Supporting Information for

Selective heterolytic P-P bond cleavage of white phosphorus by frustrated carbene-borane Lewis pairs

Dirk Holschumacher, Thomas Bannenberg, Kerstin Ibrom, Constantin G. Daniliuc, Peter G. Jones and Matthias Tamm*

* *Institut für Anorganische und Analytische Chemie, Technische Universität Carolo-Wilhelmina, Hagenring 30, D-38106 Braunschweig, Germany.*

Fax: +49 (251) 391-5309; Tel: +49 (251) 391-5387; E-mail: m.tamm@tu-bs.de

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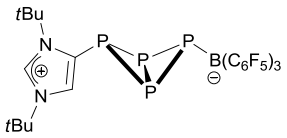
1. Experimental Details

Materials and Methods: All operations with air and moisture-sensitive compounds were performed in a glove box under a dry argon atmosphere (MBraun 200B) or on a high vacuum line using Schlenk techniques. All solvents were purified by a solvent purification system from MBraun and stored over molecular sieve (4 Å) prior to use. Elemental analysis (C, H, N) succeeded by combustion MS on a Finnigan MAT 95 (EI), Finnigan MAT 95 XL (ESI), respectively and HR-MS from Bruker-Demo QTOF micro. Unless otherwise indicated, all starting materials were obtained from Aldrich and were used without further purification. 1,3-Di-*tert.*-butylimidazolin-2-ylidene (**1**)[1] and $B(C_6F_5)_3$[2] were prepared according to literature procedures.

[1] A. J. Arduengo III., *US Patent 5 077 414*, **1991**, b) A. J. Arduengo, III; H. Bock, H. Chen, M. Denk, D. A. Dixon, J. C. Green, W. A. Herrmann, N. L. Jones, M. Wagner, R. West *J. Am. Chem. Soc.* **1994,** *116,* 6641-6649

[2] C. Wang, G. Erker, G. Kehr, K. Wedeking, R. Fröhlich, *Organometallics* **2005,** *24,* 4760-4773



(3): To 20 ml of a solution of P_4 (0.98 mmol, 121 mg) in toluene/benzene (5:1) were added $B(C_6F_5)_3$ (0.98 mmol, 0.500 g) and 1,3-Di-*tert.*-butylimidazolin-2-ylidene **1** (0.98 mmol 0.177 g). The solution was mixed at ca. 5 °C and stirred at rt for 4 hours. During this time the colour of the solution changed from yellow to purple and a smooth pale yellow precipitate was formed. The solvent was decanted carefully and the solid was washed 4 times with 3 ml toluene and following 3 times with 5 ml pentane. The crude product was dried in vacuo and recrystallized from THF/pentane at -35 °C. The product was collected as a white solid after filtration and drying in vacuo. Yield 523 mg (67 %, based on elemental analysis). Crystals for **3** were obtained from a mixture of THF/pentane at -35 °C.

elemental analysis: theoretical for $C_{29}H_{20}BF_{15}N_2P_4 \cdot 2$ THF: N 2.92, C 46.28, H 3.78, found: N 2.99, C 45.76, H 3.65.

2. NMR Characterisation

The NMR spectra were obtained on Bruker Avance II 600, DRX 400 and Avance II 300 instruments. Frequencies and referencing methods are listed in tables 1-5. For referencing the ^{19}F, ^{31}P and ^{11}B spectra the observation frequencies of a dilute solution of the reference compound in THF-d_8 (^{19}F, virtual internal referencing) or the neat external standard (^{31}P, ^{11}B, virtual external referencing) had been determined earlier. The β-deuterium atoms of THF-d_8 were always used as the lock signal. Standard two-dimensional techniques (HSQC, HMBC) as well as ^{13}C triple resonances spectra (selective decoupling for all three ^{31}P signals under ^{1}H broadband decoupling conditions) were used to assign the spectra.

Table 1 ^{1}H-NMR spectrum of **3**, 600.1 MHz, THF-d_8, δ(TMS) = 0

δ [ppm]	multiplicity	no. of H	J [Hz]	assignment
8.45	d	1	$J_{1\text{-}H,3\text{-}H}$ = 1.9	1-H
7.47	d	1		3-H
1.84	s	9		$C(CH_3)_3$ at N-1
1.54	s	9		$C(CH_3)_3$ at N-2

Table 2 ^{13}C-NMR spectrum of **3**, 150.9 MHz, THF-d_8, δ(THF-d_8) = 25.3

δ [ppm]	Type of C	multiplicity[1]	*J* [Hz][1]	assignment
148.80	C_q	"dm"	Splitting: 240.5	$B(C_6F_5)_3$: C_{ortho}
≈ 139.2	C_q	"dt"	Splittings: 246.4, ≥ 13.7	$B(C_6F_5)_3$: C_{para}
≈ 137.6	C_q	"ddd"	Splittings: 246.7, ≥ 20.9, ≥ 11.3	$B(C_6F_5)_3$: C_{meta}
≈ 136.3	C_q	dd	$J_{P\text{-}1,C}$ ≈ 106, $J_{P\text{-}4,C}$ ≈ 44*	C-2
133.98	CH	s		C-1
127.72	CH	br. s	$J_{P\text{-}2,C}$ = 8.9**	C-3
≈ 123.4	C_q	v br. m	($v_{½}$ ≈ 155 Hz)	$B(C_6F_5)_3$: C_{ipso}
63.30	C_q	s		*C*$(CH_3)_3$ at N-1
61.25	C_q	s		*C*$(CH_3)_3$ at N-2
30.33	q	d	$J_{P\text{-}2,C}$ = 9.3[2]	C(*C*$H_3)_3$ at N-1
29.21	q	s		C(*C*$H_3)_3$ at N-2

*derived from HMBC; **derived from $^{13}C\{^{31}P_{sel},^{1}H\}$, irradiation at δ(^{31}P) = -200.2 ppm

[1] Where spectra of higher order are observed merely a description of the multiplicity and splittings instead of couplings constants are given.

Table 3 ^{19}F-NMR spectrum of **3**, 376.4 MHz, THF-d_8, $\delta[(CFCl_3)_{virt.,int.}] = 0$

δ [ppm]	multiplicity	Splitting [Hz]	assignment
-126.0	"br. d"	≈ 68 ($v_{½}$ ≈ 50 Hz)	$B(C_6F_5)_3$: F_{ortho}
-162.6	"t"	20.4	$B(C_6F_5)_3$: F_{meta}
-166.1	"≈ t"	19.0	$B(C_6F_5)_3$: F_{para}

Table 4 ^{31}P-NMR spectrum of **3**, 121.5 MHz, THF-d_8, $\delta[(85\ \%\ H_3PO_4)_{virt.,\ ext.}] = 0$

δ [ppm]	multiplicity	Splitting [Hz]	assignment
-159.5	dtsept	$J_{P\text{-}1,P\text{-}4}$ = 285.3, $J_{P\text{-}2,P\text{-}4}$ = 172.7, $J_{P\text{-}4,Fortho}$ = 63.3	P-4
-200.2	br. m	$J_{P\text{-}1,P\text{-}2}$ = 173.2	P-1
-327.4	tsept	$J_{P\text{-}2,Fortho}$ = 12.3	P-2

Table 5 ^{11}B-NMR spectrum of **3**, 96.3 MHz, THF-d_8, $\delta[(BF_3{\cdot}O(CH_2CH_3)_2)_{virt.,\ ext.}] = 0$

δ [ppm]	multiplicity	Splitting [Hz]
-13.9	br. d	36 ($v_{½}$ ≈ 79 Hz)

Please note:

The following spectra, which were recorded on a 600 MHz-NMR spectrometer show impurities due to decomposition in solution during prolonged measurements within two days.

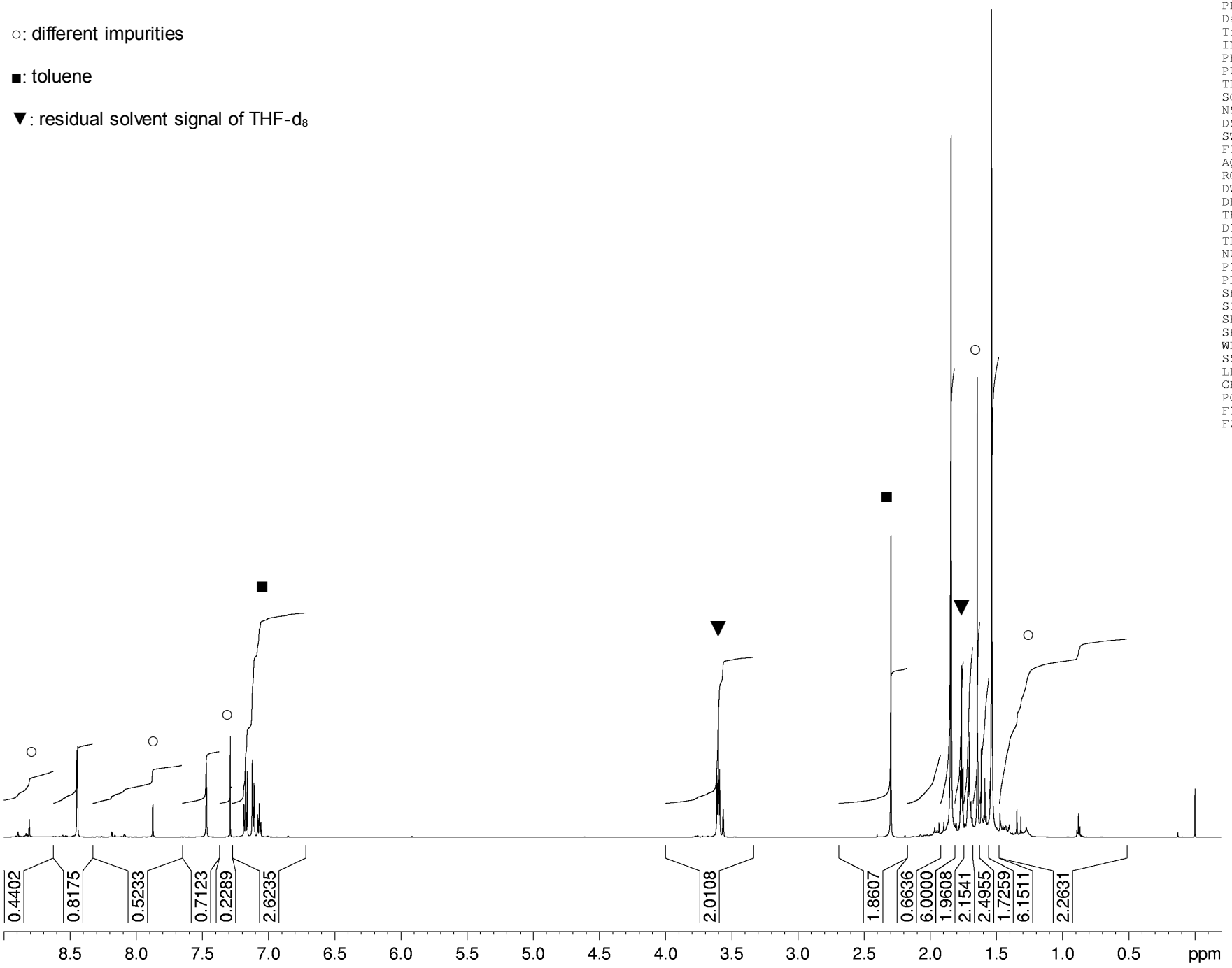
NMR spectra of freshly prepared samples measured on a 400 MHz NMR-spectrometer are also shown; these show no impurities.

^{1}H-NMR spectrum of **3**

○: different impurities

■: toluene

▼: residual solvent signal of THF-d_8



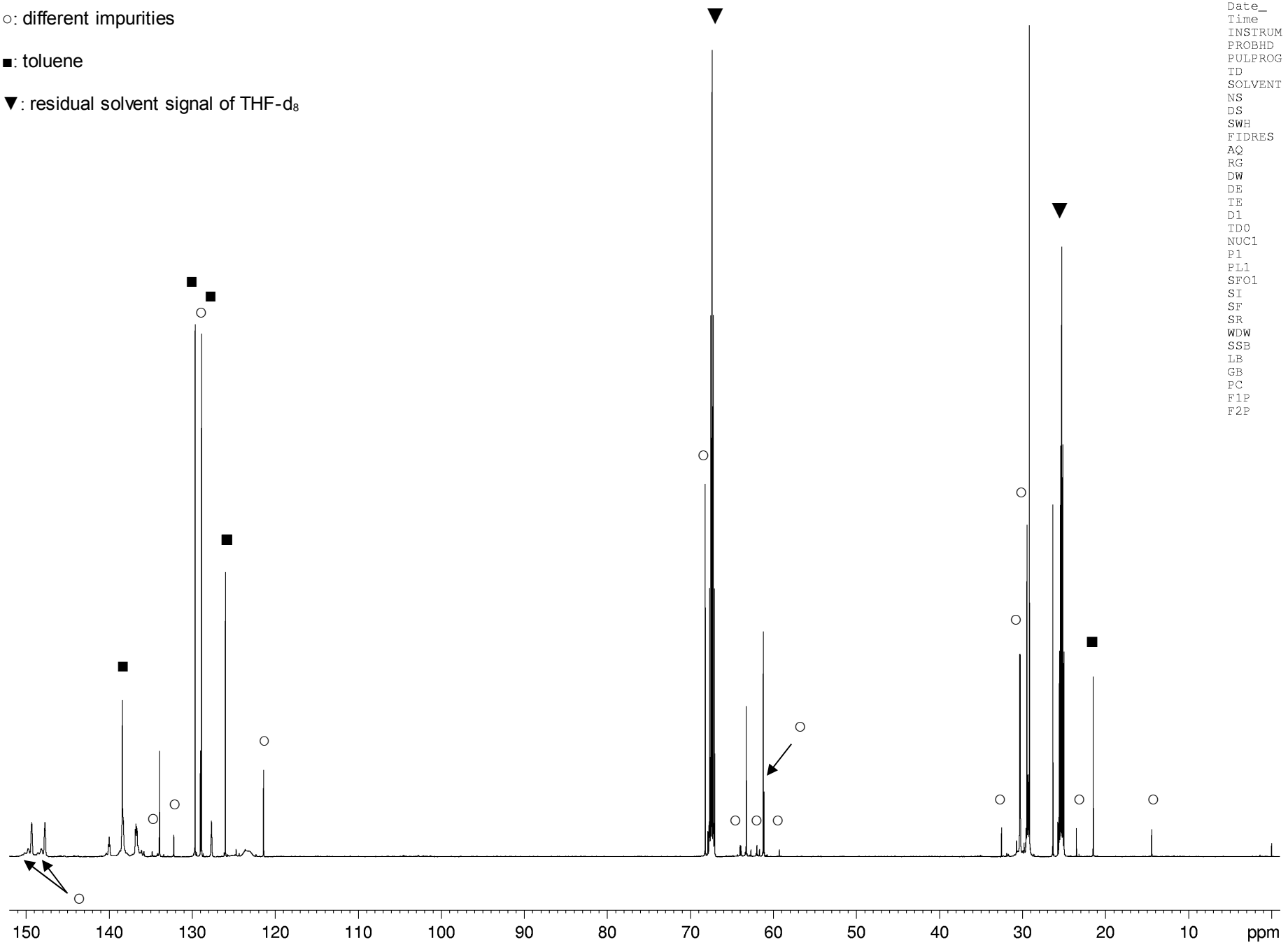
NAME	hod99193_at
EXPNO	11
PROCNO	1
Date_	20091002
Time	12.10
INSTRUM	av600
PROBHD	5 mm CPTCI 1H-
PULPROG	zg30
TD	98304
SOLVENT	THF
NS	64
DS	2
SWH	12335.526 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	40.533 use
DE	6.00 use
TE	301.2 K
D1	1.00000000 sec
TD0	1
NUC1	1H
P1	7.20 use
PL1	3.00 dB
SFO1	600.1337052 MHz
SI	131072
SF	600.1300183 MHz
SR	18.27 Hz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
F1P	9.000 ppm
F2P	-0.200 ppm

^{13}C-NMR spectrum of **3**

○: different impurities

■: toluene

▼: residual solvent signal of THF-d_8

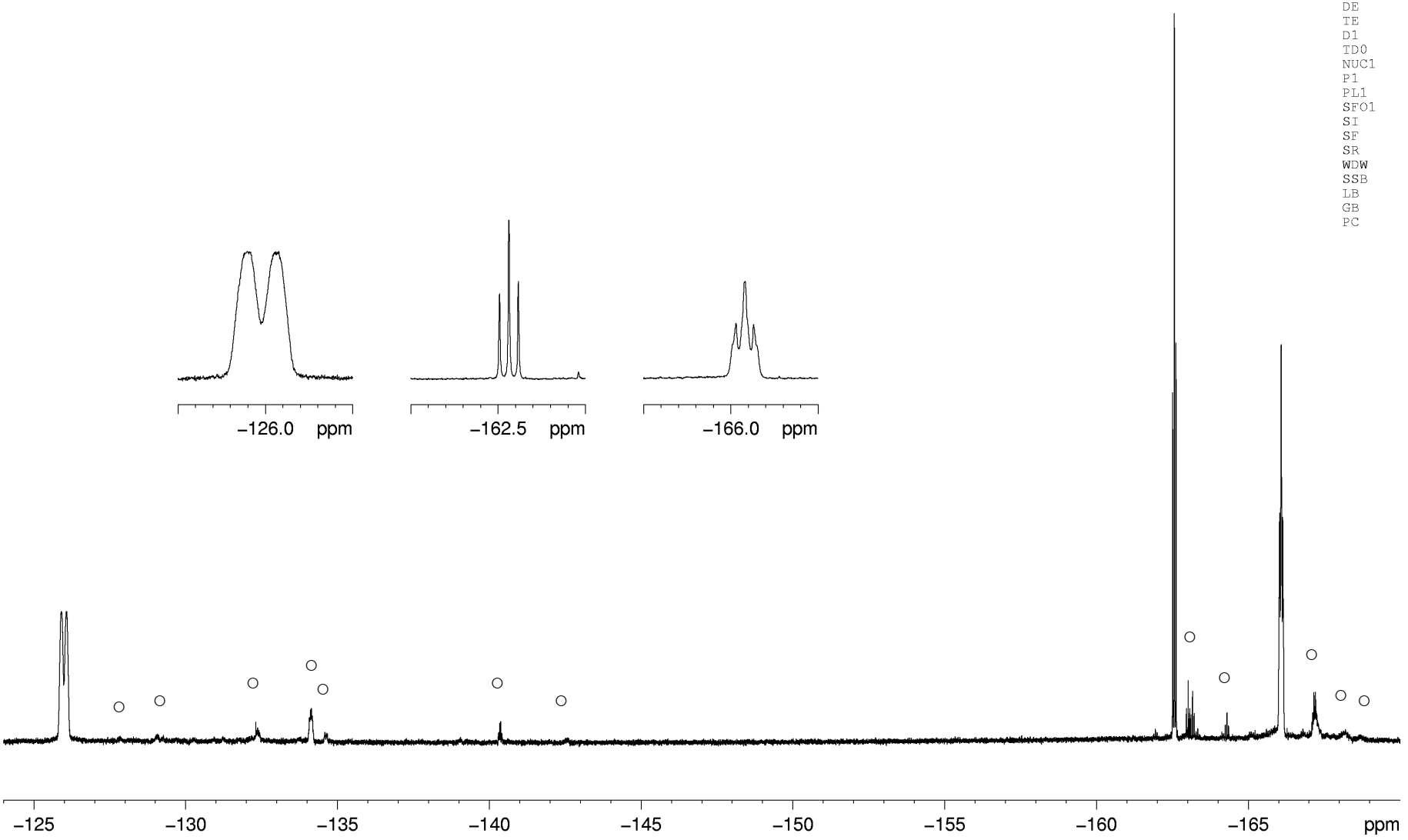


NAME	hod99193_at
EXPNO	12
PROCNO	1
Date_	20091002
Time	13.05
INSTRUM	av600
PROBHD	5 mm CPTCI 1H-
PULPROG	zgpg30
TD	196608
SOLVENT	THF
NS	7000
DS	4
SWH	39682.539 Hz
FIDRES	0.201836 Hz
AQ	2.4773109 sec
RG	256
DW	12.600 use
DE	20.00 use
TE	301.2 K
D1	2.00000000 sec
TD0	1
NUC1	13C
P1	10.80 use
PL1	-1.15 dB
SFO1	150.9195573 MHz
SI	131072
SF	150.9026601 MHz
SR	-148.95 Hz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40
F1P	152.000 ppm
F2P	-1.000 ppm

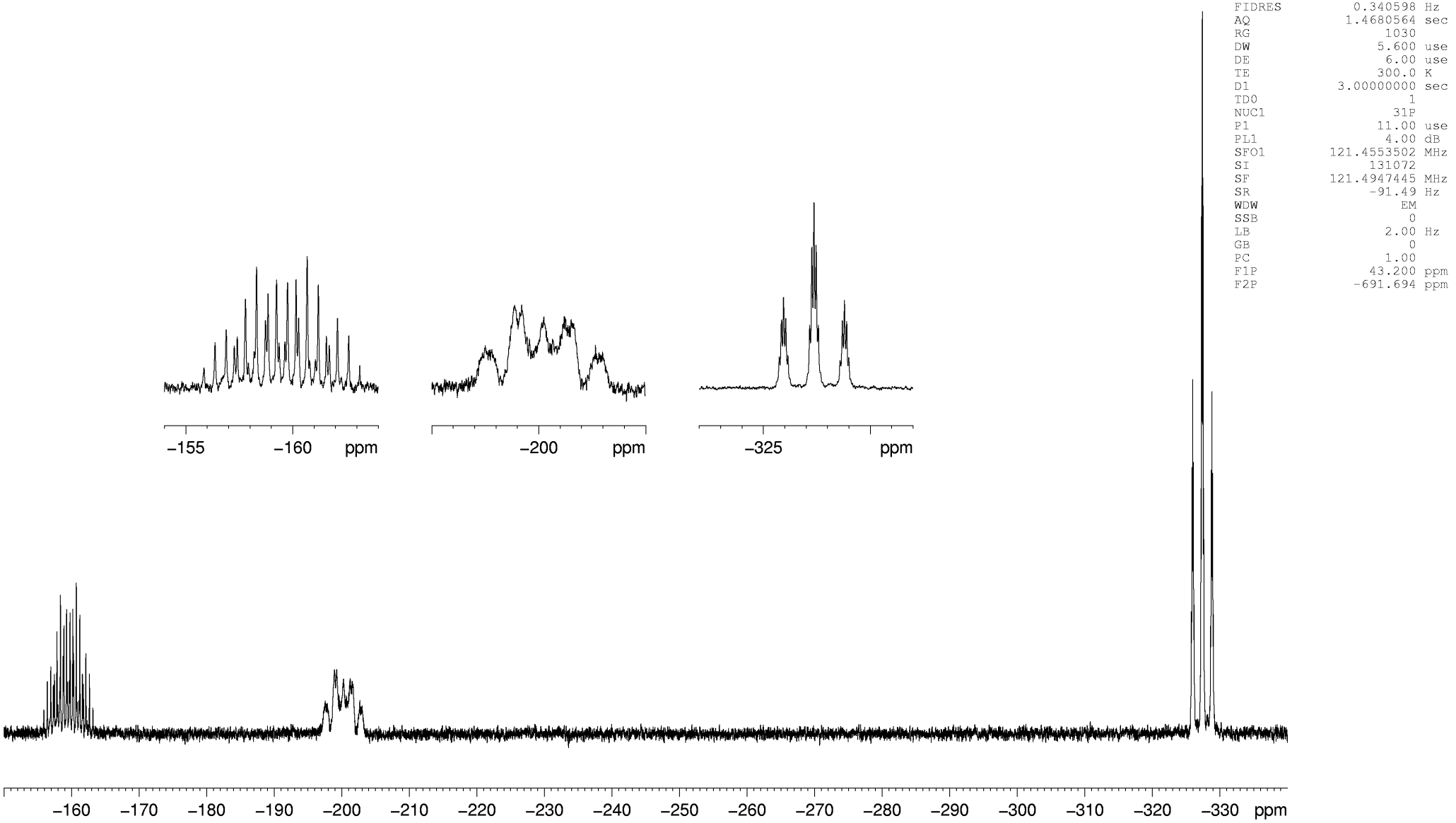
^{19}F-NMR spectrum of **3**

○: different impurities

NAME	hod97726_at
EXPNO	1
PROCNO	1
Date_	20090626
Time	13.21
INSTRUM	drx400
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn30.i
TD	262144
SOLVENT	THF
NS	64
DS	4
SWH	75187.969 Hz
FIDRES	0.286819 Hz
AQ	1.7433076 sec
RG	3251
DW	6.650 use
DE	6.00 use
TE	299.2 K
D1	2.00000000 sec
TD0	1
NUC1	19F
P1	9.40 use
PL1	-4.00 dB
SFO1	376.4043252 MHz
SI	131072
SF	376.4415429 MHz
SR	-356.11 Hz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



^{31}P-NMR spectrum of **3**



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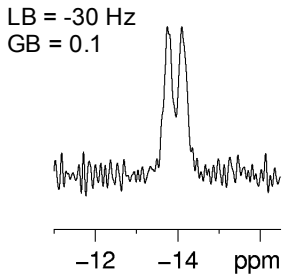
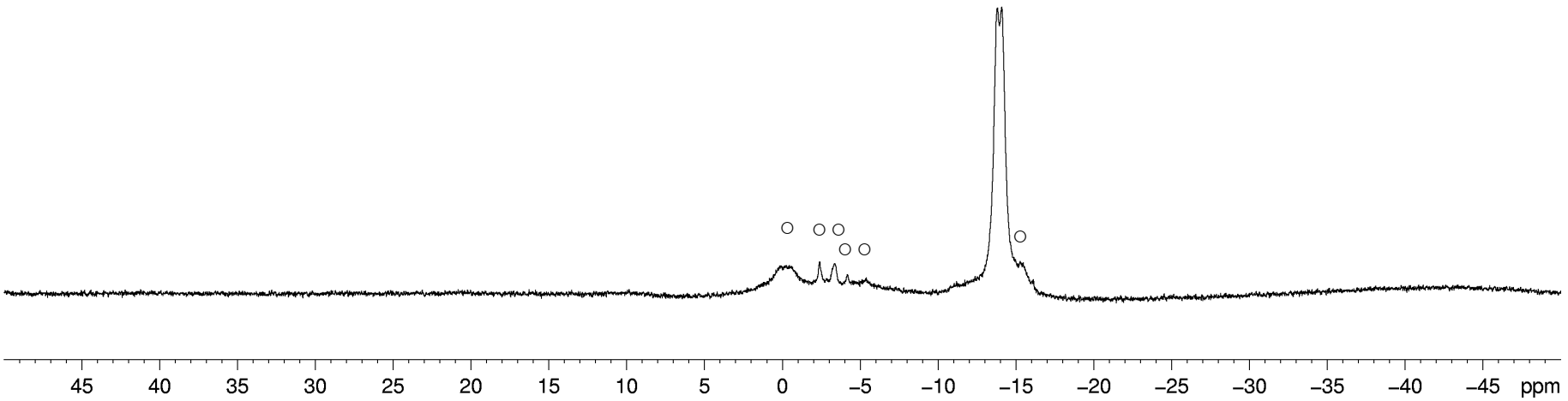
PROCNO	1
Date_	20090625
Time	15.43
INSTRUM	av300
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	262144
SOLVENT	THF
NS	512
DS	4
SWH	89285.711 Hz
FIDRES	0.340598 Hz
AQ	1.4680564 sec
RG	1030
DW	5.600 use
DE	6.00 use
TE	300.0 K
D1	3.00000000 sec
TD0	1
NUC1	31P
P1	11.00 use
PL1	4.00 dB
SFO1	121.4553502 MHz
SI	131072
SF	121.4947445 MHz
SR	-91.49 Hz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00
F1P	43.200 ppm
F2P	-691.694 ppm

^{11}B-NMR spectrum of **3**

○: different impurities and probehead background signal resp.

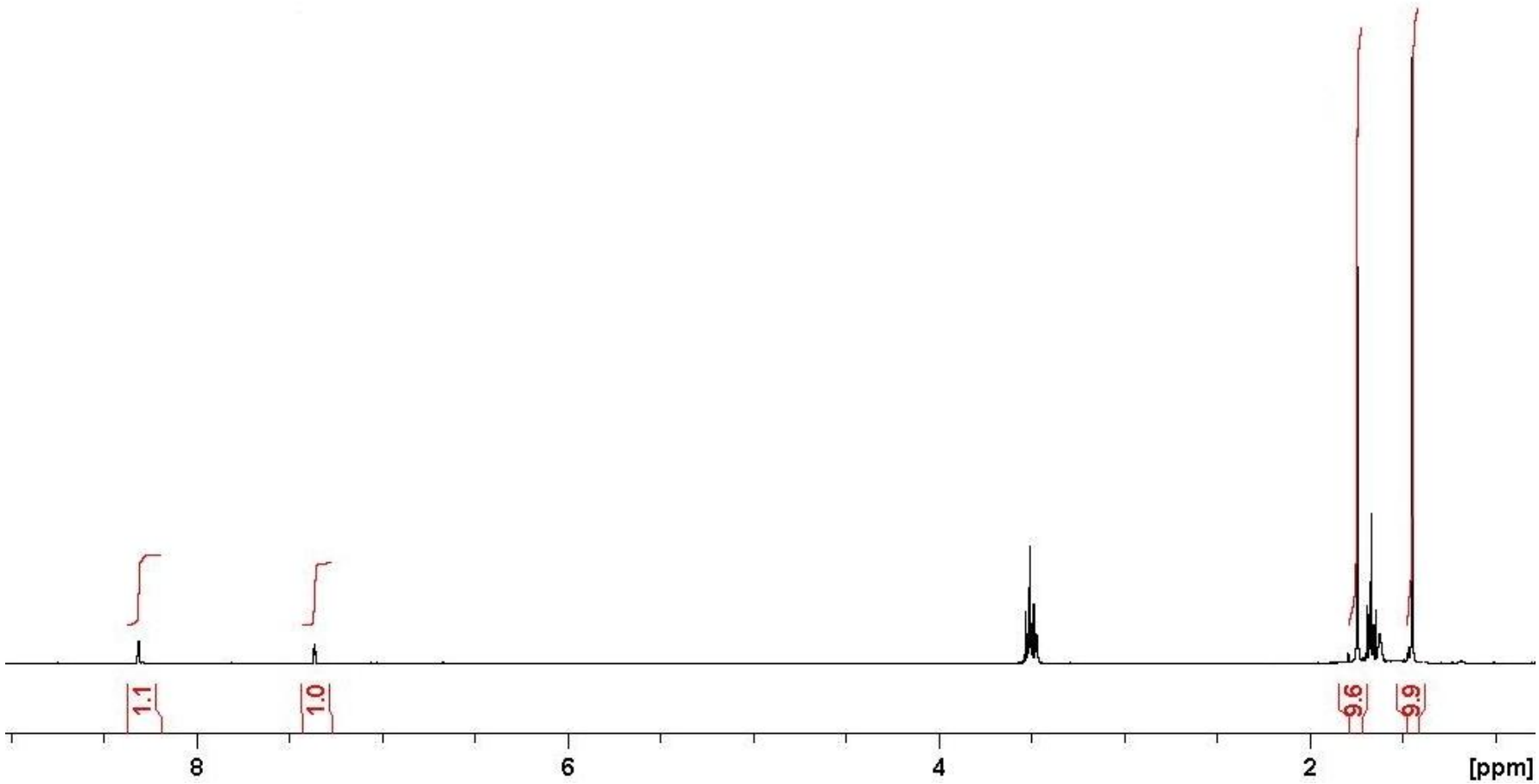
NAME	hod97726_at
EXPNO	3
PROCNO	1
Date_	20090625
Time	16.01
INSTRUM	av300
PROBHD	5 mm PABBO BB-
PULPROG	zgpg
TD	32768
SOLVENT	THF
NS	512
DS	4
SWH	21008.404 Hz
FIDRES	0.641126 Hz
AQ	0.7799284 sec
RG	287
DW	23.800 use
DE	6.00 use
TE	300.0 K
D1	1.00000000 sec
TD0	1
NUC1	11B
P1	9.70 use
PL1	4.00 dB
SFO1	96.2936310 MHz
SI	16384
SF	96.2935819 MHz
SR	-49.11 Hz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40
F1P	50.865 ppm
F2P	-49.119 ppm



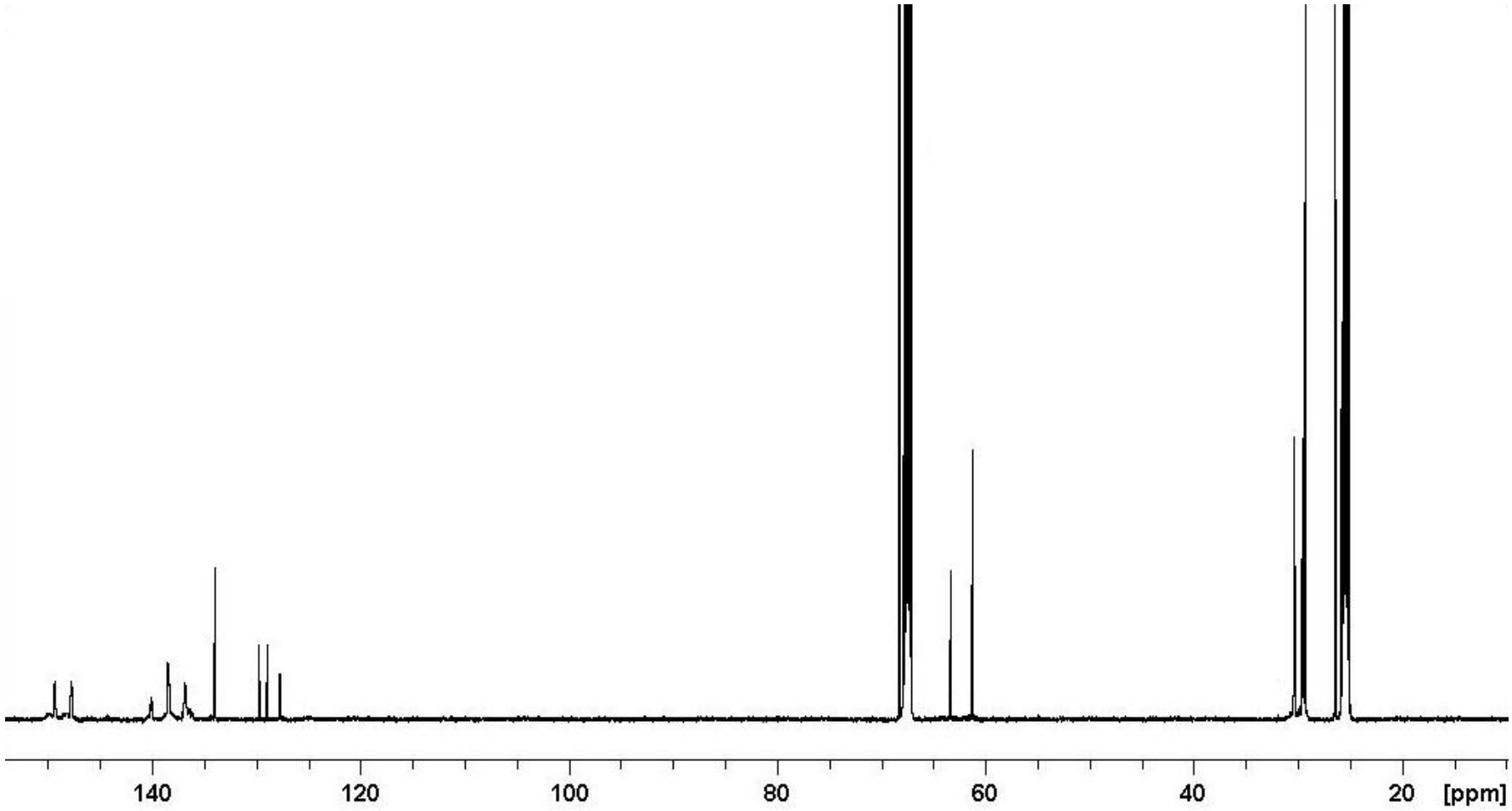


NMR spectroscopic illustration of the compound **3**, which were directly measured after synthesis on a DRX 400 spectrometer. In solution slow decomposition takes place after some hours.

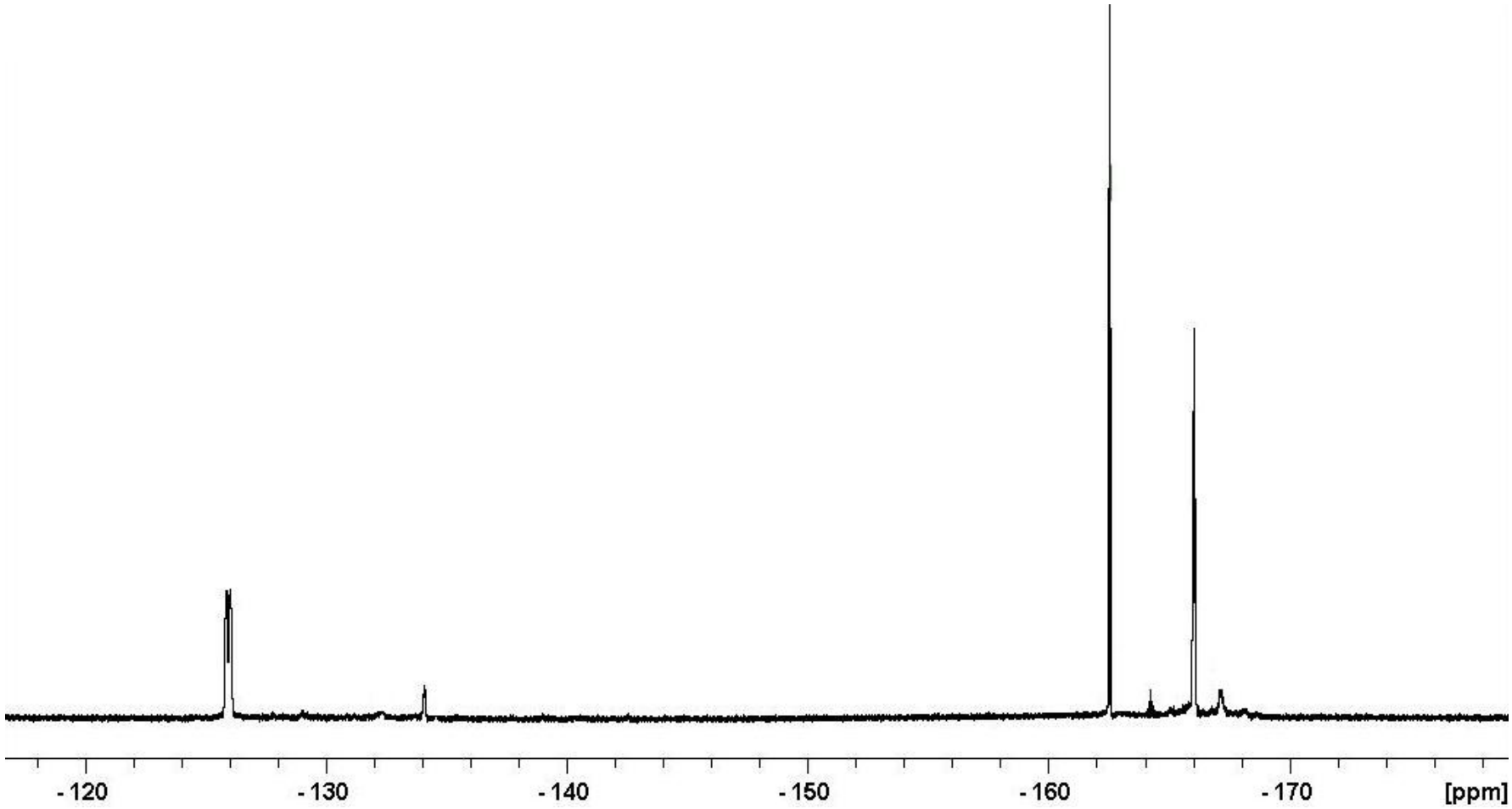
^{1}H NMR



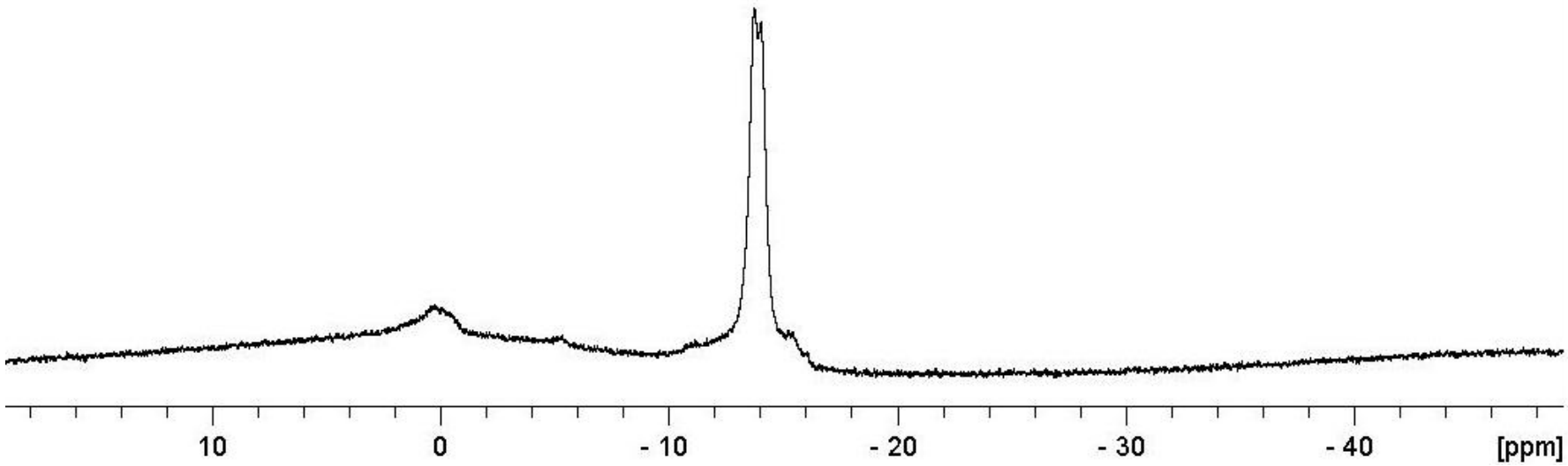
^{13}C NMR



^{19}F NMR



^{11}B NMR



3. X-Ray structure determination of 3·2THF

Crystal data: $C_{37}H_{36}BF_{15}N_2O_2P_4$, M = 960.37, monoclinic, $P2_1/n$, a = 15.2628(2), b = 12.8453(2), c = 21.2228(4) Å, β = 94.111(2)°, Z = 4, V = 4150.14(2) Å^3, D_x = 1.537 Mg m^{-3}, μ = 0.29 mm^{-1}, T = 100 K. Data collection: A crystal 0.26 × 0.16 × 0.09 mm was used to record 160687 intensities to 2θ 56.6° on an Oxford Diffraction Xcalibur E diffractometer using monochromated Mo $K\alpha$ radiation. An absorption correction was performed on the basis of multi-scans. Structure refinement: The structure was refined anisotropically on F^2 using the program SHELXL-97 (G.M. Sheldrick, University of Göttingen, Germany). Hydrogen atoms were included using rigid methyl groups or a riding model. The final $wR2$ was 0.0631 for 556 parameters and all 9886 unique reflections, with conventional $R1$ ($F > 4\sigma(F)$) 0.0298; max. Δρ 0.43 e Å^{-3}; S 0.87.

4. Computational Details

All computations were performed using the hybrid density functional method M05-2X implemented in the Gaussian09 program.[1] For all main-group elements (C, H, N, B, F) the all-electron triple-ζ basis set (6-311G**) was used.[2]

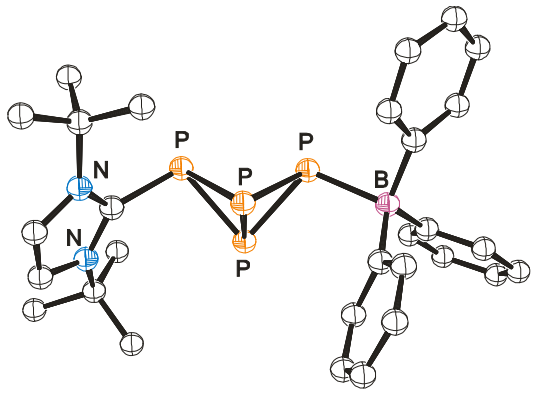
[1] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[2] X. Cao and M. Dolg, *J. Chem. Phys.* 2001, **115**, 7348.

Energies for all optimized structure:

Compound	E(0 K)[a] [Ha]	H(298 K)[b] [Ha]	G(298 K)[b] [Ha]
tBu_2ImC-P_4-BR_3 (**4**) (*trans-trans*)	-4114.484986	-4114.434616	-4114.570734
tBu_2ImCH-P_4-BR_3 (**3**) (*trans-trans*)	-4114.508198	-4114.457935	-4114.593018
tBu_2ImCH-P_4-BR_3 (**5**) (*trans-cis*)	-4114.504674	-4114.454632	-4114.587323
tBu_2ImCH-P_4-BR_3 (**6**) (*cis-trans*)	-4114.511446	-4114.460983	-4114.597554

[a]DFT energy incl. ZPE.
[b]standard conditions T = 298.15 K and p = 1 atm.

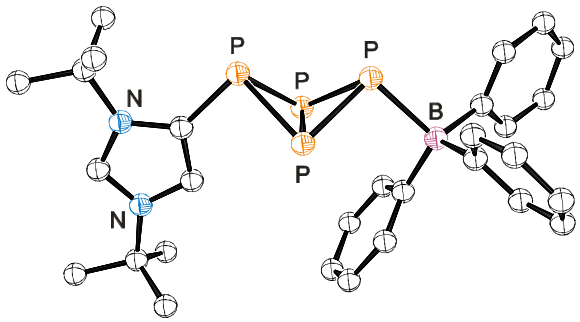


(*trans-trans*)

Structure of the carben-P_4-boran adduct (4) (atom, x-, y-, z-positions in Å):
(Hydrogen and fluorine atoms are omitted for clarity)

B	1.638200	0.064600	-0.138200
N	-5.102400	1.019100	-0.047300
N	-5.124500	-1.144100	-0.341100
P	-2.876800	0.285400	-1.655900
P	-1.603300	0.530900	0.163600
P	-1.512500	-1.340200	-0.926300
P	-0.017700	0.257100	-1.356500
F	4.001100	0.968200	-1.792600
F	4.738600	3.453400	-2.213600
F	3.363500	5.528000	-1.122000
F	1.190000	5.018400	0.436800
F	0.419600	2.535400	0.900100
F	2.230200	1.575000	2.474800
F	1.466900	0.797300	4.874200
F	0.188300	-1.568600	5.235100
F	-0.295900	-3.173200	3.083500
F	0.465100	-2.419300	0.654700
F	4.155700	-0.340200	1.021000
F	5.964700	-2.228600	0.441300
F	5.496800	-3.989800	-1.576700
F	3.182400	-3.832600	-2.991100
F	1.371000	-1.982800	-2.425400
C	-6.078800	0.497700	0.769400
C	-6.087300	-0.838100	0.594500
C	-4.473700	-0.007500	-0.684600
C	-4.994400	2.508000	-0.333600
C	-3.663300	3.103000	0.126100
C	-5.224100	2.719900	-1.830000
C	-6.113800	3.220100	0.428200
C	2.188200	1.592700	-0.376200
C	3.272900	1.915400	-1.184200
C	3.681800	3.216100	-1.435000
C	2.987100	4.272800	-0.885700
C	1.886400	4.009400	-0.093700
C	1.514000	2.700100	0.130900
C	1.264100	-0.319000	1.404500
C	1.547800	0.426900	2.543600
C	1.185200	0.029500	3.820200
C	0.545900	-1.179600	4.012000
C	0.298400	-1.987900	2.920500
C	0.681900	-1.554100	1.666300
C	2.674600	-1.079600	-0.656900
C	3.873200	-1.205300	0.033300
C	4.826800	-2.161000	-0.252000
C	4.593600	-3.055900	-1.280900
C	3.418000	-2.971400	-1.997800
C	2.489800	-1.994400	-1.676500
C	-5.045600	-2.542000	-0.917200
C	-4.232300	-3.426800	0.022400

C	-4.492400	-2.513200	-2.340000
C	-6.480700	-3.080600	-1.008600
H	-6.914300	-3.294500	-0.034000
H	-7.127400	-2.390800	-1.551100
H	-6.446900	-4.021800	-1.554000
H	-6.709300	-1.578800	1.054100
H	-3.411300	2.770700	1.132200
H	-3.770300	4.187500	0.140300
H	-2.843800	2.863900	-0.543200
H	-6.696800	1.097700	1.404700
H	-3.207400	-3.079700	0.116900
H	-4.689400	-3.450300	1.012500
H	-4.218800	-4.442600	-0.373100
H	-3.434400	-2.291500	-2.386100
H	-4.637400	-3.502700	-2.771100
H	-5.038600	-1.793000	-2.950900
H	-7.100600	2.853300	0.147000
H	-6.064300	4.273800	0.162000
H	-5.981900	3.148100	1.508000
H	-4.436700	2.272100	-2.431700
H	-5.229000	3.791100	-2.030900
H	-6.187100	2.305100	-2.129900

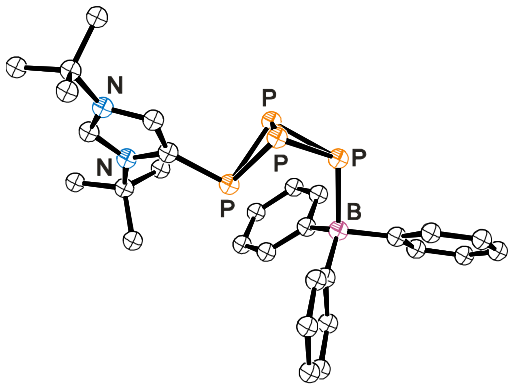


(*trans-trans*)

Structure of the abnormal carben-P_4-boran adduct (3) (atom, x-, y-, z-positions in Å):
(Hydrogen and fluorine atoms are omitted for clarity)

B	-1.806600	-0.102400	-0.138100
N	5.320800	-1.405600	-0.643300
N	5.258100	0.564800	0.276100
P	2.482700	-2.034100	-1.118100
P	1.164500	-1.213000	0.470800
P	1.248600	-0.214700	-1.476600
P	-0.490900	-1.511900	-0.964900
F	-0.690700	0.502200	2.572800
F	1.137700	2.326400	3.114600
F	2.038900	4.015300	1.192600
F	1.045500	3.821000	-1.329900
F	-0.764600	1.978700	-1.929600
F	-3.075300	2.558800	-0.946000
F	-5.045300	2.840400	-2.677500
F	-6.141500	0.682700	-3.906400
F	-5.208000	-1.809200	-3.331100
F	-3.227000	-2.129000	-1.582100
F	-3.607700	1.335600	1.471900
F	-5.113500	0.448900	3.492100
F	-4.960400	-2.152600	4.272100
F	-3.269400	-3.843700	2.980000
F	-1.770900	-2.994500	0.977500
C	-0.892800	1.175500	0.296600
C	-0.354700	1.328000	1.570500
C	0.608700	2.272200	1.887500
C	1.067700	3.134700	0.913700
C	0.555600	3.039400	-0.365200
C	-0.398500	2.077500	-0.642600

C	-2.971500	0.198900	-1.245500
C	-3.521100	1.441700	-1.536300
C	-4.568900	1.619100	-2.425000
C	-5.135200	0.524600	-3.047500
C	-4.654300	-0.737700	-2.759200
C	-3.609500	-0.870200	-1.864100
C	-2.609400	-0.773600	1.124200
C	-3.499600	0.041900	1.813900
C	-4.287300	-0.388800	2.862400
C	-4.211400	-1.710800	3.262500
C	-3.351900	-2.565000	2.604300
C	-2.578500	-2.087600	1.557400
C	6.058500	-0.414800	-0.134800
C	3.975900	-1.049500	-0.560000
C	3.967600	0.189000	0.021800
C	5.878800	-2.681700	-1.197000
C	5.329700	-3.846500	-0.375100
C	5.487100	-2.782600	-2.670000
C	7.400200	-2.656800	-1.080200
C	5.632900	1.878800	0.882100
C	4.928300	1.989900	2.233200
C	5.168800	2.978100	-0.072300
C	7.143600	1.929300	1.063800
H	7.493900	1.142000	1.732600
H	7.399700	2.886400	1.514100
H	7.666500	1.862800	0.108800
H	7.127200	-0.406800	-0.065200
H	3.130200	0.815100	0.265400
H	5.588600	-3.725900	0.676900
H	5.773400	-4.772700	-0.739600
H	4.249200	-3.932200	-0.466300
H	4.408900	-2.848400	-2.797700
H	5.932600	-3.683800	-3.090400
H	5.858200	-1.919300	-3.222600
H	7.840200	-1.844600	-1.660100
H	7.778700	-3.592700	-1.486700
H	7.727600	-2.593000	-0.041800
H	3.844500	1.990100	2.127200
H	5.212600	2.931300	2.701600
H	5.218500	1.169300	2.889000
H	5.649700	2.872300	-1.044800
H	5.433800	3.947400	0.348300
H	4.088300	2.960600	-0.208300

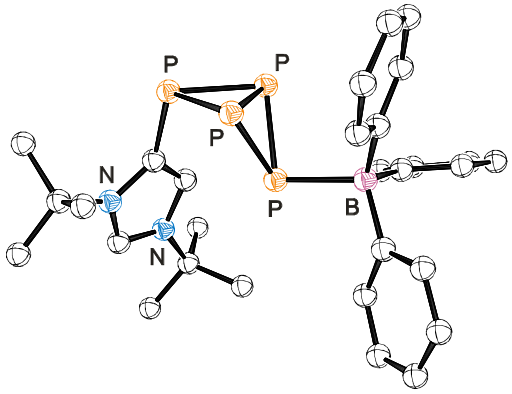


(*trans-cis*)

Structure of the abnormal carben-P_4-boran adduct (5) (atom, x-, y-, z-positions in Å):
(Hydrogen and fluorine atoms are omitted for clarity)

B	-1.630400	-0.060400	-0.322200
N	4.432500	0.446900	0.421200
N	5.665900	-0.934100	-0.721400
P	1.692000	-0.339600	-0.228600
P	1.273600	0.639300	-2.189100

P	1.259900	-1.549300	-2.018000
P	-0.654000	-0.455600	-2.131100
F	-0.181500	0.755600	2.263300
F	0.802700	3.147700	2.751000
F	0.556300	5.158100	0.960600
F	-0.776500	4.715100	-1.385700
F	-1.783200	2.309800	-1.914400
F	-3.787400	2.121000	-0.045200
F	-6.279700	1.894400	-0.896800
F	-7.134700	-0.368900	-2.121000
F	-5.407400	-2.442100	-2.479100
F	-2.882600	-2.244700	-1.631000
F	-2.897700	0.336900	2.139800
F	-3.186700	-1.367100	4.170300
F	-2.129000	-3.870100	4.017200
F	-0.792500	-4.624400	1.774400
F	-0.506500	-2.973200	-0.253000
C	-1.073700	1.402100	0.144100
C	-0.410300	1.694800	1.328100
C	0.114400	2.943400	1.616800
C	-0.001200	3.972200	0.706300
C	-0.660100	3.738500	-0.485700
C	-1.172100	2.479000	-0.731600
C	-3.184900	-0.036200	-0.849900
C	-4.112800	0.979800	-0.668700
C	-5.428600	0.884900	-1.092100
C	-5.870500	-0.266600	-1.712800
C	-4.990700	-1.316300	-1.896300
C	-3.688300	-1.181000	-1.457600
C	-1.638100	-1.194400	0.857700
C	-2.346100	-0.880700	2.015000
C	-2.516600	-1.742600	3.078900
C	-1.982700	-3.016200	3.004400
C	-1.302000	-3.392000	1.866400
C	-1.155700	-2.491900	0.821300
C	5.681600	0.075900	0.144600
C	3.556900	-0.357800	-0.308500
C	4.352300	-1.215800	-1.012100
C	4.064200	1.567400	1.355000
C	3.279100	2.609900	0.562500
C	3.256700	0.989000	2.514900
C	5.339700	2.205300	1.896700
C	6.838100	-1.648300	-1.305400
C	6.803300	-1.442100	-2.818600
C	6.714600	-3.127100	-0.944600
C	8.122100	-1.071300	-0.723000
H	3.873100	2.985900	-0.271000
H	3.029300	3.440400	1.222600
H	2.348700	2.204400	0.173100
H	2.319400	0.547300	2.185500
H	3.012100	1.795500	3.204600
H	3.839900	0.234300	3.043500
H	5.931500	1.501800	2.484000
H	5.042100	3.016000	2.558800
H	5.950400	2.636500	1.102200
H	5.895900	-1.856600	-3.255800
H	7.657800	-1.946800	-3.267900
H	6.854200	-0.381300	-3.063100
H	6.699600	-3.259700	0.136900
H	7.570400	-3.664400	-1.351500
H	5.810300	-3.566100	-1.363300
H	8.241100	-0.016900	-0.974300
H	8.962800	-1.610600	-1.155800
H	8.165900	-1.200200	0.359100
H	6.565700	0.521900	0.551800
H	4.064300	-1.995900	-1.692100



(*cis-trans*)

Structure of the abnormal carben-P_4-boran adduct (6) (atom, x-, y-, z-positions in Å):
(Hydrogen and fluorine atoms are omitted for clarity)

B	1.250400	0.021100	0.067500
N	-4.665900	0.955600	0.138400
N	-4.387200	-1.130500	-0.420200
P	-2.729300	2.331400	-1.586600
P	-0.792800	1.350600	-2.078300
P	-0.905700	2.625600	-0.307200
P	-0.758800	0.421600	-0.058500
F	2.673900	0.920900	-2.437400
F	3.768600	3.298900	-2.804000
F	3.704900	5.181000	-0.846600
F	2.475600	4.615500	1.516800
F	1.359700	2.233900	1.915800
F	3.435900	0.611200	2.134800
F	3.709000	-0.610500	4.454600
F	2.020400	-2.604700	5.191900
F	0.024700	-3.368100	3.495400
F	-0.266800	-2.172600	1.145200
F	3.890800	-0.820700	-0.365300
F	4.786300	-2.828000	-1.877700
F	3.043300	-4.347300	-3.309800
F	0.376700	-3.801300	-3.186600
F	-0.538000	-1.825700	-1.724700
C	2.020000	1.423600	-0.206600
C	2.626600	1.778200	-1.403500
C	3.196200	3.020700	-1.631600
C	3.166100	3.980300	-0.640500
C	2.551500	3.686300	0.562600
C	1.994500	2.437200	0.746000
C	1.504000	-0.646200	1.545400
C	2.532400	-0.331000	2.426100
C	2.712200	-0.968300	3.643900
C	1.861200	-1.988200	4.021600
C	0.848900	-2.368500	3.162400
C	0.709700	-1.709400	1.956800
C	1.644700	-1.182800	-0.981600
C	2.990900	-1.526200	-1.064100
C	3.481200	-2.562100	-1.833600
C	2.598100	-3.338500	-2.563300
C	1.250700	-3.055600	-2.501600
C	0.808600	-1.999700	-1.721300
C	-5.047800	-0.299100	0.381000
C	-3.688700	0.932800	-0.855500
C	-3.544200	-0.381900	-1.196400
C	-5.224500	2.155400	0.842700
C	-4.110200	2.814500	1.651600
C	-5.806800	3.100100	-0.206100
C	-6.335600	1.709300	1.789700
C	-4.413800	-2.625200	-0.390000
C	-3.095100	-3.095400	0.218600
C	-4.567900	-3.122100	-1.825300

C	-5.594900	-3.084300	0.455500
H	-3.661000	2.098000	2.339700
H	-4.533100	3.638700	2.225600
H	-3.330500	3.211900	1.009200
H	-5.042300	3.471000	-0.885500
H	-6.252000	3.955300	0.301500
H	-6.580300	2.596100	-0.786000
H	-7.151400	1.218100	1.257800
H	-6.740900	2.600100	2.265400
H	-5.959800	1.058300	2.579600
H	-2.245000	-2.757300	-0.370300
H	-3.085600	-4.185000	0.249100
H	-2.973900	-2.714600	1.232200
H	-5.465700	-2.710200	-2.286000
H	-4.647400	-4.208300	-1.812300
H	-3.701600	-2.864000	-2.432800
H	-5.482200	-2.788300	1.498900
H	-5.626800	-4.171900	0.429200
H	-6.541300	-2.708600	0.063700
H	-5.787700	-0.596200	1.095200
H	-2.864400	-0.827300	-1.897500