760 -10.81432861720698 h
10.83413213755811 1.43444418612552 -9.07666710545291 h
10.92442233879145 2.93454349214199 -4.62503721768909 h
7.16017197633940 2.52935152953134 -1.94054801057256 h

FLP 1·**3**
-2.04643118817662 3.58930543771187 3.51328649361615 c
-1.36398421416327 1.58248336309628 1.92332478919609 c
-3.42303656772692 0.40425778443737 0.75314704781220 c
-5.91791980173919 1.17660707469426 0.97713402788541 c
-6.47816978883392 3.23957128176306 2.51226801128294 c
-4.52707921105606 4.43463659442718 3.80383826625240 c
1.49418873554556 0.63221686767038 1.41778789107214 b
2.04834712662171 -2.33279302756883 1.84318997541487 c
4.35180087705241 -3.38776082334588 1.09410137636714 c
5.00373173986506 -5.90941638980338 1.39095707958186 c
3.29832089618211 -7.54098536509789 2.54894444663559 c
1.00888904156226 -6.58513712498321 3.41441745469728 c
0.43962044154522 -4.03512937805271 3.07400008415190 c
6.11008306553912 -1.88665741111857 -0.02496876691107 f
7.23050106641193 -6.79010440028517 0.53214414259184 f
3.86162706864277 -9.99404026507509 2.83705747974625 f
-0.62897718024146 -8.12429806818565 4.59701120360865 f
-1.76837467106267 -3.26760873929150 4.10156308461514 f
-3.00014918038829 -1.63893551315713 -0.71749905893955 f
-7.77858104570324 -0.03985784442290 -0.24635434943446 f
-8.86698241294518 4.03743720019511 2.76997833438741 f
-5.04808514805130 6.38736617763876 5.34252134101380 f
-0.31464758433223 4.83698999357154 4.91730298913217 f
5.24460441169257 -0.53653558702709 5.52023607871612 f
5.32525886342964 1.78860717074980 4.46574962214297 c
3.66696164822435 2.48161180674950 2.52049290255510 c
3.90051297100349 5.00703247282503 1.78363681216769 c
5.64762127743753 6.70192501818496 2.76137392996400 c
7.28741179562529 5.89499959479975 4.65373820326796 c
7.10913727971107 3.42082201714407 5.51600836310596 c
2.33458517541954 5.93357348862819 -0.02708100503139 f
5.76654110204812 9.09191052877352 1.90623587142455 f
8.99462902683376 7.48463023581014 5.63775080598595 f
8.64333114697581 2.62316411045922 7.37486340545024 f
1.77716803750733 0.74937978775629 -3.15215265319073 p
-0.29903926425445 3.01870805939198 -4.74888183381062 c
4.89615048911243 1.36005567976828 -4.57518438319733 c
0.99995064358904 -2.36457507895968 -4.45174408069825 c
-1.73478495883677 4.78364503960298 -3.38785248676176 c
-3.27444470011926 6.53598383185321 -4.60586693710453 c
-3.41379014873931 6.57119586756727 -7.23506942392673 c
-2.01934530364485 4.83819083309535 -8.64592994687202 c
-0.51205948678781 3.10837610123184 -7.38593430728649 c
2.84594679786013 -4.27720778305633 -4.32861584768571 c
2.35808578536398 -6.73436603370467 -5.12183900547140 c
-0.01186905963309 -7.35559971916344 -6.09305535486607 c
-1.86616781858853 -5.50091685470740 -6.28964523453138 c
-1.33746256598744 -3.06276598501062 -5.47612041714433 c
5.66566765686102 0.13988938579731 -6.80228158336637 c
8.00819867502507 0.67333487978428 -7.87541055198582 c
9.62066555296266 2.43261780538221 -6.75672275692303 c

8.86805144713934 3.66093324958592 -4.55293436071987 c
6.52831244546075 3.12623802433731 -3.47120985850887 c
-1.63439920019861 4.79018790473610 -1.35036795688551 h
-4.35775397665359 7.87311296658966 -3.49041695047219 h
-4.60783054311229 7.93478549469341 -8.19656472312466 h
-2.09448969426664 4.79037342455629 -10.69408914621776 h
0.76132449095974 1.40091660296774 -8.81486087309197 f
4.71935871515201 -3.80275795125294 -3.65627804967924 h
3.83407332679595 -8.15153153928624 -4.98273818736428 h
-0.41551619571997 -9.26874050646478 -6.71408900591460 h
-3.72393717839939 -5.89917445570385 -7.05932247372305 h
-3.21048317257061 -1.33844966158278 -5.73788998153111 f
4.43743201156377 -1.22051412604493 -7.70945713015743 h
8.56582052950955 -0.29088035402984 -9.59953406442689 h
11.44836123442702 2.84027716650055 -7.59682948486262 h
10.10082895191599 5.03512885101378 -3.65642423408190 h
5.99842271335789 4.08916281084072 -1.75408404794057 h

FLP 1·**4**
-1.65893950481166 4.27518193288618 2.93081195372342 c
-1.34428849151198 2.15890977360062 1.37088925743236 c
-3.55840279286108 1.42813205676181 0.12504174555280 c
-5.84941144112114 2.69383805541339 0.26322519555908 c
-6.03075183963725 4.83611985037797 1.77525327512187 c
-3.92029258990218 5.61433625948299 3.13361777341223 c
1.28194543871193 0.60951311669444 1.03181773764929 b
1.10583834463291 -2.36170741512324 1.77761373044712 c
3.02507198541585 -4.06987877650101 1.15480629070164 c
2.97653167139582 -6.63976297678682 1.66842287627139 c
0.90482220940864 -7.64639442511637 2.93475064007823 c
-1.03182755471900 -6.03538489889573 3.68201003557411 c
-0.89267270615261 -3.46354748433310 3.12122272527379 c
5.12912565064201 -3.21785042561438 -0.04270966588865 f
4.88210757545356 -8.15148363346264 0.93865826694345 f
0.78945178942324 -10.12465192969544 3.44712222321967 f
-3.01619762056880 -6.96582098608153 4.96621037218352 f
-2.82812281498191 -2.06000519111119 4.02344775284344 f
-3.53765178782375 -0.67332790028136 -1.34866207397075 f
-7.86449362977872 1.89183746349980 -1.05765591074944 f
-8.21135044426945 6.11528353050983 1.93805989098073 f
-4.08335316418610 7.64113439131265 4.65615403336409 f
0.23941962761061 5.13568669744617 4.40901124305044 f
4.90635384981996 -1.15211383200290 5.12851411726952 f
5.37946567463150 1.08158979578877 3.98144420166673 c
3.76175552197876 2.05113865261128 2.12241442961008 c
4.44623510747421 4.46343327962072 1.28436103824488 c
6.56951059530694 5.78352219257278 2.07113092881378 c
8.15682125004749 4.69196318509044 3.85923893467652 c
7.53919072520709 2.33059830410950 4.83223439341332 c
2.96355005586611 5.66724733968385 -0.43033416895924 f
7.11345708451856 8.07081768510590 1.11118982781460 f
10.23472980099384 5.90734653557292 4.64844859110441 f
9.01755877392067 1.27804475184638 6.60974846905986 f

1.91142256648440 0.57701062099860 -3.25236631108726 p
-0.60759200354371 2.21707128681175 -4.94805665988379 c
4.87362652083859 2.11724719519247 -4.12743699882571 c
2.04118853313938 -2.63042453405937 -4.51952623413629 c
-1.43608970650661 4.56682254964422 -4.01817295359843 c
-3.38012902307679 5.90305743118907 -5.17513921830796 c
-4.58289741706673 4.90578570597932 -7.29589436150988 c
-3.79210152932727 2.59866267989388 -8.28051915453680 c
-1.82214723478320 1.31329927332085 -7.11995717892392 c
0.22367234081930 -4.38951881305162 -3.69863907292790 c
0.23395523352014 -6.87949616970513 -4.53829333102505 c
2.09546015632259 -7.69674851745459 -6.21318169951172 c
3.90384842219456 -5.99749364477051 -7.08554103236355 c
3.83605315654956 -3.51066655689393 -6.25506849632647 c
5.15789415547157 3.88647248642298 -6.07609937662244 c
7.44053477508021 5.07099803775166 -6.59233247020136 c
9.56223611029955 4.46003029626591 -5.16307636276840 c
9.37486308454310 2.65973246600560 -3.24924797706807 c
7.06153032654704 1.52417689168804 -2.73687060757594 c
-0.53195443794465 5.35501184428835 -2.36618472612354 h
-3.96151183949471 7.71070942765054 -4.40090832123770 h
-6.12135186613056 5.92149148509273 -8.19591894167212 h
-4.65415096407986 1.77746376764002 -9.94930036924335 h
-1.07702186185666 -0.87150130393776 -8.22637416684896 f
-1.22099141850090 -3.78738126527512 -2.38754354649433 h
-1.20272687138509 -8.17753782523600 -3.86289744120973 h
2.13646146474272 -9.64424204067747 -6.85678603467827 h
5.35840705841229 -6.54985664452653 -8.42028017293259 h
5.58132671546672 -1.92543834107174 -7.25179918323685 f
3.18923290303947 4.49116655607842 -7.59617195975800 f
7.51723669203752 6.43440389967245 -8.12124455182502 h
11.35330745386407 5.37892604911075 -5.55836956143027 h
11.01845683639033 2.14807578099047 -2.13484120224000 h
6.93989731779961 0.14647694998916 -1.23528345535657 h

FLP 1·**5**
-1.52461849593112 4.32646560058241 3.27234641145365 c
-1.35516184943625 2.30105031516587 1.56877873928338 c
-3.62119564626136 1.81256584458823 0.29320844442539 c
-5.80255082045720 3.25890973964990 0.51132467166038 c
-5.82822204912499 5.30719454496556 2.15535557998561 c
-3.67284023393548 5.82166927280937 3.56655826293689 c
1.19243451238934 0.61771068817954 1.19440950652475 b
0.97114524090069 -2.32800897742941 1.98127612703883 c
2.85977117890165 -4.06830104762814 1.35725157025664 c
2.74969038632716 -6.63944380729804 1.85847029928712 c
0.65059145873237 -7.60172764764785 3.11719595499168 c
-1.25479025514077 -5.95288654855213 3.86167178823198 c
-1.06218984262124 -3.38487782383174 3.30172122767295 c
4.99513178206442 -3.24614026915014 0.18228657518463 f
4.63018285376643 -8.19379825726894 1.14209877427174 f
0.48025046748055 -10.08127840152511 3.61899133672045 f
-3.27119248964403 -6.85015646892250 5.11926652593244 f

-2.98659674903995 -1.93919406912396 4.15308658155367 f
-3.79055214444024 -0.21235426909481 -1.24590836591833 f
-7.87706940046913 2.68786969636513 -0.84228984072029 f
-7.90535390728993 6.73792726399979 2.40467926027041 f
-3.68539458425048 7.74450501222894 5.22869275854713 f
0.41319653212192 4.92932792949634 4.82887337309983 f
5.09407081156789 -1.13038709252765 5.06568775565586 f
5.45936101270232 1.11817906903849 3.90811753540235 c
3.72169475430888 2.06372860222850 2.15048533773205 c
4.29173645142296 4.50387092996733 1.30325504644316 c
6.41603789449619 5.87411957175781 1.99353146904459 c
8.12975950822409 4.80203352948732 3.67332513779416 c
7.63092525975225 2.41385727453413 4.64974820729165 c
2.67800647921732 5.68596728047665 -0.30578236116962 f
6.84270988600400 8.19101995631360 1.04373389754437 f
10.21788585336624 6.06277113941041 4.36054534548792 f
9.23491344925986 1.38319727200765 6.32994699592484 f
1.86984177895832 0.42881428258395 -3.08688317545648 p
-0.59038628773815 1.86146830384720 -5.01792293863822 c
4.74792065078801 2.13825237425633 -3.92159703527495 c
2.26032617939745 -2.74897592782555 -4.46698302435788 c
-1.46138855179253 4.29405390112975 -4.41038854730914 c
-3.37237390272078 5.40577923398548 -5.83867680199508 c
-4.43868819215650 4.10929405857566 -7.87095014336355 c
-3.57022233633457 1.69898226066445 -8.48841656230801 c
-1.65482995447639 0.57715262352324 -7.07246047100622 c
4.25679997249939 -3.49489696491777 -6.06251784061405 c
4.61165521452600 -5.95676171332580 -6.89803756166527 c
2.89187350298306 -7.81575153737013 -6.19510691787915 c
0.81149274415270 -7.18539491442249 -4.71754053953136 c
0.54442660783963 -4.70419479648201 -3.91972775754765 c
4.69902542380137 4.08205932355906 -5.71547601615381 c
6.89402483292885 5.42793372177469 -6.26770680466576 c
9.15544046661197 4.83894753469591 -5.05111985470628 c
9.21924702159589 2.88615667052605 -3.28089196895954 c
7.02920506551514 1.55001290646477 -2.70405812760408 c
-0.64883969149338 5.31371594032577 -2.83402446196637 h
-4.03683976439823 7.28405308180624 -5.34717142329535 h
-5.94090564109329 4.97476199597608 -8.96891888831157 h
-4.38594663871495 0.68122406243953 -10.07270007148704 h
-0.99394354673506 -1.29952955554924 -7.56583059080360 h
5.94057768856492 -1.77920605116733 -6.91439842879328 f
6.22122943325616 -6.36048054647845 -8.09948643735280 h
3.15458812635301 -9.74823683728687 -6.82765506366160 h
-0.60577222908372 -8.56056676609041 -4.17293984542226 h
-1.55165947031954 -4.14703674427301 -2.58376567041939 f
2.95260420382657 4.55017348678545 -6.67852098937358 h
6.82982100012883 6.93971689606586 -7.65395378101046 h
10.86107040446518 5.89744618910290 -5.47788429380764 h
10.97202537570633 2.41216159209650 -2.32461211945930 h
7.09931720819409 0.04996406175162 -1.31604777564158 h

FLP 1·**6**

-1.42492862711133 4.43839205123203 4.60411909128151 c
-1.36238305887712 2.40996144478776 2.89694238398208 c
-3.59161475277281 2.04335834227499 1.51851890760851 c
-5.69618187789783 3.59590330379840 1.73216339661592 c
-5.65857475756117 5.59201008487813 3.44613340165369 c
-3.51139310215245 6.00535970698114 4.91113168831231 c
1.05106818998356 0.69367215426427 2.60723240682632 b
0.80927802020070 -2.26654900400106 2.57156665663730 c
2.67877507223041 -3.85426213005961 1.55477261848051 c
2.49145393953395 -6.46857919865999 1.46769910449878 c
0.34937537736317 -7.63602035865020 2.45410024495313 c
-1.54451460909730 -6.16584133462141 3.53696232680318 c
-1.28415297824714 -3.55109614812300 3.58663205607149 c
4.80215084197891 -2.86272194689119 0.54671117879472 f
4.33499342180900 -7.87418999483387 0.44043600886712 f
0.12037189340494 -10.15263666346141 2.36943701694900 f
-3.59029196472981 -7.28589551924891 4.53447210200206 f
-3.15942257672289 -2.27658969888645 4.74654897493449 f
-3.74479247630547 0.14679750095412 -0.16572250459345 f
-7.75320617608182 3.20566130902774 0.29350067313126 f
-7.67570603011854 7.09917647185285 3.69012986602286 f
-3.48188228111682 7.89993764659210 6.60060947898774 f
0.57412172514653 4.91684855450783 6.12091022214570 f
5.38479595929496 -1.16846812182735 5.55882868329350 f
5.68577336483077 1.03054878724898 4.29799410692148 c
3.69843575726670 2.02426114567251 2.85374372964069 c
4.18381534280576 4.38862613124379 1.75423799754239 c
6.47144224466758 5.65381921506605 1.99726632219364 c
8.39559453657252 4.56615546074930 3.42253931314040 c
7.99707412357614 2.24183611450837 4.59558161876186 c
2.40532210447796 5.52661431242511 0.33448615126807 f
6.85825917195773 7.87913214945968 0.84737033977001 f
10.62421088603011 5.74110817220635 3.65759627102301 f
9.83666778874688 1.21382600209141 6.01151153692804 f
1.82739721008574 0.56287097530166 -3.59300634730133 p
-0.43506970484093 1.77520971139015 -5.93830947122173 c
4.72103680679020 2.28122858508999 -4.38628239203420 c
2.25992237036803 -2.71561597627878 -4.68394031476944 c
-2.14227960204600 3.67143205967076 -5.23140095483928 c
-4.02871231621739 4.61757041874153 -6.78405190248808 c
-4.23680429766173 3.64925890576391 -9.22368097295557 c
-2.55812592911122 1.80891621016683 -10.07591667004632 c
-0.69864967474100 0.94023722080863 -8.44103061273023 c
4.38732821742981 -3.81518984239977 -5.81969207740174 c
4.57877980132636 -6.37456471942290 -6.36623626867284 c
2.55313089863502 -7.95995071214634 -5.81437152997132 c
0.36120443545902 -6.97931840372155 -4.73488631879244 c
0.28663245226141 -4.41711851419848 -4.20053834250474 c
4.75064509328914 4.23660506513694 -6.16933164383902 c
6.93273993137689 5.66439018363405 -6.54801400191724 c
9.11329141203305 5.15171967469345 -5.16207709232241 c
9.09859121531486 3.20727449460334 -3.38001120695703 c
6.91393117284531 1.80291942714800 -2.96969184809334 c

-1.90996803855702 4.68660478825557 -2.89288260779072 f
-5.28119707165694 6.07643772423671 -6.07733266928754 h
-5.70025566944687 4.35083090626706 -10.47737434156899 h
-2.64690567203932 1.05631989725893 -11.97968179763243 h
0.95712159282780 -0.77392925213337 -9.37074026412060 f
6.37117874125449 -2.34714673673465 -6.47808013039178 f
6.29685196063234 -7.07462752466185 -7.23596289212080 h
2.67823512413001 -9.96274930560491 -6.23486499428161 h
-1.26379368067931 -8.14923012181333 -4.30057510889787 h
-1.86591270028193 -3.47753262878857 -3.16601368073824 f
3.06915879106745 4.64751510671955 -7.26903607826745 h
6.92455112279218 7.17570591036780 -7.93707735264157 h
10.81173091187173 6.26452146103093 -5.45933772593155 h
10.78727551412141 2.79756934931464 -2.28661185039381 h
6.91954208828126 0.31257771974550 -1.56430490852582 h

FLP 1·**7**
-1.66391477274404 4.67502426264830 4.67006768683780 c
-1.59644470940908 2.37693415152308 3.35172638308655 c
-3.82486248884085 1.74023824677615 2.06680059373472 c
-5.94652114887219 3.28559886168861 2.02493017704640 c
-5.91754059313624 5.55091127974386 3.36473843975674 c
-3.76516447255149 6.24687002032974 4.71564679956935 c
0.80397821667483 0.64446345261657 3.30794917450497 b
0.45710107953970 -2.28858858437456 3.52809284113895 c
2.00416551635464 -4.02774549671119 2.25563584593358 c
1.63275706213712 -6.62514486307625 2.34657861527789 c
-0.33015153498360 -7.59545790920176 3.80814844069079 c
-1.88987227165860 -5.95612134368241 5.15538959396272 c
-1.48248829406226 -3.36787239629787 4.98428846814418 c
3.92831393935545 -3.21220059089376 0.81281640592571 f
3.14182044368534 -8.20594970238661 1.05761269248366 f
-0.70530601434340 -10.09187003178945 3.93131981322936 f
-3.75588332537959 -6.89208615204587 6.59653556106690 f
-3.03162342586444 -1.88757696583543 6.36603839966659 f
-3.95898668875783 -0.41795011342129 0.72737553320260 f
-8.00891842381035 2.63252986624083 0.69819456340387 f
-7.94935181311162 7.05566393926223 3.35722688559035 f
-3.74968015410328 8.41625667094929 6.03171976052128 f
0.35956187854773 5.42713469136927 6.03132998323070 f
5.37841473727507 -1.27787071457709 5.76446670653346 f
5.61439982306212 0.82229450541508 4.34002192405444 c
3.49204042996531 1.86734091004275 3.13770370909967 c
3.95432872337150 4.11020636394767 1.79023494021241 c
6.32816489761662 5.21424431875448 1.60437844117720 c
8.37372114945852 4.08410672162885 2.81569214196904 c
8.01500228123375 1.87701237855818 4.20520452634180 c
2.07167183254682 5.28465676318583 0.54588456054097 f
6.67247691097492 7.34252265985243 0.27175570368015 f
10.67618822282424 5.11377131803247 2.64327541438621 f
9.98239179231117 0.80438180822161 5.39427107354433 f
2.10065113904087 0.77965010880108 -4.01298767927644 p
-0.24407058919110 1.89999523588741 -6.31799732777946 c

5.00868149068110 2.52102205025837 -4.76260746519796 c
2.62006111831123 -2.44099480174974 -5.23091781284730 c
-2.39264252522410 3.17482728061401 -5.45350032268300 c
-4.38046325336408 3.90948929818630 -6.99789618799332 c
-4.22631475072432 3.36959842153012 -9.56973046720956 c
-2.11427028406938 2.14375311483230 -10.56133846531502 c
-0.18444443129596 1.45853238846863 -8.92682107662528 c
4.59945225395244 -3.40983889118645 -6.69485112881844 c
4.83693493006308 -5.95255044733148 -7.30311348161252 c
3.00739085723867 -7.64609384282721 -6.46211243876117 c
0.96140910992744 -6.79515734147808 -5.03704778214803 c
0.83603903695793 -4.24461672979436 -4.46813332046573 c
5.19706805183267 4.82707297894354 -6.04817575504399 c
7.43044120437122 6.18817889918095 -6.27314872863781 c
9.61784004898738 5.25077946733677 -5.15471688436128 c
9.55148502333764 2.98336836874006 -3.81304409886185 c
7.27058651140731 1.71742847295672 -3.64083026596152 c
-2.53943552438722 3.76476230227472 -2.96466437650729 f
-5.98895482597162 4.88129153837785 -6.18218962761265 h
-5.75693669892312 3.92366177965674 -10.81742753611814 h
-1.93438907917199 1.73819977634771 -12.56174692624262 h
1.88670785252020 0.34392601536366 -9.93085830100282 f
6.38767899517001 -1.82793037387385 -7.60956884277621 f
6.43220548659158 -6.55709846385881 -8.43824004012526 h
3.16848078376176 -9.63645533966590 -6.92827727224376 h
-0.50553505338309 -8.05844109798838 -4.36698116672644 h
-1.16475072768524 -3.41732243988674 -3.07878022591222 f
3.10886472758850 5.84301835429778 -7.13433234814001 f
7.41367043523042 7.95569941346564 -7.30927425487826 h
11.37481006110185 6.29582467163851 -5.30972213281962 h
11.21305372622563 2.20234702313218 -2.90378159174177 h
7.20543909378616 -0.47075951714408 -2.29442146709852 f

FLP 1·**8**
-2.17709183056986 3.31800440314001 3.18523594612218 c
-1.33725008756981 1.21261249663655 1.80983612029215 c
-3.30446870847458 -0.31728805229194 0.91648491895622 c
-5.85891967519950 0.19095827517831 1.22012257774025 c
-6.58463265242864 2.34472694626536 2.54636698589170 c
-4.72329837003531 3.90179592556457 3.55157353182945 c
1.61581212354949 0.56074338349677 1.23678034590766 b
2.50792651395688 -2.29858287349649 1.92037807774485 c
4.95883851776288 -3.10774908280204 1.34507303183716 c
5.94511505117452 -5.45856380125978 1.97108130616179 c
4.45329025299066 -7.15353769815551 3.31559677033341 c
2.03429087566397 -6.42076650703828 4.03507574753793 c
1.12982053810476 -4.03938337325604 3.36742474936834 c
6.55162530756326 -1.52054367924369 0.12014064789249 f
8.30783255772670 -6.09912864704433 1.29464591152726 f
5.34457557813770 -9.43995309183863 3.93991723548139 f
0.60063723051786 -7.99911184657368 5.41666751107340 f
-1.15881943219463 -3.45330370450255 4.34068664229054 f
-2.74812285286936 -2.47359857249029 -0.34515749642628 f

-7.61838420191735 -1.37208960085247 0.27247415960020 f
-9.03363691049670 2.88986276120285 2.87287686467482 f
-5.38935894647088 5.96849493806559 4.86710039544799 f
-0.54536639339940 4.96516557069938 4.25331234182230 f
4.56952797055946 0.09547532741334 5.98327411030626 f
4.90238482980691 2.23466720413853 4.62585484455541 c
3.58983178391508 2.64115430262038 2.36206884270960 c
4.00636721301701 5.02382119883684 1.31093275196642 c
5.63998786512480 6.83141788327251 2.28974427995028 c
6.94640398915988 6.30275631432796 4.51009043626471 c
6.55548853013870 3.98836128925059 5.69083206319062 c
2.74696591784319 5.69157697307075 -0.82527945973955 f
5.95824198065293 9.06652117940252 1.12373108354615 f
8.53501343956222 8.00562292311408 5.50469563800973 f
7.75785545414425 3.46708974513820 7.86477406659569 f
1.80530547429324 0.73604208109566 -3.04305176687818 p
-0.03272491113450 3.24238113226199 -4.61179328659949 c
4.88016925964675 1.00430382172683 -4.62289683471990 c
0.56449191657077 -2.21063016706137 -4.45115967607489 c
-2.00117759540770 4.50388516514155 -3.37125964656779 c
-3.36725911098518 6.38218161097119 -4.60475131621121 c
-2.79376379071786 7.02913035305132 -7.09373939353883 c
-0.82811017759585 5.79235297287415 -8.33636999955769 c
0.55241510846369 3.91849551553759 -7.10440265371098 c
2.04276760622069 -4.40966527512157 -4.53765321969305 c
1.17719822303106 -6.68216350910689 -5.53733470362134 c
-1.26312057112078 -6.82977160849754 -6.50602578571791 c
-2.79664539896681 -4.69357301363122 -6.45651034379069 c
-1.88715523112958 -2.44583681929902 -5.43729176537248 c
5.24702452084548 -0.05437072398506 -7.02772484105064 c
7.51468059899698 0.30062213510989 -8.31373514271737 c
9.44865096976608 1.71854290716992 -7.22039949968785 c
9.10310489381308 2.76344169517855 -4.82760077852417 c
6.83801478773046 2.40927846678407 -3.53441546677537 c
-2.47580153620177 4.02877620233217 -1.44426638378337 h
-4.88214307421505 7.34207848927526 -3.60728431388155 h
-3.86155083314286 8.49588624271681 -8.05296908348364 h
-0.34743736215203 6.29110574375618 -10.26829363130347 h
2.10073017092990 3.01219678378210 -8.09096050011106 h
4.44075894179894 -4.39666631313837 -3.70063961399459 f
2.68912636036724 -8.71361753340148 -5.59044051821816 f
-2.12626346979289 -8.99746129433861 -7.46825530914536 f
-5.16120513237373 -4.81950722620906 -7.35337600104610 f
-3.53118095027245 -0.51594332775245 -5.37477758395666 f
3.76177367354139 -1.16430152680367 -7.90461094010713 h
7.76670769292473 -0.54017104449503 -10.16871847016631 h
11.21952215980025 1.99084837620281 -8.22076474459225 h
10.60380910146160 3.85009551746971 -3.94596112878083 h
6.63580422555945 3.18080566041417 -1.65397863708217 h

FLP-$H_2$ [1-H][H-**2**]
-2.21770909205054 1.74499233384065 3.27136549145313 c
-0.43731124501351 -0.05803899132945 2.53210000873792 c

-1.45764788557955 -2.08938084015774 1.18529260390079 c
-4.00320454143906 -2.34487830455045 0.56972018104779 c
-5.69470821473938 -0.48465383544744 1.34390582974172 c
-4.78888273628847 1.56928285751293 2.71516004969687 c
2.62252260662069 0.02832524091578 2.98959119837658 b
3.65400754309295 -2.21867643056693 4.82290025329223 c
6.13468322763834 -3.06897644120558 4.54134652817278 c
7.19481373029437 -5.00115362176187 5.97510622385568 c
5.72798097918713 -6.18252916533346 7.81225024971567 c
3.24288494377140 -5.40231641117457 8.17400134505799 c
2.27009487726752 -3.45444757193604 6.69294180043233 c
7.65938286823984 -1.98662806139704 2.77350043323011 f
9.60552788150377 -5.74723754575134 5.60783059733492 f
6.70553742204511 -8.05763260612811 9.22518236723238 f
1.81574388107488 -6.53315427232858 9.95607949043234 f
-0.15645577790490 -2.77566133491924 7.16757619420759 f
0.09126162586654 -3.98548967602901 0.39994824637550 f
-4.84646275487685 -4.35591203888913 -0.75048279549332 f
-8.16265519590889 -0.66199769601552 0.75882665735950 f
-6.40810280160338 3.39943499992775 3.44045910789319 f
-1.51645004584125 3.82565838460382 4.57766581816762 f
2.82623034252665 2.19873642406369 8.17297356764043 f
3.80273460458002 3.64425952255444 6.30449964630706 c
3.72747778478430 2.78635154717763 3.81007135259246 c
4.73481797936187 4.46748862459138 2.05761949057836 c
5.73447295106771 6.82321281999485 2.66354584885257 c
5.76664726269270 7.58501127909166 5.17832059367572 c
4.79246647920528 5.97489765784181 7.01916156974887 c
4.78463914659442 3.85595745008724 -0.45733720185376 f
6.66754389580818 8.36221563419713 0.85196311678480 f
6.72280108125276 9.85067409053696 5.82353735437812 f
4.79987197719214 6.70738092350294 9.45674847061635 f
1.69428497393521 0.43124183382869 -4.19164047794836 p
0.28339120984018 3.50680007911714 -4.10363129979206 c
4.59025186414096 0.42120191368762 -5.93527885665795 c
-0.51286156466711 -1.78254388177262 -5.50932948157497 c
-1.94767918091508 3.82954355522137 -2.70817799537689 c
-2.97794166217888 6.23333164593874 -2.44387534782900 c
-1.79107524397550 8.30505798790016 -3.56858105004114 c
0.42575793187232 7.97950556731672 -4.95908960639529 c
1.47870962420298 5.58186006771878 -5.22863066340635 c
0.12091256916945 -4.34941979421808 -5.52981278447135 c
-1.50056319949935 -6.18864760494434 -6.44267684586101 c
-3.84433915648856 -5.43277961394115 -7.38197596415048 c
-4.52655489138472 -2.88414745012702 -7.41454653195724 c
-2.87146724879755 -1.06437877088097 -6.48609642120765 c
4.57990241634466 0.63542198292053 -8.57736499505365 c
6.86277422889937 0.63616356436573 -9.88209232333985 c
9.13735677933107 0.41039370780779 -8.55915639256190 c
9.13986615618555 0.17735762437083 -5.93293641879194 c
6.86767621445128 0.18025882838292 -4.60250960895782 c
-2.84452053708370 2.21850061217759 -1.81094301392029 h
-4.68449113004032 6.48718849298641 -1.33461184939395 h

-2.58785199428201 10.18253703581717 -3.34327937746771 h
1.35596903548443 9.59694132207176 -5.81113318272898 h
3.23367808620206 5.32970275062496 -6.25861903204002 h
2.41178033163108 -5.03411395214817 -4.62879664311795 f
-0.93127077287946 -8.15649805067186 -6.39153435230971 h
-5.14678330708137 -6.85182866807696 -8.08731640087838 h
-6.35408315121874 -2.31524018921593 -8.14854851225777 h
-3.39639555123976 0.91728635922390 -6.49508722702858 h
2.80386641565869 0.78695339060767 -9.59724241054064 h
6.87049904831692 0.80207950588721 -11.92692596971227 h
10.91458530401099 0.40554101557228 -9.58537562685982 h
10.90881753069779 -0.01258494158503 -4.91237429476156 h
6.85652598981434 -0.00315511793754 -2.55934017037963 h
3.56642565950814 -0.45483984897164 0.93594819237821 h
2.35496042161192 -0.30427090457389 -1.69271375314844 h

FLP-$H_2$ [1-H][H-**3**]
-2.19146369133698 4.09544647373965 3.83742129109299 c
-1.19598616575708 2.35203140388157 2.12674389163462 c
-2.97147900066524 1.38023409834970 0.43666665652308 c
-5.51345279440978 2.02703253547285 0.38673294777384 c
-6.40922258000093 3.77315175337951 2.14012227054924 c
-4.73167217229653 4.81066417173088 3.87676870352176 c
1.77149003243117 1.57117072572502 1.80533463837983 b
2.29301074109789 -1.48160336875013 1.70303315187807 c
4.48732088043847 -2.37662307078454 0.54747263592259 c
5.10938261532163 -4.91811619829468 0.30680629071998 c
3.45686402703435 -6.73118378723691 1.24650264119086 c
1.25133032266613 -5.95063904038267 2.44576697116646 c
0.73071074919909 -3.37672635842931 2.66778470966921 c
6.16506533931362 -0.70257587380166 -0.47673576109355 f
7.25469256410365 -5.64667636345138 -0.87937806836543 f
3.97825474839466 -9.20741390092988 0.97725724393649 f
-0.35394851075960 -7.69442412464995 3.37377175959252 f
-1.43224406532477 -2.77802430319691 3.88846077365127 f
-2.20542879218960 -0.33473852301272 -1.34420136241440 f
-7.10257540208983 1.01215909503998 -1.32929976846303 f
-8.85865605424834 4.45434199280769 2.14113388517561 f
-5.57713439117833 6.50799600404328 5.57427387808847 f
-0.69942688450508 5.22051607624167 5.58389816184201 f
2.48171996434840 0.27062934967054 7.15784541078986 f
4.03490628781622 2.08951552262310 6.24171364457126 c
3.76453905078760 2.87820732905941 3.74136196315636 c
5.42777786532606 4.77444662131292 2.99253106832278 c
7.24285234795979 5.83285638735344 4.57768702394843 c
7.43394896263699 4.98138732012782 7.05770103910138 c
5.81134538004335 3.08770541565752 7.90255236048773 c
5.34818388140926 5.70865743574779 0.58879532445605 f
8.81207057947562 7.66253696255052 3.74217415345450 f
9.16930716570875 5.97749324144862 8.62590690838960 f
5.98293576606526 2.26263363138590 10.30495315999036 f
2.06109598775823 0.39212424224774 -5.44058348647391 p
-0.32980138014392 2.48794546628985 -6.58582981237871 c

5.09905210884071 1.12680444778451 -6.73953108997770 c
1.42089251795780 -2.90769910292838 -5.85223099832303 c
-1.30558516632883 4.31992189772778 -4.93180854152846 c
-3.13245774278048 6.01065583470995 -5.77906617764995 c
-3.98539747851603 5.89301286634591 -8.27225849850325 c
-3.02087498488098 4.09826636646895 -9.95090673255696 c
-1.20528980778966 2.43618475024145 -9.07156275565595 c
3.46744039313601 -4.58893586621331 -5.60439470977939 c
3.08029082387060 -7.18510643982212 -5.64953149409790 c
0.64040309235303 -8.14458564519697 -5.94692571929432 c
-1.41351630611885 -6.51891685918380 -6.21457022651228 c
-0.99892631674562 -3.93115037378133 -6.15929850909417 c
5.85119240010461 0.24066192544838 -9.12180733917652 c
8.20296907053734 0.93733040571596 -10.06914856837623 c
9.78689286403326 2.50955857679332 -8.65698163396813 c
9.03077109721890 3.39053041087284 -6.28989857524711 c
6.68338328831472 2.70569097362679 -5.31457420413433 c
-0.64068731227606 4.39030970906975 -2.99140395575466 h
-3.89748573324045 7.40632475310880 -4.48732547597831 h
-5.41861063572766 7.20603583625043 -8.92801882503742 h
-3.65983142761559 3.97550750072373 -11.89424931779450 h
-0.24022007624966 0.66734446040148 -10.66412818278349 f
5.35845673630864 -3.83994592935588 -5.34179653595914 h
4.67494353212584 -8.45045719275563 -5.41478572862227 h
0.32818157753528 -10.17183081437338 -5.96311599485193 h
-3.32688511442976 -7.21556153824731 -6.44721564041560 h
-3.00789130034014 -2.38365930293345 -6.41776907506998 f
4.61498207390593 -0.98393029866109 -10.20778913189103 h
8.80291268167398 0.25287291163352 -11.90776536138581 h
11.62306321650419 3.04024510129620 -9.40436983363700 h
10.26926168152009 4.59699684056170 -5.18641774120959 h
6.10510184579991 3.36337046493234 -3.45886208671585 h
2.33776782998258 2.38807057090688 -0.28536709523643 h
2.21566019688617 1.02405641586554 -2.83997254356980 h

FLP-$H_2$ [1-H][H-**4**]
-2.28730749468839 3.88928050571629 5.53113620520887 c
-1.65910896531674 2.07320314018191 3.72754156402911 c
-3.56317494294195 1.56377688103119 1.97911957780254 c
-5.89840033880703 2.76671059683426 1.93793397118748 c
-6.42212543221420 4.58580217272943 3.76522562629721 c
-4.60295919441301 5.14599066323722 5.58124479430372 c
1.07568804587936 0.70037546078518 3.43424819032811 b
1.11533577881402 -2.27328659421894 4.20814042414449 c
2.78450905224383 -3.91021073975208 2.99322323731587 c
2.85431250304746 -6.50831972444031 3.37769926628797 c
1.18516991078207 -7.58178000242404 5.10516342260569 c
-0.50129016074005 -6.03146969162899 6.39890070091520 c
-0.49960546202447 -3.43800510316854 5.93429705516571 c
4.47488219886961 -2.96943527927668 1.27766072107171 f
4.49167466210135 -7.99092667403891 2.10082139740883 f
1.20601493150376 -10.09011754212714 5.51952899204752 f
-2.10918955036178 -7.05921356235231 8.08178914149136 f

-2.17229807248906 -2.04321857869535 7.27496843771942 f
-3.16368388888473 -0.20374742113232 0.13350202371154 f
-7.64052898115333 2.21355336056463 0.15821408940705 f
-8.66383243616320 5.78531068536497 3.77417228405552 f
-5.10666654462182 6.89352255982823 7.36062040790594 f
-0.61818511067500 4.51205986389462 7.36574754490910 f
4.25334059181459 -0.17638841391468 8.12830107151872 f
4.91319641307499 1.76532918429537 6.59999212195573 c
3.46399601368411 2.33312641012693 4.47323604840397 c
4.31395029961870 4.41091009053329 3.09354493619461 c
6.45451467923377 5.81163515084444 3.69186488851009 c
7.85474346549342 5.14689545641038 5.81809784094220 c
7.07107920024122 3.11177794710823 7.28917473994561 c
3.02220080627838 5.15506312724640 0.98056034936385 f
7.19712442256463 7.77647644405901 2.24383490613881 f
9.94030551306403 6.46062108922177 6.44202167345081 f
8.40910426135824 2.47156898836793 9.35659388155950 f
2.08501721310320 0.61604108450541 -4.12260467739469 p
-0.44769533961962 2.51035085706368 -5.31541439118457 c
5.15314385730263 1.97459431862192 -4.52610501529262 c
1.89572021498836 -2.66099232066481 -4.92688629787039 c
-1.49192848298214 4.31570968217835 -3.66471183925873 c
-3.53835352563481 5.77188047230061 -4.43188910765316 c
-4.56672945289646 5.43672239002853 -6.83917299800669 c
-3.55979236898671 3.65626460505302 -8.50209685133223 c
-1.51405556861953 2.22447296204025 -7.71258086272573 c
0.55432244474739 -4.24392779124810 -3.26284991532880 c
0.44065967881557 -6.82921094912369 -3.71078042068416 c
1.66737668103368 -7.85906304495776 -5.80817444130894 c
3.00768245691952 -6.32197191725252 -7.47899140769008 c
3.09811190392337 -3.74708233359197 -7.01030004463109 c
5.92645576684050 3.27078653158860 -6.69084487353347 c
8.28111659519181 4.40374412718305 -6.86358896039439 c
9.91575894471124 4.23021613308448 -4.80256871088256 c
9.19962893983432 2.94266389279589 -2.61300765246717 c
6.82896001949891 1.82204684824063 -2.46628976004978 c
-0.70825342294679 4.54134997912488 -1.78211951032209 h
-4.34737246438050 7.14268985013432 -3.14066903831138 h
-6.17784578222367 6.56045057826706 -7.43053400791790 h
-4.33258474951135 3.36376749090480 -10.37767376253206 h
-0.52838761140913 0.48853291288896 -9.30844525250858 f
-0.36136994501652 -3.43629290728381 -1.61448163103044 h
-0.57565786042381 -8.03977889042160 -2.40594905717883 h
1.59500358428034 -9.88112370114918 -6.14616244954039 h
3.97771771823624 -7.08545089369553 -9.11507430045780 h
4.40458065262774 -2.24164086813007 -8.60998586676081 f
4.32223507806998 3.43836281217227 -8.67346668660882 f
8.79881221328651 5.39946257946535 -8.57845872477022 h
11.75934544569709 5.12361288152191 -4.90862079233934 h
10.47128091955935 2.83939492624429 -1.00871899727396 h
6.24624901123449 0.85130932828107 -0.75545376991218 h
1.71936680441070 0.64497111414157 -1.45426403901298 h
1.41268022384015 0.66363979512008 1.15550458947155 h

FLP-$H_2$ [1-H][H-**5**]
-1.86656749938171 3.49277921831492 6.27605289366512 c
-2.19970129941300 2.34414781027185 3.92677876234834 c
-4.46937061250580 2.92047083898682 2.72785831081050 c
-6.29492246317275 4.51858212017400 3.74927040995390 c
-5.87126597054142 5.61570710992386 6.10017342807237 c
-3.63093761620839 5.09649273222874 7.38212570530582 c
-0.01517807324170 0.62007693980387 2.61609911486891 b
0.32661502918360 -2.23650036056681 3.72988601169883 c
1.99137477611586 -3.89011558577763 2.53650438468526 c
2.33769211137913 -6.40919577141522 3.17123234295738 c
0.94060748078082 -7.41647855847843 5.15985470836469 c
-0.75336043796661 -5.86327849910050 6.43309592668109 c
-1.03005594203650 -3.34162302724212 5.70371329207839 c
3.42976019338960 -3.02293585766499 0.55790712058681 f
3.98228143050938 -7.88281869538551 1.88343001677452 f
1.21895701110800 -9.85497836443802 5.82525285089663 f
-2.12364520026114 -6.81551242457875 8.35501344827741 f
-2.74196795350716 -1.99268667832335 7.04111718838491 f
-5.01440642729000 1.92236322323706 0.41395369761515 f
-8.45616141731217 5.02059960135799 2.48877848750349 f
-7.60771068378576 7.16436822829642 7.12592989785026 f
-3.21403889249619 6.14569436598816 9.66476365972460 f
0.27252503569567 3.02891735581493 7.60817232916624 f
5.04496566342782 -0.11981614118349 5.39749234539956 f
4.82509921867455 1.88205717195280 3.82192357365344 c
2.58813010820547 2.30356669164302 2.48872181852159 c
2.62909123005773 4.46184993943207 0.97308340551871 c
4.66799979485155 6.10682069553546 0.77127220491771 c
6.86078961004234 5.58039413143145 2.11882996930293 c
6.94000921044803 3.44375932097812 3.64793879623453 c
0.56227913980033 5.05157499866435 -0.45705211234554 f
4.55638606050353 8.16845758876282 -0.72800380834049 f
8.89206442229565 7.09944053975866 1.91855022009422 f
9.07129100101031 2.91023042876923 4.93909322082679 f
2.14449045971217 0.23505178372706 -4.36388080308625 p
0.04272831811111 1.87368787353170 -6.43988880144467 c
5.17617619437389 1.73026358685458 -4.16072404676465 c
2.51113748793430 -3.01028591860695 -5.30563318205604 c
-2.16865826001366 2.90316859132756 -5.40206911016484 c
-3.85953575278400 4.16621338216764 -6.97809901604706 c
-3.34858285406059 4.39637124639770 -9.55323327883294 c
-1.14678497177837 3.35859686650253 -10.58149528214189 c
0.55592917434044 2.08753568769483 -9.03463174347991 c
4.35441336648566 -3.85201606312238 -7.00942883674593 c
4.70793889571397 -6.37943385469151 -7.58952799598163 c
3.13274697311457 -8.15994368636416 -6.44808287076294 c
1.21912726631431 -7.42745654655570 -4.79226498085496 c
0.93415674790357 -4.87778699852666 -4.27598478476429 c
5.58315784334095 4.07030219953924 -5.32673147142659 c
7.92337526418456 5.24960993132247 -5.07423262032766 c
9.83403811981806 4.10825233154378 -3.66540248729072 c

9.41471517672967 1.77955274655747 -2.49378368673725 c
7.09174117012309 0.57658070768496 -2.73345104800199 c
-2.56014115351713 2.72212615302483 -3.39705816253117 h
-5.57248683797065 4.96572466687147 -6.18228330839126 h
-4.67144376863186 5.38445616367309 -10.77206756589215 h
-0.76265070106798 3.53765337724717 -12.58884960294913 h
2.26601254876290 1.27373041185722 -9.82614899217800 h
5.84247297345606 -2.11293184153231 -8.15454818695637 f
6.17991957192039 -6.91823621373033 -8.90797614570023 h
3.39069839147525 -10.14954808866062 -6.87151750431851 h
-0.03121020755427 -8.78397225946980 -3.90316575647605 h
-0.94194997654283 -4.13526365054334 -2.72382000867344 f
4.07942438261861 4.97398524395354 -6.38719540070762 h
8.23707710362045 7.07552359296380 -5.95324579892625 h
11.64497246675726 5.04690640134241 -3.44889274547510 h
10.89073388186732 0.91184255168238 -1.36434813773074 h
6.75859562296665 -1.21641845031495 -1.79815451907514 h
-0.69595174478651 0.29692053580236 0.42869273948454 h
0.92330478870360 0.17563245167710 -1.96927347864523 h

FLP-$H_2$ [1-H][H-**6**]
-1.79035205317263 3.94873622483678 5.36029854763384 c
-1.93941729995795 2.12051624848039 3.46844913892799 c
-4.36647170411279 1.70132485685114 2.52741487013319 c
-6.49841465946190 3.00601365723733 3.34712752370471 c
-6.24381892233882 4.82969045685928 5.22473465188260 c
-3.86636586667643 5.30273523367893 6.24561835325205 c
0.45805282266014 0.59491569025984 2.29344831169499 b
0.82266109091375 -2.24980994933196 3.42234954207066 c
1.96717179673828 -4.10876963559796 1.95758405155616 c
2.26082528150988 -6.61732167435392 2.66900958458717 c
1.37824138756135 -7.37368409235061 5.02794315610675 c
0.24147695687366 -5.59358911191396 6.59531181297583 c
-0.00732061627465 -3.09970511362287 5.77740519852446 c
2.91698294231987 -3.48815812839023 -0.37740421655642 f
3.37452321720174 -8.31041525016582 1.11214647412108 f
1.62730772103703 -9.78900447552063 5.78188995372128 f
-0.59831810507764 -6.30385359481809 8.89017608521606 f
-1.09470806443434 -1.48213414889726 7.43073514753360 f
-4.74660647272171 -0.06656731632939 0.70224192313366 f
-8.79784410461478 2.53256035371620 2.34660299161448 f
-8.27709614012739 6.11743547352299 6.04937282720771 f
-3.60940804398954 7.05114555128443 8.08140721646389 f
0.46158552931324 4.47116876049854 6.46865105556163 f
5.45148280754095 -0.19157041289943 5.12070970216704 f
5.26042115199265 1.83537839599838 3.56880081129726 c
3.03318335488232 2.30497895107217 2.23665582768809 c
3.11149748505734 4.47446829471030 0.73819002915342 c
5.17532573999251 6.08862717784481 0.55916647630420 c
7.35312657927238 5.52285111572795 1.91603247634495 c
7.39650587597583 3.37204098725890 3.42506987697282 c
1.06206367797305 5.10290315194951 -0.69492414060372 f
5.10806130648304 8.15662001196311 -0.93475403083522 f

9.41026407008559 7.00881454329641 1.72578918356781 f
9.51487862689928 2.79351742102714 4.71933189478342 f
1.97804148033609 0.42734301161016 -4.91028028010141 p
0.03182179685476 2.22740278705900 -7.02422711462481 c
5.07796818196328 1.74810667618704 -4.63077853262502 c
2.05698275861065 -2.81117635431412 -5.92167258073650 c
-2.19972107078527 3.41680216119417 -6.21630199992088 c
-3.73368780433689 4.77801255357066 -7.85264232026671 c
-3.04265368676882 4.94965594266037 -10.38689696580932 c
-0.86231091106390 3.77256964355641 -11.29726207838785 c
0.61088120502357 2.43610550120807 -9.60151115067833 c
4.03592443033736 -3.97962099500674 -7.23909474049048 c
4.04056321363375 -6.54428900199182 -7.77808691238401 c
1.99482572055971 -8.00905716704414 -6.99721623600332 c
-0.04552204740007 -6.93636717214166 -5.71803606620570 c
0.02832893439615 -4.37196110249875 -5.22153481109181 c
5.70952039643018 4.01058894835319 -5.84266010077721 c
8.10452570782478 5.04220780862473 -5.48208931281607 c
9.84679827196047 3.82648798895113 -3.92566687276549 c
9.20003187443226 1.57665268973372 -2.70406676783500 c
6.81745116735481 0.52536456165902 -3.04249732137598 c
-2.88540193556670 3.21105955379690 -3.78961124695167 f
-5.43126624157640 5.66388617033681 -7.12550039471919 h
-4.22754317821095 6.00880307724558 -11.68288394431207 h
-0.31036819653731 3.87457515479253 -13.26695284933104 h
2.71927993916205 1.25719222201298 -10.44101928143598 f
6.01674137935705 -2.57669985533431 -8.00875489807024 f
5.63012338165357 -7.35276168382592 -8.78567216058102 h
1.98721112745506 -10.02019733944525 -7.39667983924546 h
-1.65189529532486 -8.04504925195256 -5.09828827736743 h
-1.92669684358121 -3.27840526544720 -4.00297647213682 f
4.34163614164301 4.97654759182155 -7.02470577265297 h
8.59403612037406 6.81041134016321 -6.39780131819523 h
11.70156854261220 4.65053393486049 -3.62875661603422 h
10.54306202604181 0.65453295814721 -1.45823556554231 h
6.30110853166739 -1.20028060947162 -2.06402942017150 h
0.76095225385719 0.41799548091754 -2.48706777717959 h
-0.12813674171217 0.25919638612923 0.07586669091466 h

FLP-$H_2$ [1-H][H-**7**]
-1.80976420880272 4.23872173346921 4.95458960709354 c
-1.85462479669168 2.26885534693459 3.20651291603809 c
-4.20371560401397 1.83888126411843 2.08858554071507 c
-6.35246355129848 3.26328124137807 2.59975629395473 c
-6.20343865409581 5.22623435529232 4.34439371739621 c
-3.91122511135464 5.71487186487967 5.53701723398092 c
0.55287174496257 0.55623562317221 2.36678056325437 b
0.44695171077093 -2.32453002899280 3.43997304657568 c
1.57115386825767 -4.28054473502663 2.08430999920826 c
1.44826630337602 -6.81631377966449 2.75278694441122 c
0.15207361706238 -7.49484050432538 4.93829870154985 c
-0.97594085371947 -5.61566124370949 6.39148936267322 c
-0.80516853554180 -3.09908781437329 5.62737174265349 c

2.90550559725259 -3.73563766202836 -0.05674807290449 f
2.55731942830338 -8.61588961329214 1.31546465889497 f
0.00030144860356 -9.93490374846321 5.63836359287827 f
-2.21330974594958 -6.25264358862678 8.52318562779508 f
-1.91546731329865 -1.38178273511593 7.16456583231941 f
-4.47237059521914 -0.06470284448271 0.38212069033649 f
-8.56681797559583 2.77612367661587 1.42672916378819 f
-8.25629071179106 6.63269106817483 4.87394615248508 f
-3.75754373724333 7.59996137565766 7.24406131639139 f
0.34974311612119 4.79621747443802 6.21918427392700 f
5.05049392296288 -0.82965429069136 5.72076145238423 f
5.27275149723058 1.21965665829927 4.20849648425403 c
3.26876806619951 1.98399363194209 2.67452690896401 c
3.75526957175967 4.15640097019109 1.25988538357184 c
6.01099941789956 5.49725534012830 1.32510870410818 c
7.96426253701151 4.63170821325870 2.85690217889361 c
7.58993706438801 2.47461326693384 4.31070146899499 c
1.94149285982722 5.06970020598151 -0.33146787616796 f
6.35337002557124 7.58090424988424 -0.11061387969144 f
10.19923061806741 5.85175545029677 2.89920792544656 f
9.47333598769924 1.62559718146447 5.79902029746589 f
2.25355624276255 0.63670621730720 -4.87415663019657 p
-0.12657680817444 2.03076242262584 -6.83746688879358 c
5.18596256147013 2.33498143191700 -4.93363419723573 c
2.65027340296470 -2.59098314200234 -5.83999662286523 c
-2.21487252135951 3.30358605772975 -5.81390325710720 c
-4.16196038830502 4.23031466440607 -7.30639225034211 c
-4.02022953337853 3.89683503115627 -9.91350568776708 c
-1.96810875723663 2.66782597362156 -11.03133833030392 c
-0.07297551466510 1.77247072279721 -9.47287869151910 c
4.70213177143671 -3.61068830509340 -7.16322819623216 c
4.90761563082649 -6.17019792634021 -7.67634132700536 c
2.99015063622208 -7.78517361817039 -6.86280081058662 c
0.87990952308194 -6.86428766522218 -5.58096355503781 c
0.75515705467567 -4.29722408300853 -5.11093845260344 c
5.63419914761396 4.60579647358578 -6.22653170364003 c
7.91853162759466 5.87598291543541 -6.08625957424340 c
9.84638577543590 4.87099376455424 -4.60062449053390 c
9.50689610880889 2.61946034032016 -3.27474366726108 c
7.19758550477901 1.41434945895479 -3.46654779151887 c
-2.32272614456828 3.64094154431999 -3.30758405576336 f
-5.73795810483097 5.18625135425795 -6.41330968987884 h
-5.52913846793304 4.61435695020613 -11.10239629394431 h
-1.82223733998489 2.41724814861536 -13.05879028161610 h
1.95744396230133 0.61746552955127 -10.51265201385979 f
6.55327415547207 -2.05475284630725 -7.97609666244613 f
6.54745979145316 -6.86034963867888 -8.69119411646233 h
3.14103130780692 -9.79500576158314 -7.23919209259971 h
-0.62697953998721 -8.08967605974698 -4.93234639225501 h
-1.27579582972616 -3.33910660713362 -3.90019286100356 f
3.78270492011772 5.61702632678785 -7.66224636948167 f
8.14521914421271 7.63479696272911 -7.11056167488036 h
11.63210792276569 5.86685495305228 -4.45528379914391 h

10.97064027046236 1.81763346855760 -2.08810171306076 h
6.81975341134538 -0.76591587560199 -2.20316056614271 f
0.26933078955997 0.30877726297655 0.06232482433923 h
1.26780327826846 0.55911894970469 -2.31141007064723 h

FLP-$H_2$ [1-H][H-**8**]
-2.21367176597740 1.86035799476202 1.16476966812613 c
-0.46797611828337 -0.01485526450174 0.52807132515134 c
-1.52880825998606 -2.08101264748172 -0.72943627950971 c
-4.07329673626441 -2.30330762894475 -1.36123362042931 c
-5.73405097279876 -0.38641474231382 -0.66505735726940 c
-4.78798927904398 1.70431591431115 0.62008795329697 c
2.58675152096289 -0.00777351031935 1.03680453307986 b
3.50314334857637 -2.16664335163555 3.03035549648736 c
5.97040150330949 -3.08640988214807 2.87451230141502 c
6.94605422704106 -4.94334467452046 4.45895261398336 c
5.40294781505724 -5.97026526409316 6.32661338454767 c
2.92772945659332 -5.11515043989021 6.56646501092415 c
2.03984074722000 -3.24793837592436 4.93528929545135 c
7.56501892464712 -2.15160495459745 1.08527000211400 f
9.34714366101045 -5.76229292613675 4.20915416612735 f
6.29845494888937 -7.76918846214244 7.88372699961738 f
1.42678277795668 -6.09511906330119 8.37576296274692 f
-0.38305973131670 -2.49094845164909 5.29414414334269 f
-0.02761419567708 -4.05909469144511 -1.39406331479684 f
-4.94287226272939 -4.34507044769793 -2.62567125935222 f
-8.20119441707270 -0.53720070224639 -1.25279125951279 f
-6.37033422785357 3.59663189255364 1.25889713658684 f
-1.47456494873309 3.99574292182725 2.35380566372671 f
2.50146898537269 2.53449757673615 6.02715085687586 f
3.70508145939829 3.78742119044966 4.15444083045127 c
3.78859299421949 2.74501943393792 1.73068097752213 c
5.05421755697720 4.22367914747756 -0.03443671113490 c
6.12948943077522 6.56683323747117 0.48317202561371 c
5.98285540947289 7.52367825427934 2.92564511029203 c
4.76191083949920 6.11277816425859 4.78371198201526 c
5.32268570488197 3.40363804128701 -2.47874088019538 f
7.30765010158891 7.90460503016798 -1.34594520174107 f
7.00631458878272 9.78132846480940 3.48598215792248 f
4.60111678929002 7.03037494556434 7.15096689584290 f
1.93087435422922 0.54741607523447 -6.08294641222967 p
0.38376848581935 3.53507904122754 -5.78796227025424 c
4.74574899586541 0.74115260087160 -7.94219690608090 c
-0.11960780233677 -1.85471840681772 -7.37339038226571 c
-2.03228504850114 3.65277236309003 -4.71014094725387 c
-3.11760154519285 5.99403728500475 -4.22084065490191 c
-1.79561846639187 8.20565063448114 -4.79135609467516 c
0.61182218872819 8.08419210023921 -5.85930372822727 c
1.71802620055030 5.74996793803447 -6.36153041792869 c
0.58666534959321 -4.37365691999139 -6.93419544922667 c
-0.90435550744118 -6.39478001180727 -7.69200105933913 c
-3.16066269929327 -5.91091215863453 -8.96924649700120 c
-3.87662412064504 -3.43223496475408 -9.51075384092199 c

-2.34673487831869 -1.43722568326480 -8.74097583890054 c
4.63246328704982 1.50780152916229 -10.47883703473321 c
6.84546057187947 1.61417998638562 -11.89264006121462 c
9.15081262829891 0.95017352913026 -10.78690709141363 c
9.25446380360381 0.17713504045678 -8.26896287896157 c
7.05277970501110 0.06529118096340 -6.82887721209134 c
-3.04358002109742 1.93131407649848 -4.24239895143404 h
-4.97908176052135 6.08991419260590 -3.36652845136383 h
-2.64208985378675 10.03032558665851 -4.38662758163543 h
1.64530677394505 9.80466380539854 -6.28132379918427 h
3.61098101525642 5.64871159481842 -7.14040885068950 h
2.79045148620995 -4.85474254438414 -5.77825999772029 f
-0.19726316958444 -8.77165403208244 -7.22996385620206 f
-4.61424879482503 -7.82465713126982 -9.71578275614098 f
-6.00818478981185 -2.98907353654094 -10.79483977859189 f
-3.06331164354877 0.91034879069012 -9.38719387615934 f
2.83573575501774 2.02295434336685 -11.32959589042259 h
6.77563539526131 2.21196578590252 -13.85373365637940 h
10.87346676585264 1.03660375527850 -11.89868497192996 h
11.04809276420138 -0.33539329953580 -7.41673669517266 h
7.12201502965211 -0.52124930312778 -4.86444999801666 h
2.65925867594396 -0.34611817795398 -3.64457538973512 h
3.55177199354081 -0.65595879423853 -0.96405333091969 h