Reactions of Phosphorus/Boron frustrated LEWIS Pairs with SO_2

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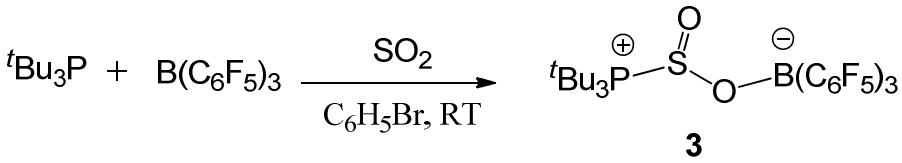
Supporting Information

General Procedures. All syntheses involving air- and moisture-sensitive compounds were carried out using standard Schlenk-type glassware (or in a glove box) under an atmosphere of argon. Solvents were dried with the procedure according to Grubbs (Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518-1520) or were distilled from appropriate drying agents and stored under an argon atmosphere. The following instruments were used for physical characterization of the compounds: NMR spectra: *Varian* Inova 500 (^{1}H: 500 MHz, ^{13}C: 126 MHz, ^{19}F: 470 MHz, ^{11}B: 160 MHz, ^{31}P: 202 MHz), *Varian* UnityPlus 600 (^{1}H: 600 MHz, ^{13}C: 151 MHz, ^{19}F: 564 MHz, ^{11}B: 192 MHz, ^{31}P: 243 MHz). ^{1}H NMR and ^{13}C NMR: chemical shift δ is given relative to TMS and referenced to the solvent signal. ^{19}F NMT: chemical shift δ is given relative to $CFCl_3$ (external reference); ^{11}B NMR: chemical shift δ is given relative to $BF_3{\cdot}Et_2O$ (external reference). NMR assignments are supported by additional 2D NMR experiments. Elemental analyses were performed on a *Elementar Vario El III*. IR spectra were recorded on a *Varian* 2100 FT-IR (Excalibur Series). Melting points were obtained with a DSC Q20 (*TA Instruments*).

X-Ray Crystal Structure Analyses. Data sets were collected with a Nonius KappaCCD diffractometer (for compounds **4b** und **6**) and with a Bruker Kappa Apex II diffractometer (for compound **3**). Programs used: data collection, COLLECT (Nonius B.V., 1998) and BRUKER SMART CCD Diffractometer; data reduction Denzo-SMN (Z. Otwinowski, W. Minor, *Methods Enzymol.* **1997**, *276*, 307-326); absorption correction, Denzo (Z. Otwinowski, D. Borek, W. Majewski, W. Minor, *Acta Crystallogr*. **2003**, *A59*, 228-234); structure solution SHELXS-97 (G. M. Sheldrick, *Acta Crystallogr*. **1990**, *A46*, 467-473); structure refinement SHELXL-97 (G. M. Sheldrick, *Acta Crystallogr*. **2008**, *A64*, 112-122) and graphics, XP (BrukerAXS, 2000). *R*-values are given for observed reflections, and wR^2 values are given for all reflections. *Exceptions and special features*: For the compound **4b** an unidentified disordered solvent molecule was found in the asymmetrical unit and could not be satisfactorily refined. The program SQUEEZE (A. L. Spek *J. Appl. Cryst*., **2003**, *36*, 7-13) was therefore used to remove mathematically the effect of the solvent. Two molecules of **4b** were found in the asymmetric unit. For the compound **6** the O2 atom at the S1 was found disordered over two positions. Several restraints (SAME, SIMU and SADI) were used in order to improve refinement stability.

Materials. Dimesitylvinylphoshine (Spies, P; Erker, G.; Kehr, G.; Bergander, K., Fröhlich, R., Grimme, S.; Stephan, D. W., *Chem. Commun*. **2007**, 5072-5074), bis(pentafluorophenyl)-borane (Parks, D. J.; Spence, R. E. V H.; Piers, W. E., *Angew. Chem*. **1995**, *107*, 895-897;

Angew. Chem. Int. Ed. Engl. **1995**, *34*, 809-811; Piers, W. E.; Parks, D. J.; Yap, G. P. A., *Organometallics* **1998**, *17*, 5492-5503), tris(pentafluorophenyl)borane (Massay, A. G.; Park, A. J., *J. Organomet. Chem*. **1964**, *2*, 245-250) and {2-[Bis(pentafluorophenyl)boryl]-ethyl}dimesitylphosphine (**2a**) (Spies, P.; Erker, G.; Kehr, G.; Bergander, K., Fröhlich, R.; Grimme, S.; Stephan, D. W.; *Chem. Commun*. **2007**, 5072-5074) were prepared according to modified literature procedures.



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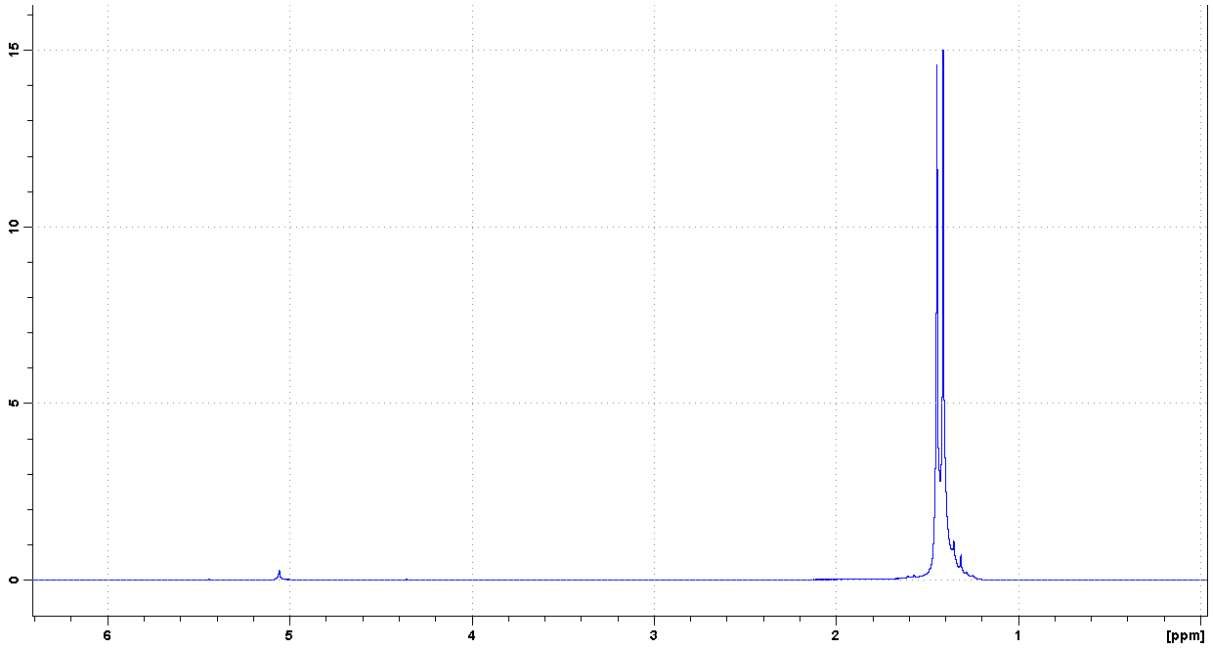
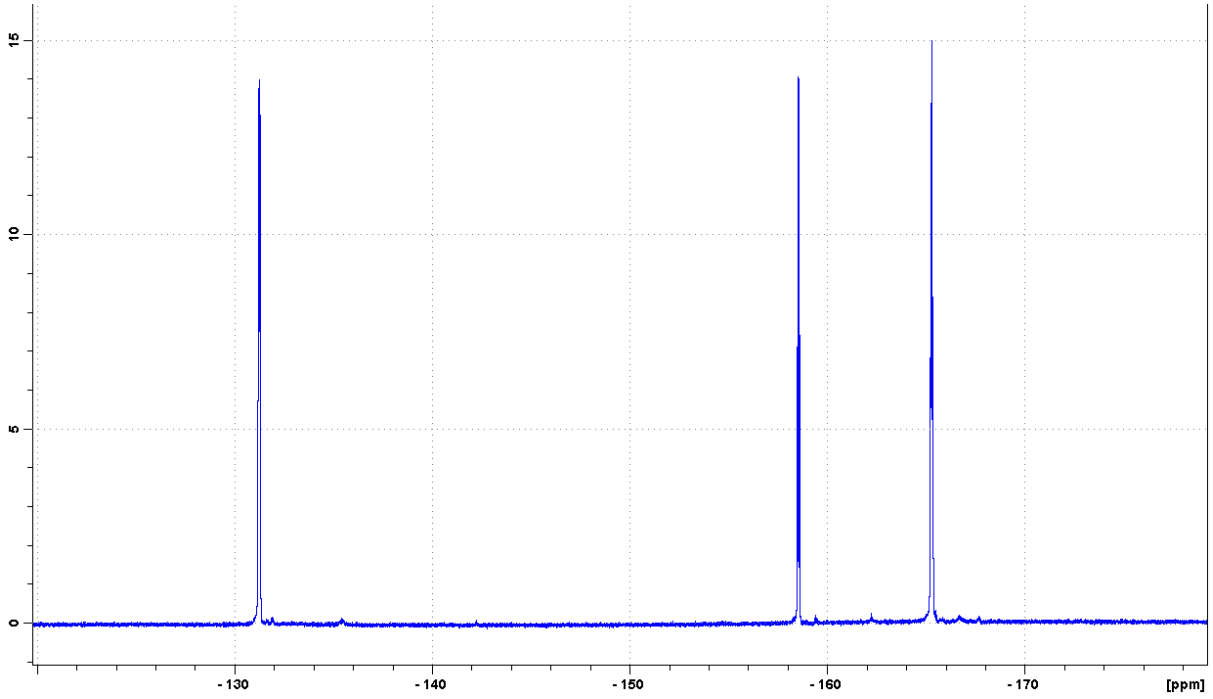
[*t*Bu$_3$PS(O)OB(C$_6$F$_5$)$_3$] (3)

A solution of B(C$_6$F$_5$)$_3$ (25 mg, 0.049 mmol) and *t*Bu$_3$P (10 mg, 0.049 mmol) in C$_6$H$_5$Br (1 mL) was degassed and the J-Young NMR tube was filled with SO$_2$ (1 bar). A colorless crystal precipitated after 30min. The reaction mixture was allowed to sit under SO$_2$ (1 bar) overnight. Pentane (2 mL) was added, after which the supernatant was decanted. The residue was washed with pentane (2 mL) and dried in vacuo to afford *t*Bu$_3$PS(O)OB(C$_6$F$_5$)$_3$ (**3**) as a white powder (31 mg, 0.039 mmol, 80%). Crystals suitable for X-ray crystal structure analysis were obtained by recrystallization from CH$_2$Cl$_2$.

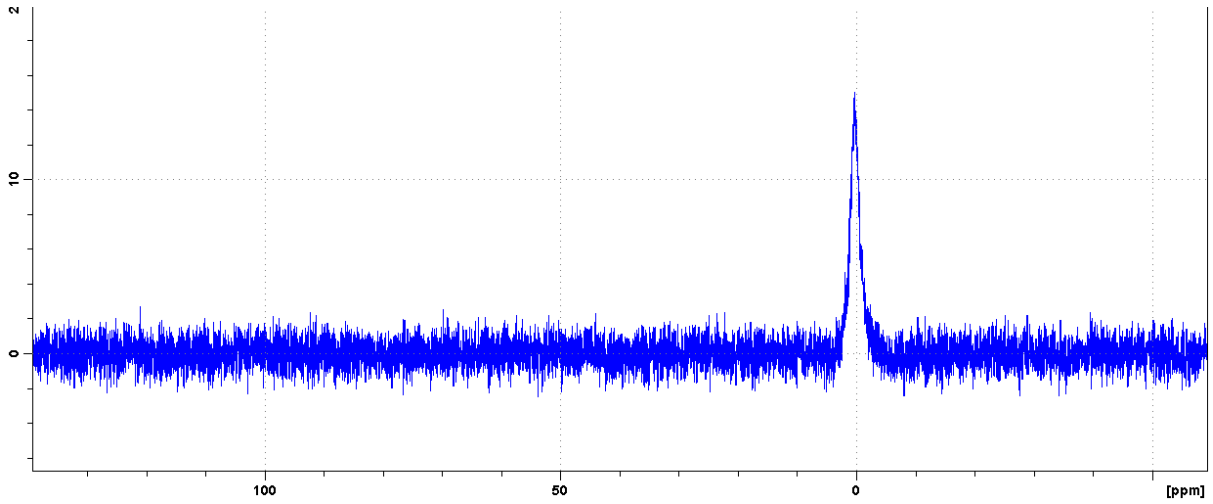
^{1}H NMR (400 MHz, CD$_2$Cl$_2$, 298 K): δ = 1.43 (d, J_{PH} = 14.1 Hz, 27H, *t*Bu).



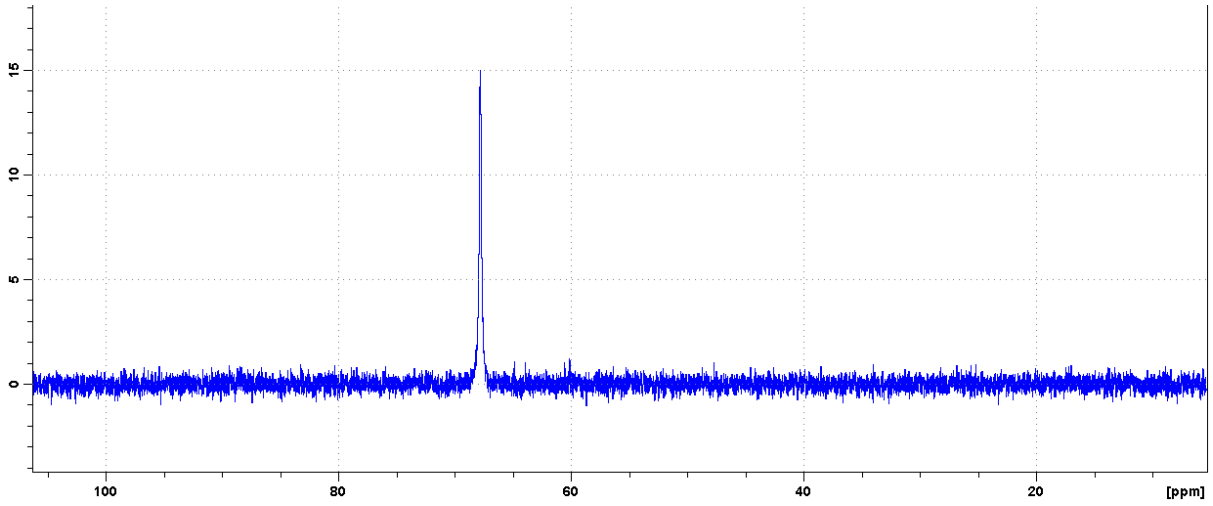
^{19}F NMR (377 MHz, CD$_2$Cl$_2$, 298 K): δ = -131.2 (d, ^3J = 21.9 Hz, 6F, *o*-C$_6$F$_5$); -158.5 (t, ^3J = 20.7 Hz, 3F, *p*- C$_6$F$_5$); -165.3 (m, 6F, *m*-C$_6$F$_5$).



^{11}B NMR (128 MHz, CD_2Cl_2, 298 K): δ = 0.32 (br s, $\nu_{1/2}$ = 195 Hz).



^{31}P NMR (162 MHz, CD_2Cl_2, 298 K): δ = 67.8 (s).



Elemental Analysis $C_{30}H_{27}BF_{15}O_2PS$ requires C: 46.29, H: 3.50; found C: 45.84, H: 3.40.

X-ray crystal structure analysis of 3: formula $C_{30}H_{27}BF_{15}O_2PS$, M = 778.36, colourless crystal, 0.24 x 0.22 x 0.19 mm, a = 9.4942(4), b = 29.0008(13), c = 11.5368(5) Å, β = 90.018(2)°, V = 3176.5(2) Å^3, ρ_{calc} = 1.628 gcm^{-3}, μ = 0.270 mm^{-1}, empirical absorption correction ($0.937 \leq T \leq 0.950$), Z = 4, monoclinic, space group $P2_1/c$ (No. 14), λ = 0.71073 Å, T = 150(2) K, ω and φ scans, 30506 reflections collected ($\pm h, \pm k, \pm l$), 8222 independent (R_{int} = 0.040) and 6900 observed reflections [$I>2\sigma(I)$], 452 refined parameters, R = 0.034, wR^2 = 0.072, max. (min.) residual electron density 0.37 (-0.43) e.Å^{-3}, hydrogen atoms calculated and refined as riding atoms.

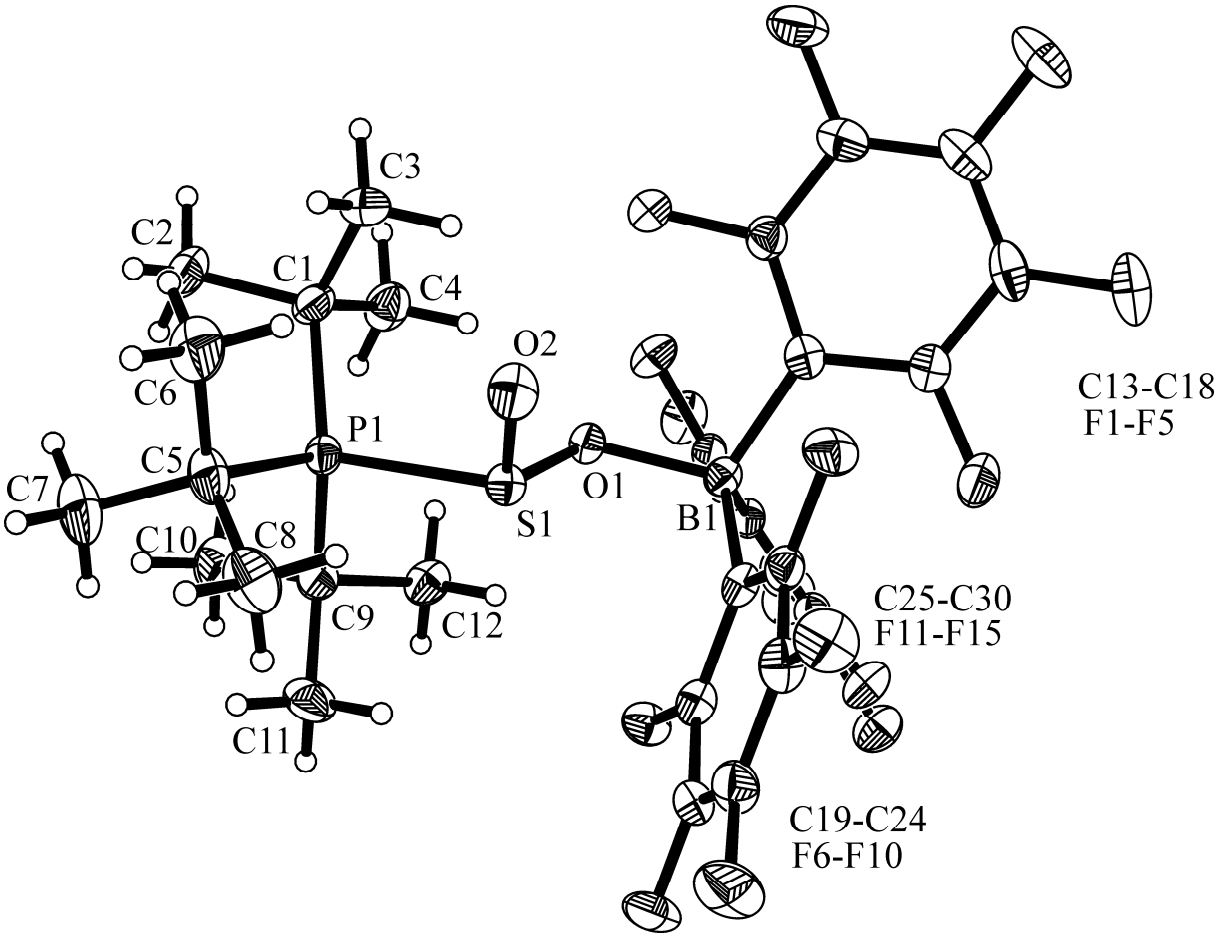
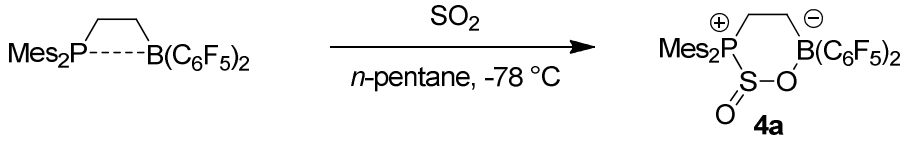


Figure 1. Poffray drawing of [$tBu_3PS(O)OB(C_6F_5)_3$] (**3**). S: yellow, O: red, B: yellow-green, C: black, F: pink, P: orange. Selected bond distances (Å)and angles (°): S-O(1) 1.5298(19), S-O(2) 1.5376(19), O(1)-B 1.541(4), P-S 1.530(4), O(1)-S-O(2) 101.47(10), P-S-O(1) 100.86(11), P-S-O(2) 101.70(11), S-O(1)-B 126.16(17)

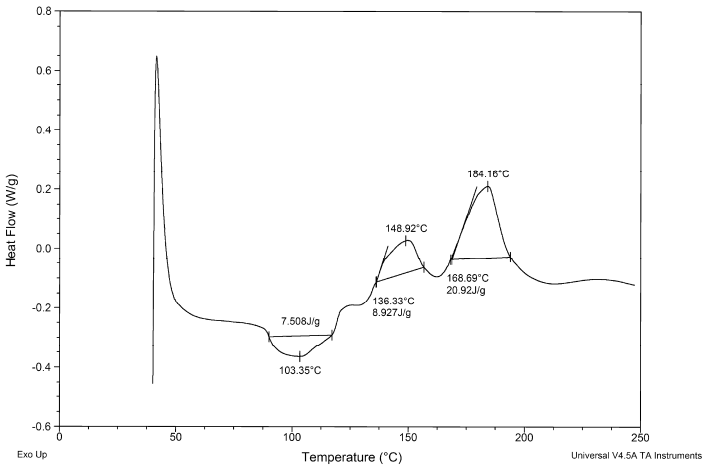
Reaction of 2a with SO_2



A suspension of bis(pentafluorophenyl)borane (117 mg, 0.34 mmol, 1.0 eq) in *n*-pentane (3 mL) was added to a solution of dimesitylvinylphosphine (100 mg, 0.34 mmol, 1.0 eq) in *n*-pentane (3 mL). After stirring for one hour the reaction mixture was cooled down to −78 °C and sulfur dioxide (0.8 bar) was introduced for ten minutes whereupon a white powder precipitated immediately. After stirring the reaction mixture for 1.5 h all volatiles were removed *in vacuo* to yield **4a** (198 mg, 83%) as white solid. [Compound **4a** was not stable in CD_2Cl_2 and C_7D_8 solution, respectively]

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3675 (w), 3649 (w), 3587 (w), 3154 (w), 3032 (w), 2967 (m), 2930 (m), 2741 (w), 2559 (w), 2476 (w), 2361 (w), 1734 (w), 1700 (w), 1645 (s), 1606 (s), 1558 (m), 1515 (s), 1463 (s), 1398 (m), 1382 (m), 1283 (s), 1153 (s), 1139 (s), 1092 (s), 1028 (m), 978 (s), 948 (s), 870 (s), 798 (s), 766 (m), 742 (s), 694 (s), 653 (w), 639 (m), 612 (w), 578 (w), 552 (w), 526 (w), 470 (m), 453 (w), 448 (w), 413 (w).

Melting point (DSC): 103 °C.



DSC of compound **4a**.

Elemental analysis: Calc.: C: 54.41, H: 3.71; Found: C: 54.88, H: 3.91.

^{1}H NMR (500 MHz, CD_2Cl_2, 298 K): δ = 7.00 (d, $^4J_{PH}$ = 3.6 Hz, 4H, *m*-Mes^A), 6.99 (d, $^4J_{PH}$ = 3.9 Hz, 4H, *m*-Mes^B), 3.75, 2.93 (each m, each 1H, CH_2^P), 2.45 (br s, 6H, *o*-CH_3^{MesA}), 2.41 (br s, 6H, *o*-CH_3^{MesB}), 2.31 (s, 6H, *p*-$CH_3^{MesA,B}$), 1.88, 1.23 (each m, each 1H, CH_2^B).

$^{13}C\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2, 298 K): δ = 147.7 (dm, $^{1}J_{FC}$ ~ 238 Hz, C_6F_5), 144.9, 144.8 (each s, *p*-$Mes^{A,B}$), 144.1 (d, $^{2}J_{PC}$ = 7.0 Hz, *o*-Mes^{B}), 143.4 (d, $^{2}J_{PC}$ = 5.6 Hz, *o*-Mes^{A}), 139.5 (dm, $^{1}J_{FC}$ ~ 238 Hz, C_6F_5), 137.2 (dm, $^{1}J_{FC}$ ~ 247 Hz, C_6F_5), 132.2 (d, $^{3}J_{PC}$ = 10.8 Hz, *m*-Mes^{B}), 131.6 (d, $^{3}J_{PC}$ = 9.8 Hz, *m*-Mes^{A}), 122.2 (d, $^{1}J_{PC}$ = 39.3 Hz, *i*-Mes^{A}), 121.6 (br, *i*-C_6F_5), 118.3 (d, $^{1}J_{PC}$ = 52.5 Hz, *i*-Mes^{B}), 23.4 (br, *o*-CH_3^{MesA}), 23.1 (br, *o*-CH_3^{MesB}), 22.7 (d, $^{1}J_{PC}$ = 22.9 Hz, CH_2^{P}), 21.3, 21.2 (each s, *p*-$CH_3^{MesA,B}$), 11.4 (br, CH_2^{B}).

$^{11}B\{^{1}H\}$ NMR (160 MHz, CD_2Cl_2, 298 K): δ = 1.2 ($\nu_{1/2}$ ≈ 400 Hz).

^{19}F NMR (470 MHz, CD_2Cl_2, 298 K): δ = −134.9 (m, 2F, *o*), −160.6 (m, 1F, *p*), −165.7 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 5.1 [$C_6F_5^{A}$]; −135.5 (m, 2F, *o*), −160.7 (m, 1F, *p*), −165.7 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 4.7 [$C_6F_5^{B}$].

^{19}F / ^{19}F GCOSY (470 MHz / 470 MHz, CD_2Cl_2, 298 K): δ ^{19}F / δ ^{19}F = −134.9 / −160.6, −165.7 (*o* / *m*, *p*), −160.6 / −134.9, −165.7 (*p* / *o*, *m*), −165.7 / −134.9, −160.6 (*m* / *o*, *p*) [$C_6F_5^{A}$]; −135.5 / −160.7, −165.7 (*o* / *m*, *p*), −160.7 / −135.5, −165.7 (*p* / *o*, *m*), −165.7 / −135.5, −160.7 (*m* / *o*, *p*) [$C_6F_5^{B}$].

$^{31}P\{^{1}H\}$ NMR (202 MHz, CD_2Cl_2, 298 K): δ = 33.3 ($\nu_{1/2}$ ≈ 20 Hz).

^{1}H / ^{13}C GHSQC (500 MHz / 126 MHz, CD_2Cl_2, 298 K): δ ^{1}H / δ ^{13}C = 7.00 / 131.6 (*m*-Mes^{A}), 6.99 / 132.2 (*m*-Mes^{B}), 3.75 / 22.7 (CH_2^{P}), 2.93 / 22.7 (CH_2^{P}), 2.45 / 23.4 (*o*-CH_3^{MesA}), 2.41 / 23.1 (*o*-CH_3^{MesB}), 2.31 / 21.3, 21.2 (*p*-$CH_3^{MesA,B}$), 1.88 / 11.4 (CH_2^{B}), 1.23 / 11.4 (CH_2^{B}).

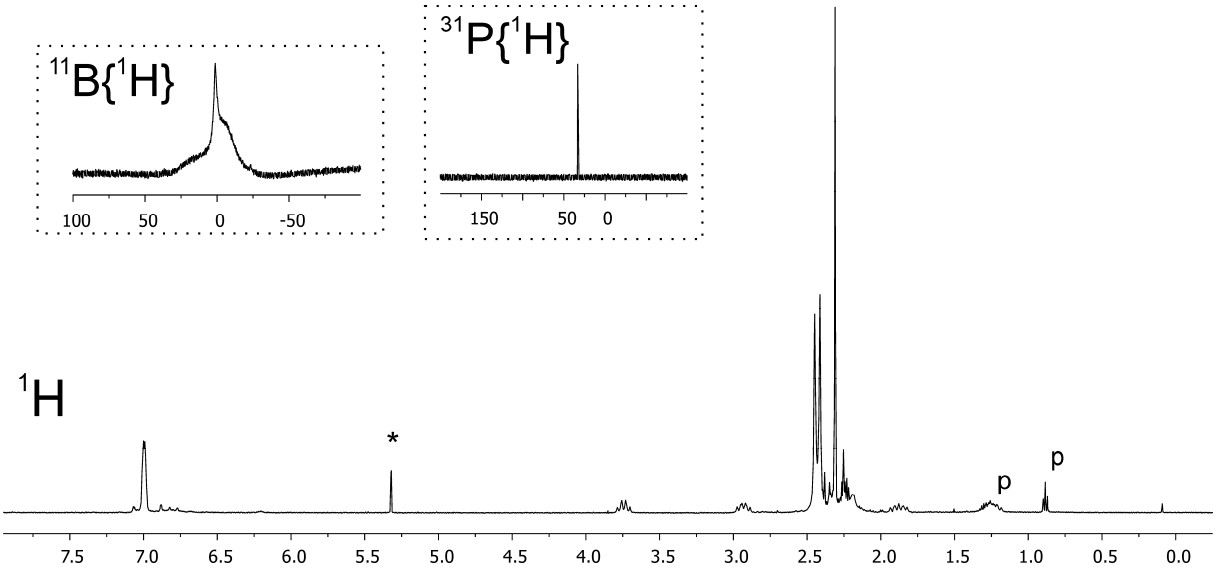
^{1}H / ^{13}C GHMBC (500 MHz / 126 MHz CD_2Cl_2, 298 K): δ ^{1}H / δ ^{13}C = 7.00 / 131.6, 122.2, 23.4, 21.3, 21.2 (*m*-Mes^{A} / *m*-Mes^{A}, *i*-Mes^{A}, *o*-CH_3^{MesA}, *p*-CH_3^{MesA}), 6.99 / 132.2, 118.3, 23.1, 21.3, 21.2 (*m*-Mes^{B} / *m*-Mes^{B}, *i*-Mes^{B}, *o*-CH_3^{MesB}, *p*-CH_3^{MesB}), 2.45 / 143.4, 131.6, 122.2 (*o*-CH_3^{MesA} / *o*-Mes^{A}, *m*-Mes^{A}, *i*-Mes^{A}), 2.41 / 144.1, 132.2, 118.3 (*o*-CH_3^{MesB} / *o*-Mes^{B}, *m*-Mes^{B}, *i*-Mes^{B}), 2.31 / 144.9, 144.8, 132.2, 131.6, 122.2, 118.3 (*p*-$CH_3^{MesA,B}$ / *p*-Mes^{A}, *p*-Mes^{B}, *m*-Mes^{B}, *m*-Mes^{A}, *i*-Mes^{A}, *i*-Mes^{B}).

^{1}H / ^{1}H GCOSY (500 MHz / 500 MHz, CD_2Cl_2, 298 K): δ ^{1}H / δ ^{1}H = 7.00 / 2.45, 2.31 (*m*-Mes^{A} / *o*-CH_3^{MesA}, *p*-CH_3^{MesA}), 6.99 / 2.41, 2.31 (*m*-Mes^{B} / *o*-CH_3^{MesB}, *p*-CH_3^{MesB}), 3.75 / 2.93, 1.23 (CH_2^{P} / CH_2^{P}, CH_2^{B}), 2.93 / 3.75, 1.88 (CH_2^{P} / CH_2^{P}, CH_2^{B}), 2.45 / 7.00, 2.31 (*o*-CH_3^{MesA} / *m*-Mes^{A}, *p*-CH_3^{MesA}), 2.41 / 6.99, 2.31 (*o*-CH_3^{MesB} / *m*-Mes^{B}, *p*-CH_3^{MesB}), 2.31 / 7.00, 6.99, 2.45, 2.41 (*p*-$CH_3^{MesA,B}$ / *m*-Mes^{A}, *m*-Mes^{B}, *o*-CH_3^{MesA}, *o*-CH_3^{MesB}), 1.88 / 2.93, 1.23 (CH_2^{B} / CH_2^{P}, CH_2^{B}), 1.23 / 3.75, 1.88 (CH_2^{B} / CH_2^{P}, CH_2^{B}).

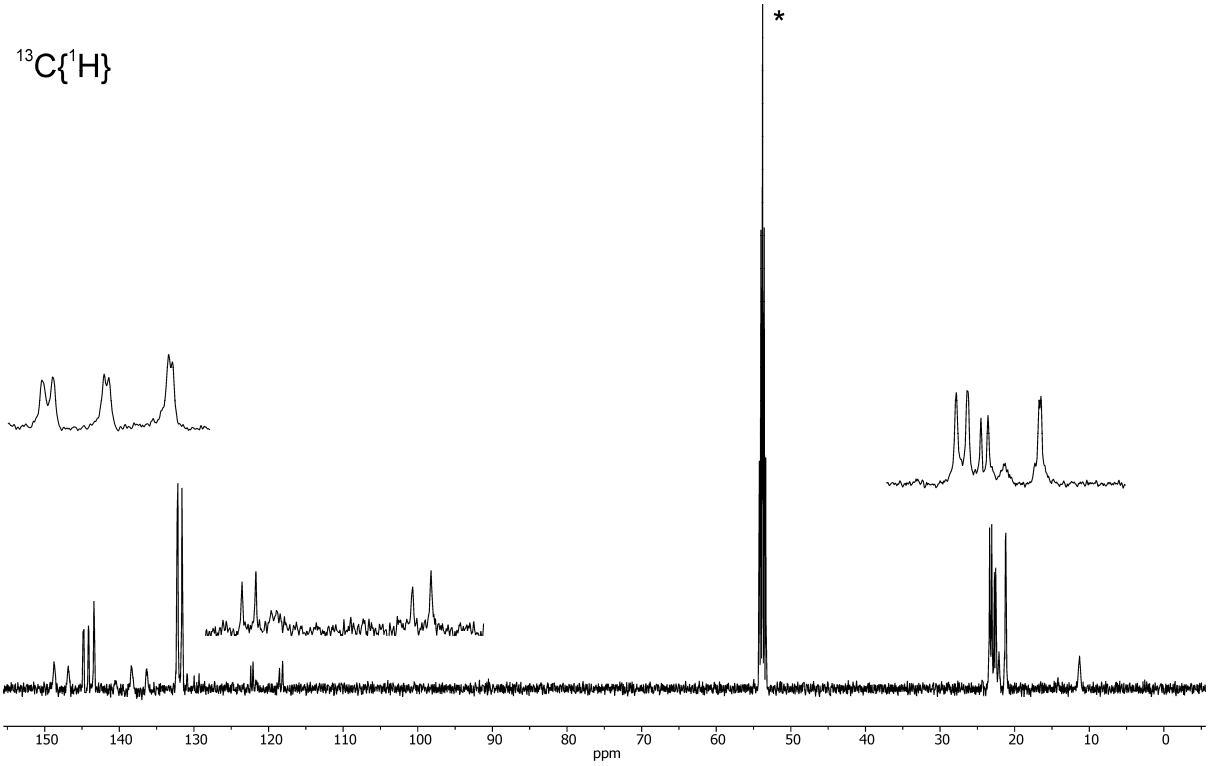
$^{1}H\{^{1}H\}$ NOE (500 MHz, CD_2Cl_2, 298 K): δ $^{1}H_{irr}$ / δ $^{1}H_{res}$ = 7.00 / 2.45, 2.41, 2.31 (*m*-Mes^{A} / *o*-CH_3^{MesA}, *o*-CH_3^{MesB}, *p*-$CH_3^{MesA,B}$), 3.75 / 2.93, 2.45, 2.41 (CH_2^{P} / CH_2^{P},*o*-CH_3^{MesA}, *o*-CH_3^{MesB}), 2.93 / 3.75 (CH_2^{P} / CH_2^{P}), 2.43 / 7.00, 6.99, 2.45, 2.41 (*o*-CH_3^{MesA}, *o*-CH_3^{MesB} / *m*-

Mes^{A}, *m*-Mes^{B}, *o*-CH_3^{MesA}, *o*-CH_3^{MesB}), 2.31 / 7.00, 6.99 (*p*-$CH_3^{MesA,B}$ / *m*-Mes^{A}, *m*-Mes^{B}), 1.88 / 2.45, 2.41, 1.23 (CH_2^{B} / *o*-CH_3^{MesA}, *o*-CH_3^{MesB}, CH_2^{B}), 1.23 / 1.88 (CH_2^{B} / CH_2^{B}).

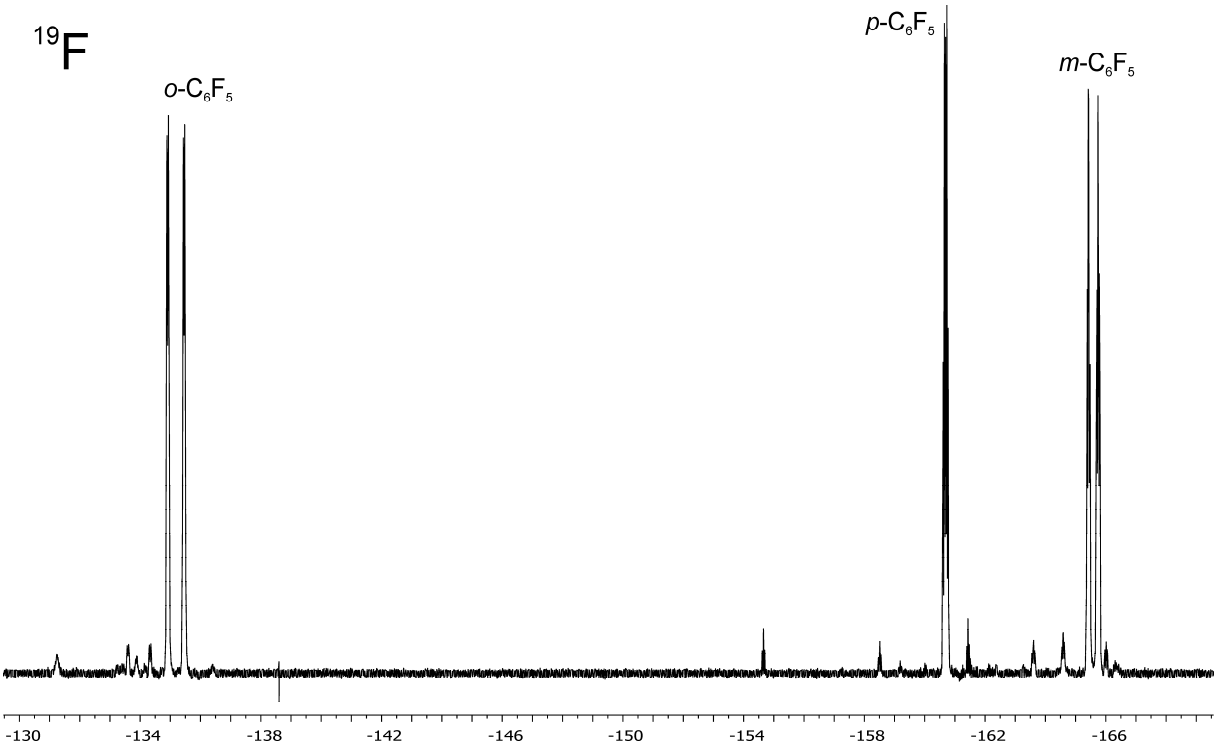
^{1}H{^{1}H} TOCSY (500 MHz, CD_2Cl_2, 298 K): δ $^{1}H_{irr}$ / δ $^{1}H_{res}$ = 7.00 / 2.45, 2.41, 2.31 (*m*-Mes^{A}, *m*-Mes^{B} / *o*-CH_3^{MesA}, *o*-CH_3^{MesB}, *p*-CH_3^{MesA}, *p*-CH_3^{MesB}), 3.75 / 2.93, 1.88, 1.23 (CH_2^{P} / CH_2^{P}, CH_2^{B}, CH_2^{B}), 2.93 / 3.75, 2.31, 1.88, 1.23 (CH_2^{P} / CH_2^{P}, *p*-$CH_3^{MesA,B}$, CH_2^{B}, CH_2^{B}), 2.43 / 2.31 (*o*-CH_3^{MesA}, *o*-CH_3^{MesB} / *p*-$CH_3^{MesA,B}$), 2.31 / 2.45, 2.41 (*p*-$CH_3^{MesA,B+}$ / *o*-CH_3^{MesA}, *o*-CH_3^{MesB}), 1.88 / 3.75, 2.93, 1.23 (CH_2^{B} / CH_2^{P}, CH_2^{P}, CH_2^{B}), 1.23 / 3.75, 2.93, 1.88 (CH_2^{B} / CH_2^{P}, CH_2^{P}, CH_2^{B}).



^{1}H NMR (500 MHz, CD_2Cl_2, 298 K), **^{11}B{^{1}H} NMR** (160 MHz, CD_2Cl_2, 298 K) and **^{31}P{^{1}H} NMR** (202 MHz, CD_2Cl_2, 298 K) [p: *n*-pentane].



$^{13}C\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2, 298 K) spectrum of compound **4a.**



^{19}F NMR (470 MHz, CD_2Cl_2, 298 K) spectrum of compound **4a**.

Low temperature messurements:

^{1}H NMR (500 MHz, C_7D_8, 298 K): δ = 6.36, 6.29 (br, each 2H, *m*-Mes), 3.58, 2.58 (each m, each 1H, CH_2^P), 2.08, 1.95 (each br, each 6H, *o*-CH_3^{Mes}), 1.82, 1.78 (each br, each 3H, *p*-CH_3^{Mes}), n.o., 1.14 (m, 1H, CH_2^B).

^{1}H NMR (500 MHz, C_7D_8, 273 K): δ = 6.33 (d, $^4J_{PH}$ = 3.2 Hz, 2H, *m*-Mes^A), 6.25 (d, $^4J_{PH}$ = 3.4 Hz, 2H, *m*-Mes^B), 3.60, 2.55 (each m, each 1H, CH_2^P), 2.07 (br, 6H, *o*-CH_3^{MesA}), 2.05, 1.14 (each m, each 1H, CH_2^B)[1], 1.94 (br s, 6H, *o*-CH_3^{MesB}), 1.82 (s, 3H, *p*-CH_3^{MesA}), 1.76 (s, 3H, *p*-CH_3^{MesB}), [[1] from the ghsqc experiment].

^{1}H NMR (500 MHz, C_7D_8, 183 K): δ = 6.22, 6.03, 6.01, 5.86 (each br, each 1H, *m*-Mes), 3.93, 2.52 (each br, each 1H, CH_2^P), 2.69, 2.09, 1.78, 1.65, 1.57, 1.40 (each s, each 3H, CH_3^{Mes}), n.o. (CH_2^B).

^{13}C{^{1}H} NMR (126 MHz, C_7D_8, 273 K): δ = 143.9 (d, $^4J_{PC}$ = 2.8 Hz, *p*-Mes^A), 143.8 (d, $^4J_{PC}$ = 2.8 Hz, *p*-Mes^B), 143.5 (br, *o*-Mes^B), 143.1 (br, *o*-Mes^A), 131.8 (d, $^3J_{PC}$ = 11.2 Hz, *m*-Mes^B), 131.1 (d, $^3J_{PC}$ = 9.6 Hz, *m*-Mes^A), 122.2 (d, $^1J_{PC}$ = 36.8 Hz, *i*-Mes^A), 118.4 (d, $^1J_{PC}$ = 52.0 Hz, *i*-Mes^B), 22.9 (br, *o*-CH_3^{MesA}), 22.5 (br, *o*-CH_3^{MesB}), 21.9 (d, $^1J_{PC}$ = 21.9 Hz, CH_2^P), 20.70, 20.68 (*p*-$CH_3^{MesA,B}$), 11.6 (br, CH_2^B), [C_6F_5 not listed].

^{11}B{^{1}H} NMR (160 MHz, C_7D_8, 298 K): δ = 1.6.

^{11}B{^{1}H} NMR (160 MHz, 273 K, C_7D_8): δ = 6.4.

^{11}B{^{1}H} NMR (160 MHz, C_7D_8, 183 K): δ = -2.5.

^{19}F NMR (470 MHz, C_7D_8, 273 K): δ = −134.3 (m, 2F, *o*), −159.2 (t, J_{FF} = 20.7 Hz, 1F, *p*), −164.8 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 5.6 [$C_6F_5^A$]; −134.9 (m, 2F, *o*), −159.5 (t, J_{FF} = 20.7 Hz, 1F, *p*), −164.3 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 4.8 [$C_6F_5^B$].

^{19}F NMR (470 MHz, C_7D_8, 273 K): δ = −134.4 (m, 2F, *o*), −159.1 (t, J_{FF} = 20.7 Hz, 1F, *p*), −164.7 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 5.6 [$C_6F_5^A$]; −135.0 (m, 2F, *o*), −159.4 (t, J_{FF} = 20.7 Hz, 1F, *p*), −164.2 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 4.8 [$C_6F_5^B$].

^{19}F / ^{19}F GCOSY (470 MHz / 470 MHz, C_7D_8, 273 K): δ ^{19}F / δ ^{19}F = −134.4 / −164.7 (*o* / *m*), −159.1 / −164.7 (*p* / *m*), −164.7 / −134.4, −159.1 (*m* / *o*, *p*) [$C_6F_5^A$]; −135.0 / −164.2 (*o* / *m*), −159.4 / −164.2 (*p* / *m*), −164.2 / −135.0, −159.4 (*m* / *o*, *p*) [$C_6F_5^B$].

^{19}F NMR (470 MHz, C_7D_8, 183 K): all resonances are broad.

^{31}P{^{1}H} NMR (202 MHz, C_7D_8, 298 K): δ = 29.4 ($\nu_{1/2} \approx 20$ Hz).

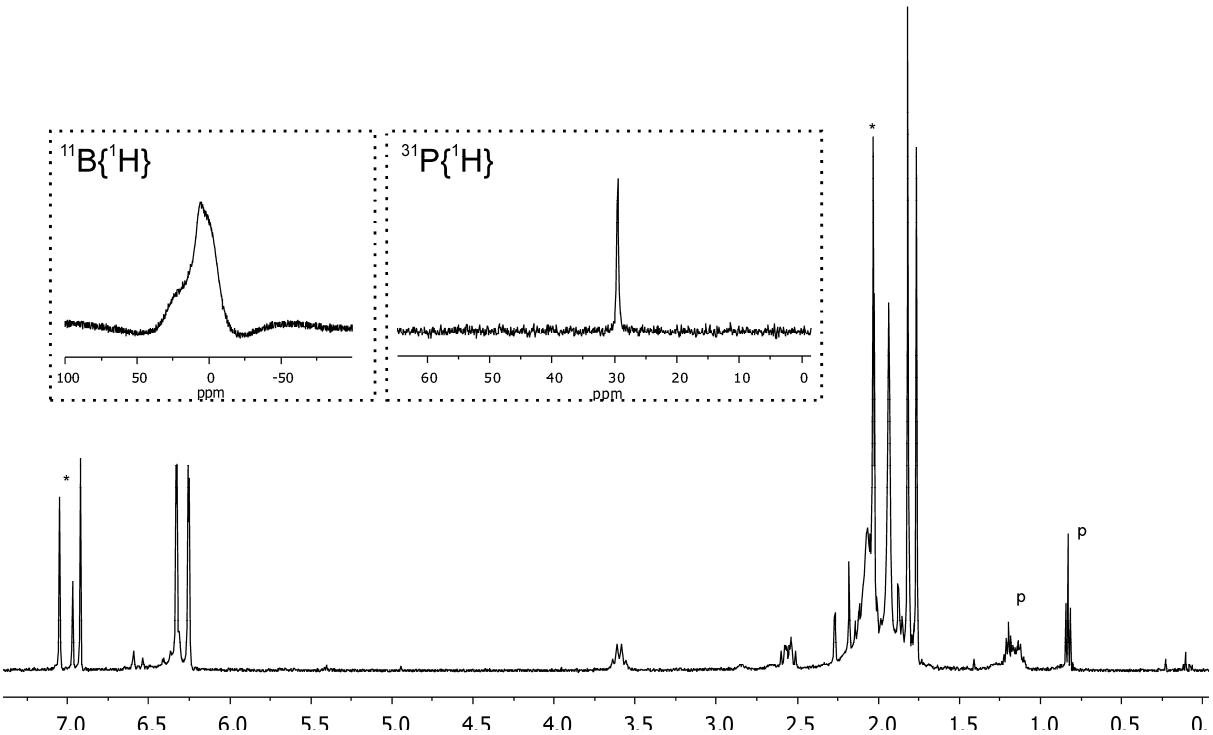
^{31}P{^{1}H} NMR (202 MHz, C_7D_8, 273 K): δ = 29.5 ($\nu_{1/2} \approx 55$ Hz).

^{31}P{^{1}H} NMR (202 MHz, C_7D_8, 183 K): δ = 38.0 ($\nu_{1/2} \approx 20$ Hz; 18%), 26.8 ($\nu_{1/2} \approx 15$ Hz; 82%).

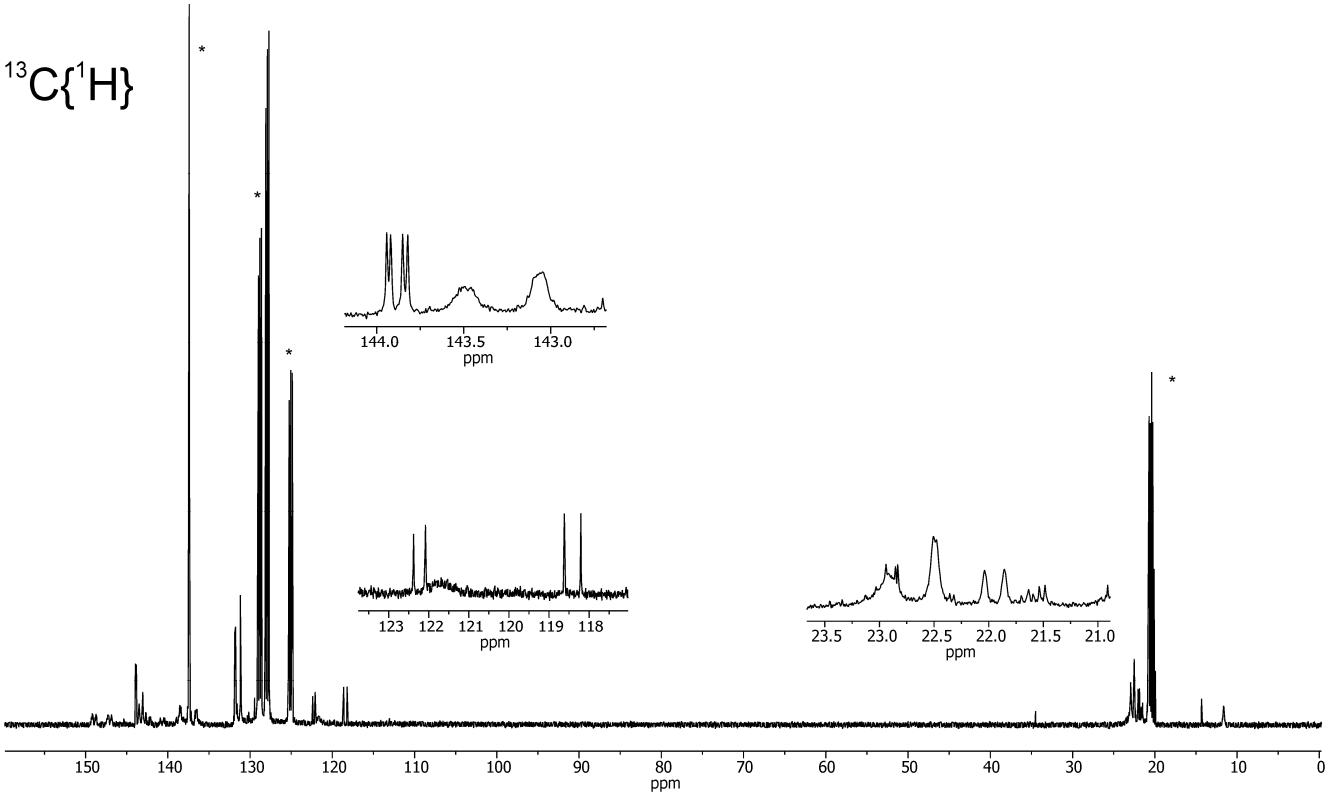
^{1}H / ^{13}C GHSQC (500 MHz / 126 MHz, C_7D_8, 273 K): δ ^{1}H / δ ^{13}C = 6.33 / 131.1 (*m*-Mes^{A}), 6.25 / 131.8 (*m*-Mes^{B}), 3.60, 2.55 / 21.9 (CH_2^{P}), 2.07 / 22.9 (*o*-CH_3^{MesA}), 2.05, 1.14 / 11.6 (CH_2^{B}), 1.94 / 22.5 (*o*-CH_3^{MesB}), 1.82, 1.76 / 20.70, 20.68 (*p*-CH_3^{MesA}, *p*-CH_3^{MesB}).

^{1}H / ^{13}C GHMBC (500 MHz / 126 MHz, C_7D_8, 273 K): δ ^{1}H / δ ^{13}C = 6.33 / 122.2, 22.9, 20.70, 20.68 (*m*-Mes^{A} / *i*-Mes^{A}, *o*-CH_3^{MesA}, *p*-CH_3^{MesA}), 6.25 / 118.4, 22.5, 20.70, 20.68 (*m*-Mes^{B} / *i*-Mes^{B}, *o*-CH_3^{MesB}, *p*-CH_3^{MesB}), 2.07 / 143.1, 131.1 (*o*-CH_3^{MesA} / *o*-Mes^{A}, *m*-Mes^{A}), 1.94 / 143.5, 131.8 (*o*-CH_3^{MesB} / *o*-Mes^{B}, *m*-Mes^{B}), 1.82 / 143.9, 131.1 (*p*-CH_3^{MesA} / *p*-Mes^{A}, *m*-Mes^{A}), 1.76 / 143.8, 131.8, 118.4 (*p*-CH_3^{MesB} / *p*-Mes^{B}, *m*-Mes^{B}, *i*-Mes^{B}).

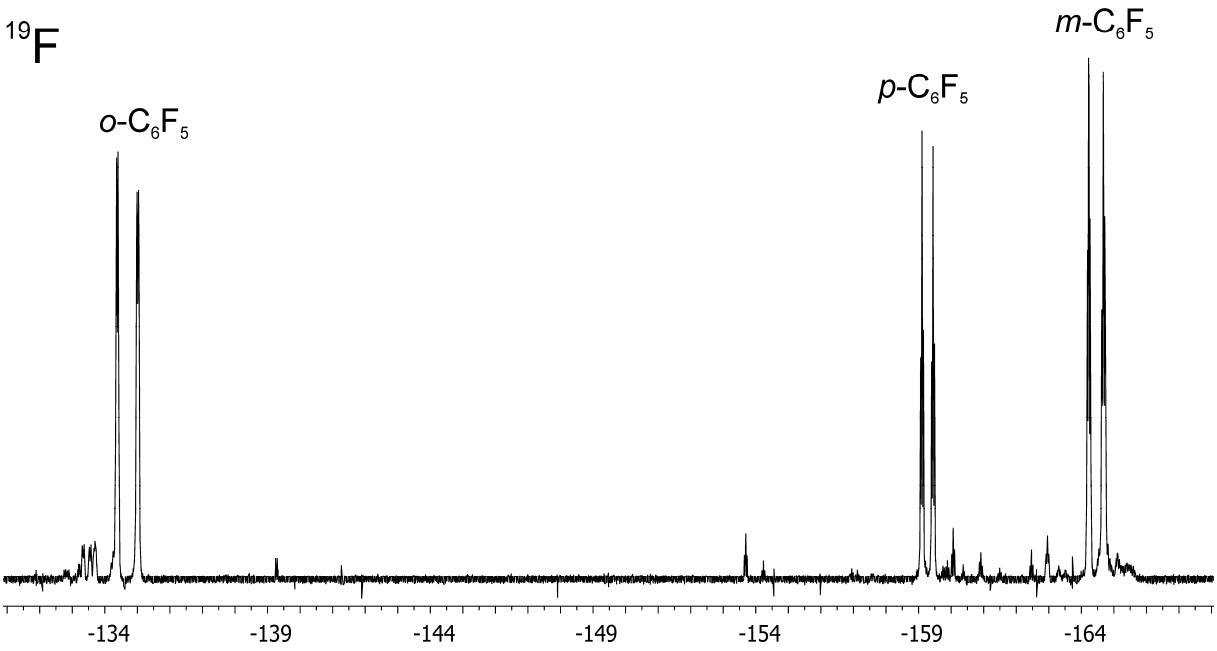
^{1}H / ^{1}H GCOSY (500 MHz / 500 MHz, C_7D_8, 273 K): δ ^{1}H / δ ^{1}H = 6.33 / 1.82 (*m*-Mes^{A} / *p*-CH_3^{MesA}), 6.25 / 1.94, 1.76 (*m*-Mes^{B} / *o*-CH_3^{MesB}, *p*-CH_3^{MesB}), 3.60 / 2.55, 1.14 (CH_2^{P} / CH_2^{P}, CH_2^{B}), 2.55 / 3.60, 2.05 (CH_2^{P} / CH_2^{P}, CH_2^{B}), 1.82 / 6.33 (*p*-CH_3^{MesA} / *m*-Mes^{A}), 1.76 / 6.25 (*p*-CH_3^{MesB} / *m*-Mes^{B}), 1.14 / 3.60, 2.05 (CH_2^{B} / CH_2^{P}, CH_2^{B}).



^{1}H NMR (500 MHz, C_7D_8, 273 K) of compound **4a** [p: pentane]. **^{11}B{^{1}H} NMR** (160 MHz, C_7D_8, 273 K) and **^{31}P{^{1}H} NMR** (202 MHz, C_7D_8, 273 K) spectra.



$^{13}C\{^{1}H\}$ NMR (126 MHz, C_7D_8, 273 K) spectrum of compound **4a**.



^{19}F NMR (470 MHz, C_7D_8, 273 K) spectrum of compound **4a**.

Dynamic ^{19}F NMR of compound **4a**:

$\Delta G^{\neq} = RT_c(22.96 + \ln (T_c/\delta\nu)$ [Jmol^{-1}]

R = 8.314 J(mol K)$^{-1}$

1 cal = 4.187 J

$\Delta G^{\neq}_{diss}$ (T_c = 331 K; $\Delta\nu$(*o*-C_6F_5, 298 K) =273 Hz) = 15.2 kcal/mol

$\Delta G^{\neq}_{diss}$ (T_c = 333 K; $\Delta\nu$(*o*-C_6F_5, 298 K) =273 Hz) = 15.3 kcal/mol

average value: $\Delta G^{\neq}_{diss}$ (*o*-C_6F_5) = 15.25 ± 0.07 kcal/mol

$\Delta G^{\neq}_{diss}$ (T_c = 333 K; $\Delta\nu$(*o*-C_6F_5, 298 K) =227 Hz) = 15.4 kcal/mol

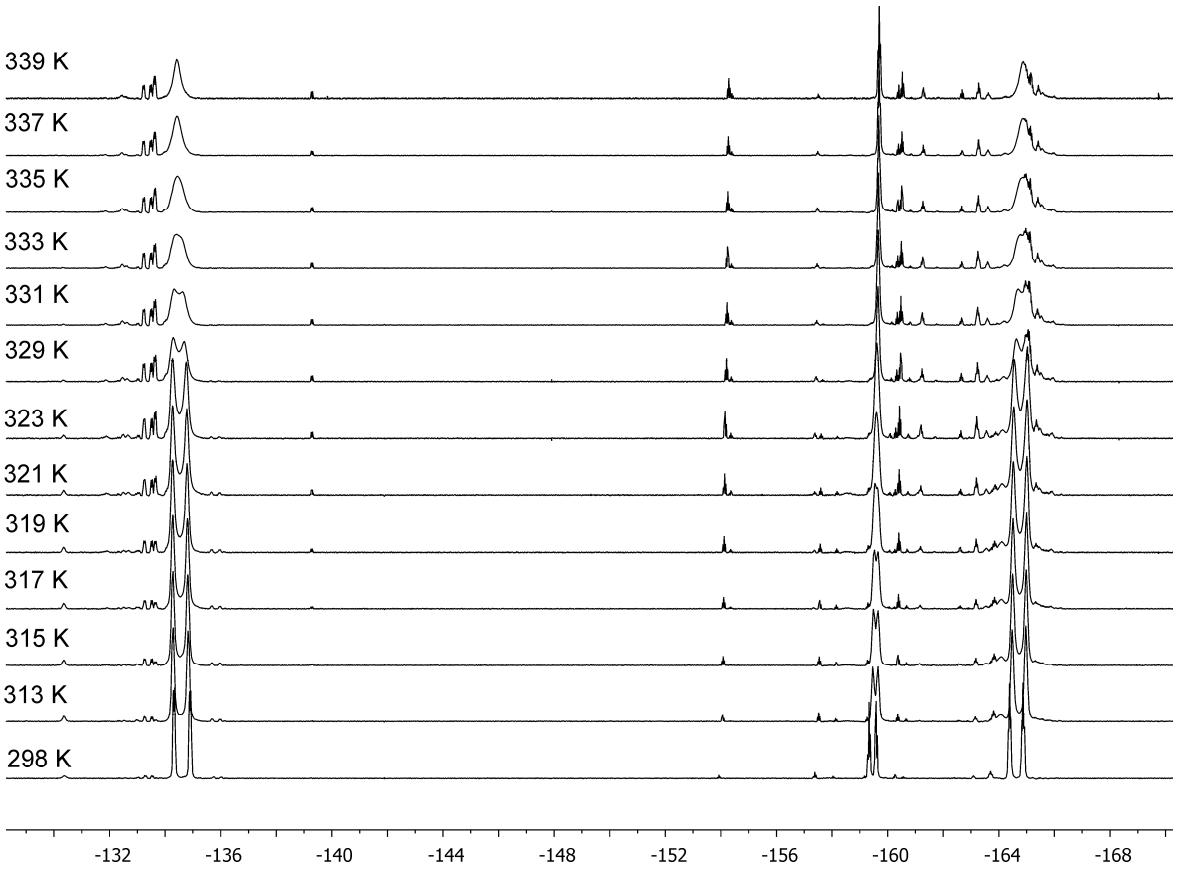
$\Delta G^{\neq}_{diss}$ (T_c = 335 K; $\Delta\nu$(*o*-C_6F_5, 298 K) =227 Hz) = 15.5 kcal/mol

average value: $\Delta G^{\neq}_{diss}$ (*o*-C_6F_5) = 15.45 ± 0.07 kcal/mol

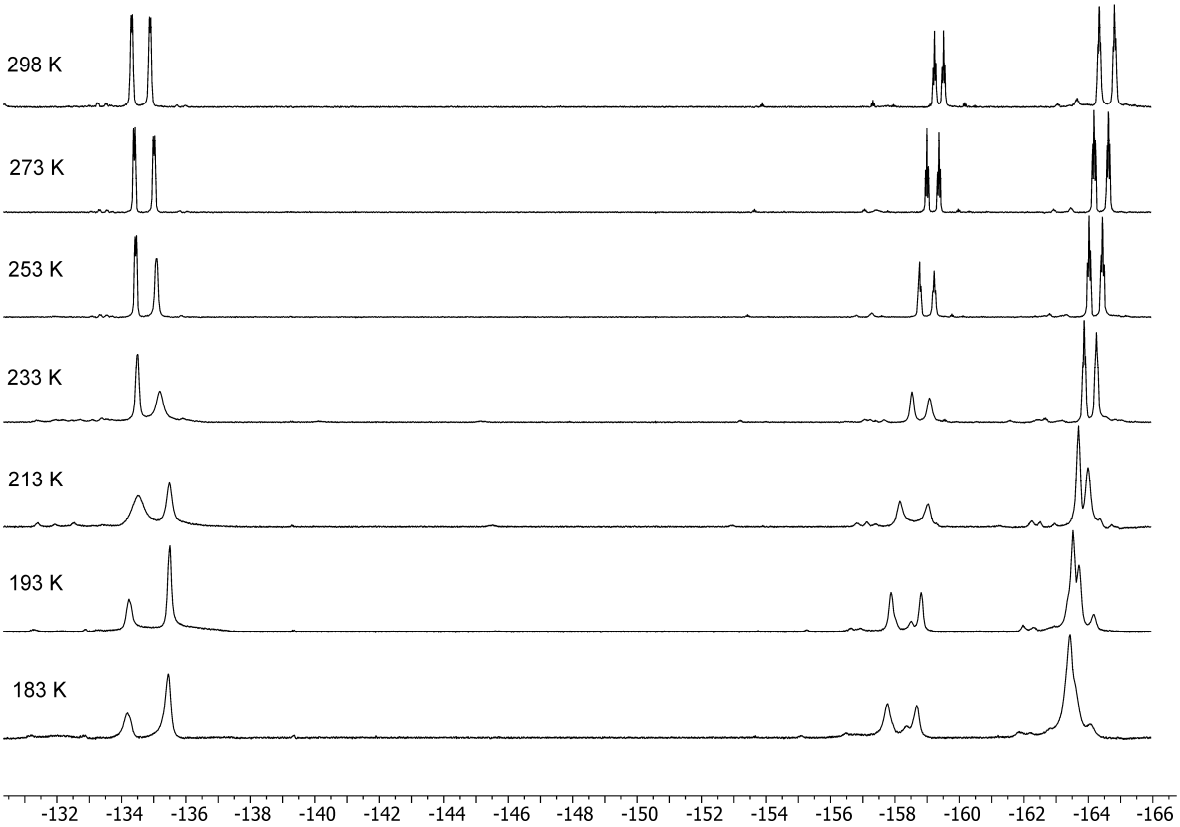
$\Delta G^{\neq}_{diss}$ (T_c = 319 K; $\Delta\nu$(*p*-C_6F_5, 298 K) =119 Hz) = 15.2 kcal/mol

$\Delta G^{\neq}_{diss}$ (T_c = 321 K; $\Delta\nu$(*p*-C_6F_5, 298 K) =119 Hz) = 15.3 kcal/mol

average value: $\Delta G^{\neq}_{diss}$ (*p*-C_6F_5) = 15.25 ± 0.07 kcal/mol



^{19}F NMR (470 MHz, C_7D_8, VT) spectra of compound **4a**.



^{19}F NMR (470 MHz, VT, [d_8]-toluene) spectra of compound **4a**.

Calculation of $\Delta G^{\neq}(^{31}P)$ of **4a**:

$\Delta G^{\neq} = RT(23.76 + \ln (T/k_{rate})$ [Jmol^{-1}]

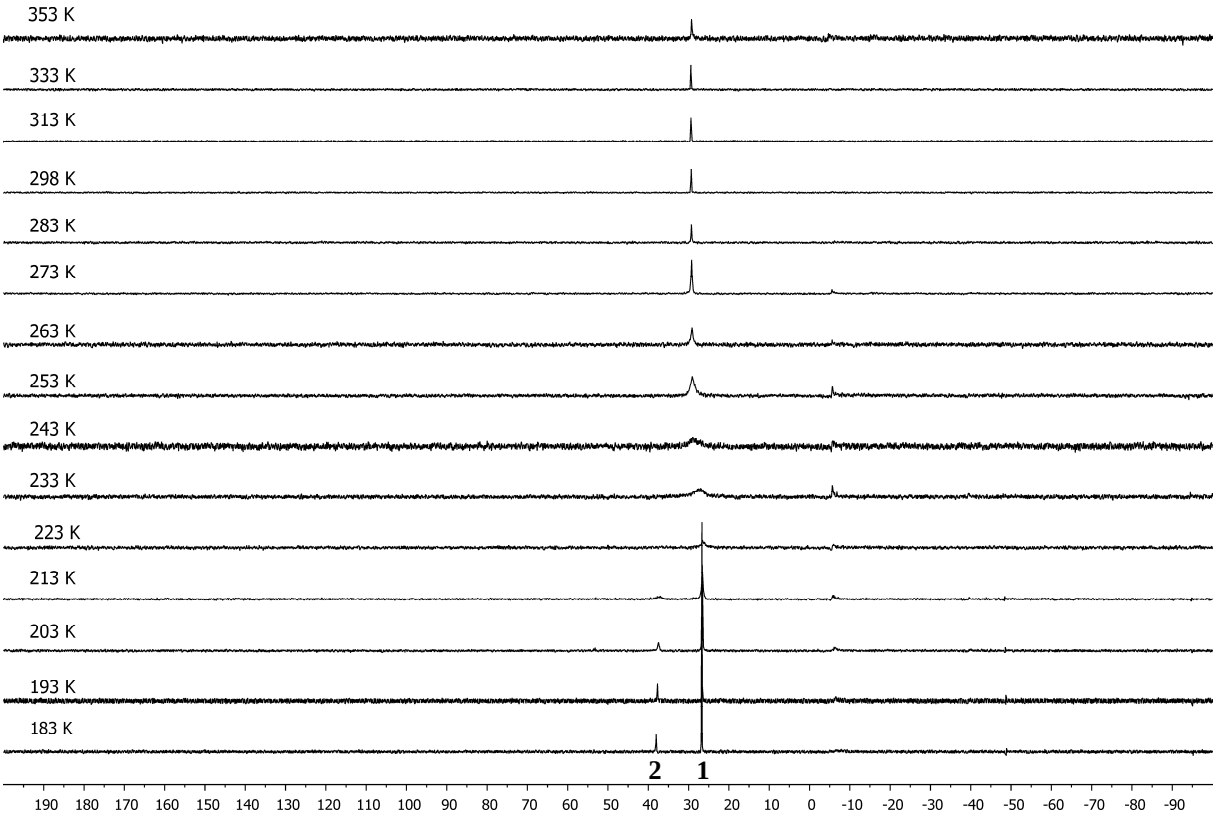
R = 8.314 J(mol K)$^{-1}$

1 cal = 4.187 J

k_{rate} was calculated by simulating the phosphorus NMR spectra using DNMR simulation of SpinWorks 3.1.8 (2011) by KIRK MARAT, University of Manitaba. [Reference: D. S. Stephenson, G. Binsch, *J. Magn. Reson.* 1978, **30**, 625.]

Tab. 1: $\Delta G_{1,2}^{\neq}$ of **4a**.

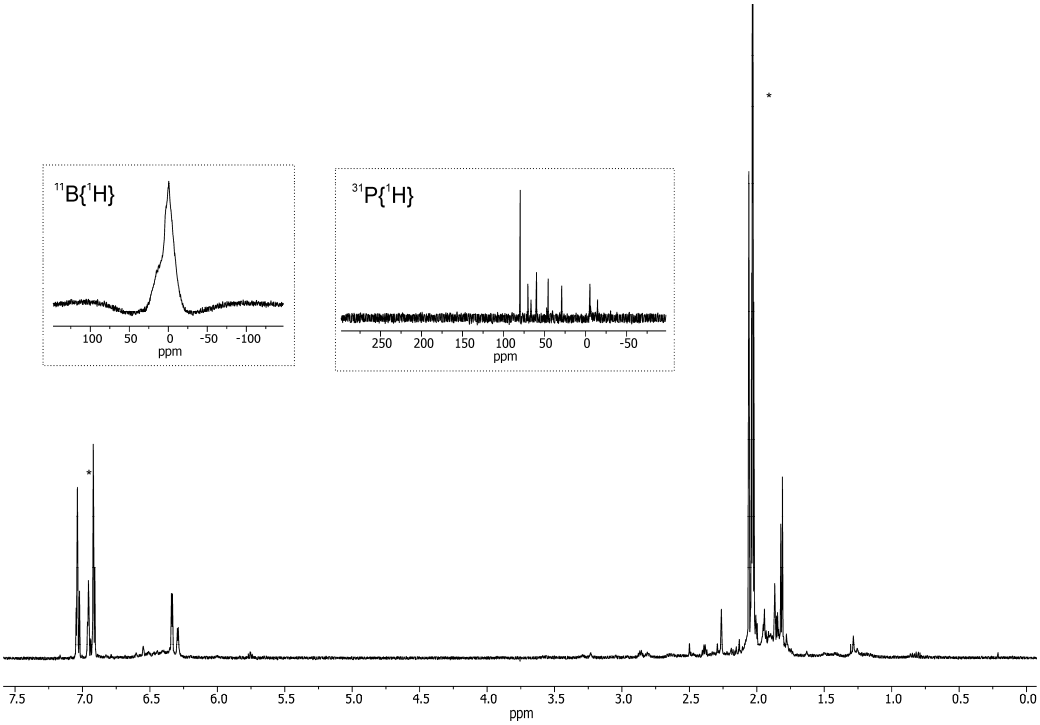
Temp [K]	k_{rate}	$\Delta G_{1,2}^{\neq}$ [kcal/mol]
183 (75%:25%)	35	9.2
203	40	9.7
213	90	9.9
223	750	10.0
233	2500	9.9
243	4000	10.1
253	12500	10.0
263	28000	10.0
273	50000	10.1
283	80000	10.2
298	200000	10.2
313	200000	10.8



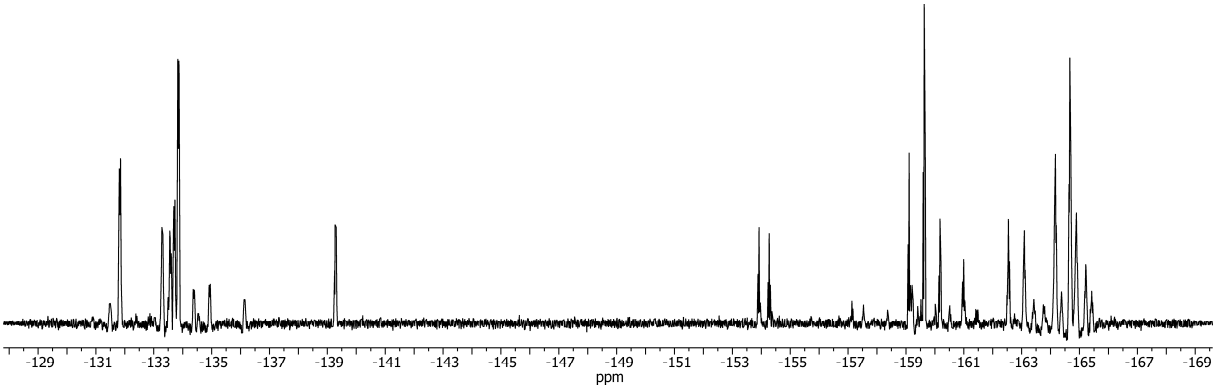
$^{31}P\{^{1}H\}$ NMR (202 MHz, C_7D_8, VT) spectra of compound **4a**.

Thermal stability of **4a:**

Compound **4a** was melted by heating the solid to 110 °C for 30 min. Then the following NMR spetra were measured.

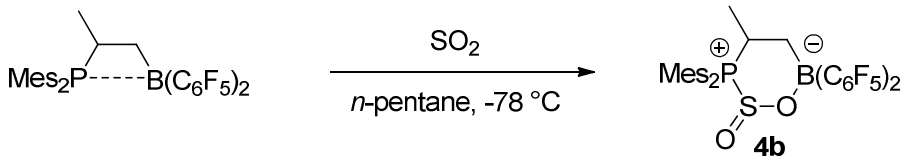


^{1}H NMR (600 MHz, 299 K, C_7D_8), **$^{11}B\{^{1}H\}$** NMR (192 MHz, 299 K, C_7D_8) und **$^{31}P\{^{1}H\}$** NMR (243 MHz, 299 K, C_7D_8) of **4a** after melting.



^{19}F NMR (564 MHz, 299 K, C_7D_8) of **4a** after melting.

Preperation of compound 4b



A suspension of bis(pentafluorophenyl)borane (27.6 mg, 0.08 mmol, 1.0 eq) in toluene (1 mL) was added to a solution of (1-methylethenyl)dimesitylphosphane (24.8 mg, 0.08 mmol, 1.0 eq) in toluene (1 mL). The reaction mixture was cooled down to −78 °C and sulfur dioxide (1.8 bar) was introduced for five minutes whereupon the reaction mixture got yellow. After stirring the solution for 45 min at −78 °C the Schlenkflask was flushed with argon whereupon the reaction mixture got colourless. This solution was overlaid with precooled n-pentane (5 mL) and storred at -36 °C, where crystals of compound **4b** suitable for X-ray crystal structure analysis were obtained. Two diastereomers of **4b** were found in CD_2Cl_2 solution at 299K (ratio: 84/16) [Compound **4b** was not stable in CD_2Cl_2 solution].

The compound could not be obtained completely pure: **Elemental analysis:** Calc.: C: 55.02, H: 3.92; Found: C: 57.86, H: 4.26.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3837 (w), 3806 (w), 3750 (w), 3675 (w), 3649 (w), 3028 (w), 2973 (m), 2931 (m), 2875 (m), 2736 (w), 2360 (w), 2339 (w), 1644 (s), 1605 (s), 1558 (m), 1515 (s), 1464 (s), 1404 (m), 1381 (s), 1281 (s), 1155 (s), 1134 (m), 1094 (s), 1058 (m), 1030 (m), 975 (s), 941 (s), 862 (s), 807 (m), 765 (m), 744 (m), 729 (m), 700 (m), 670 (s), 641 (m), 615 (w), 598 (w), 572 (w), 556 (m), 543 (m), 474 (m), 441 (m), 417 (m).

Melting point (DSC): 126 °C.

^{1}H NMR (500 MHz, CD_2Cl_2, 299 K): δ[84%] = 7.02 (d, $^4J_{PH}$ = 3.6 Hz, 2H, *m*-Mes^A), 7.00 (d, $^4J_{PH}$ = 3.6 Hz, 2H, *m*-Mes^B), 4.14 (m, 1H, CH^P), 2.38 (br, 6H, *o*-CH_3^{MesA}), 2.35 (br, 6H, *o*-CH_3^{MesB}), 2.325 (br m, 3H, *p*-CH_3^{MesA}), 2.318 (br m, 3H, *p*-CH_3^{MesB}), 1.82 (dd, $^3J_{PH}$ = 27.8 Hz, $^3J_{HH}$ = 16.4 Hz, 1H, CH_2^B), 1.414 (dd, $^3J_{PH}$ = 18.1 Hz, $^3J_{HH}$ = 7.0 Hz, 3H, CH_3^P), 1.30 (m, 1H, CH_2^B).

^{1}H NMR (500 MHz, CD_2Cl_2, 299 K): δ[16%] = 7.04 (d, $^4J_{PH}$ = 3.7 Hz, 2H, *m*-Mes^A), 7.01 (d, $^4J_{PH}$ = 3.6 Hz, 2H, *m*-Mes^B), 3.36 (m, 1H, CH^P), 2.37 (br, 6H, *o*-CH_3^{MesA}), 2.34 (br, 6H, *p*-$CH_3^{MesA,B}$), 2.27 (br, 6H, *o*-CH_3^{MesB}), 2.04 (m, 1H, CH_2^B), 1.68 (dd, $^3J_{PH}$ = 27.5 Hz, $^3J_{HH}$ = 16.4 Hz, 1H, CH_2^B), 1.406 (dd, $^3J_{PH}$ = 17.9 Hz, $^3J_{HH}$ = 7.1 Hz, 3H, CH_3^P).

^{13}C{^{1}H} NMR (126 MHz, CD_2Cl_2, 299 K): δ[84%] = 144.6 (d, $^4J_{PC}$ = 3.1 Hz, *p*-Mes^A), 144.3 (d, $^4J_{PC}$ = 3.8 Hz *p*-Mes^B), 144.0 (d, $^2J_{PC}$ = 5.6 Hz *o*-Mes^A), 143.6 (br d, $^2J_{PC}$ = 6.6 Hz

o-Mes^{B}), 132.5 (br d, $^{3}J_{PC}$ = 11.4 Hz, *m*-Mes^{B}), 131.69 (d, $^{3}J_{PC}$ = 9.9 Hz, *m*-Mes^{A}), 120.4 (d, $^{1}J_{PC}$ = 49.6 Hz, *i*-Mes^{B}), 120.3 (d, $^{1}J_{PC}$ = 36.1 Hz, *i*-Mes^{A}) 31.1 (d, $^{1}J_{PC}$ = 15.0 Hz, CH^{P}), 24.6 (br, *o*-CH$_3$^{MesA})^{t}, 23.3 (d, $^{3}J_{PC}$ = 4.1 Hz, *o*-CH$_3$^{MesB})^{t}, 22.3 (br d, $^{2}J_{PC}$ = 7.9 Hz, CH$_3$^{P}), 21.19, 21.18 (each d, each $^{5}J_{PC}$ = 1.8 Hz, *p*-CH$_3$^{MesA,B}), 21.1 (br, CH$_2$^{B}), [C_6F_5 not listed].

^{13}C{^{1}H} NMR (126 MHz, CD_2Cl_2, 299 K): δ[16%] = 144.4 (d, $^{4}J_{PC}$ = 3.3 Hz), 144.3^{t} (d, $^{4}J_{PC}$ = 3.8 Hz) (*p*-Mes^{A,B}), 144.1 (d, $^{2}J_{PC}$ = 6.3 Hz, *o*-Mes^{A}), 142.9 (d, $^{2}J_{PC}$ = 6.3 Hz, *o*-Mes^{B}), 132.2 (d, $^{3}J_{PC}$ = 10.6 Hz, *m*-Mes^{B}), 131.67 (d, $^{3}J_{PC}$ = 10.8 Hz, *m*-Mes^{A}), 121.5 (d, $^{1}J_{PC}$ = 44.8 Hz, *i*-Mes^{B}), 121.1 (d, $^{1}J_{PC}$ = 34.5 Hz, *i*-Mes^{A}), 33.6 (d, $^{1}J_{PC}$ = 11.7 Hz, CH^{P}), 24.4 (br, *o*-CH$_3$^{MesA}), 23.7 (d, $^{3}J_{PC}$ = 3.5 Hz, *o*-CH$_3$^{MesB}), 21.6 (d, $^{2}J_{PC}$ = 12.6 Hz, CH$_3$^{P}), n.o. (*p*-CH$_3$^{Mes}), 20.2 (br, CH$_2$^{B}), [C_6F_5 not listed; ^{t} tentative assignment].

^{11}B{^{1}H} NMR (160 MHz, CD_2Cl_2, 299 K): δ = 1.3 ($\nu_{1/2}$ ≈ 450 Hz).

^{19}F NMR (470 MHz, 299 K, CD_2Cl_2): δ[84%] = −135.4 (m, 2F, *o*), −160.6 (t, $^{1}J_{FC}$ = 20.4 Hz, 1F, *p*), −165.7 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 5.1 [C_6F_5^{A}]; −135.6 (m, 2F, *o*), −161.1 (t, $^{1}J_{FC}$ = 20.4 Hz, 1F, *p*), −165.5 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 4.4 [C_6F_5^{B}]; δ[16%] = −134.5 (m, 2F, *o*), −161.0 (t, $^{1}J_{FC}$ = 20.4 Hz, 1F, *p*), −165.9 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 5.1 [C_6F_5^{A}]; −134.7 (m, 2F, *o*), −159.9 (t, $^{1}J_{FC}$ = 20.4 Hz, 1F, *p*), −165.0 (m, 2F, *m*), $\Delta\delta^{19}F_{p,m}$ = 4.4 [C_6F_5^{B}].

^{19}F / ^{19}F GCOSY (470 MHz / 470 MHz, CD_2Cl_2, 299 K): δ[84%]= −135.4 / −165.7 (*o* / *m*), −160.6 / −165.7 (*p* / *m*), −165.7 / −135.4, −160.6 (*m* / *o*, *p*) [C_6F_5^{A}]; −135.6 / −165.5 (*o* / *m*), −161.1 / −165.5 (*p* / *m*), −165.5 / −135.6, −161.1 (*m* / *o*, *p*) [C_6F_5^{B}]; δ[16%]= −134.5 / −165.9 (*o* / *m*), −161.0 / −165.9 (*p* / *m*), −165.9 / −134.5, −161.0 (*m* / *o*, *p*) [C_6F_5^{A}]; −134.7 / −165.0 (*o* / *m*), −159.9 / −165.0 (*p* / *m*), −165.0 / −134.7, −159.9 (*m* / *o*, *p*) [C_6F_5^{B}].

^{31}P{^{1}H} NMR (202 MHz, CD_2Cl_2, 299 K): δ = 51.2 ($\nu_{1/2}$ ≈ 10 Hz, 16%), 39.5 ($\nu_{1/2}$ ≈ 10 Hz, 84%).

^{31}P{^{1}H} NMR (202 MHz, CD_2Cl_2, 198 K): δ = 55.4($\nu_{1/2}$ ≈ 15 Hz, 8%), 50.3 ($\nu_{1/2}$ ≈ 35 Hz, 3%), 39.0 ($\nu_{1/2}$ ≈ 25 Hz, 58%), 37.8 ($\nu_{1/2}$ ≈ 30 Hz, 31%).

^{1}H / ^{13}C GHSQC (500 MHz / 126 MHz, CD_2Cl_2, 299 K): δ ^{1}H / δ ^{13}C [84%] = 7.02 / 131.69 (*m*-Mes^{A}), 7.00 / 132.5 (*m*-Mes^{B}), 4.14 / 31.1 (CH^{P}), 2.38 / 24.6 (*o*-CH$_3$^{MesA}), 2.35 / 23.3 (*o*-CH$_3$^{MesB}), 2.325, 2.318 / 21.19, 21.18 (*p*-CH$_3$^{MesA}, *p*-CH$_3$^{MesB}), 1.82 / 21.1 (CH$_2$^{B}), 1.414 / 22.3 (CH$_3$^{P}), 1.30 / 21.1 (CH$_2$^{B}).

^{1}H / ^{13}C GHSQC (500 MHz / 126 MHz, CD_2Cl_2, 299 K): δ ^{1}H / δ ^{13}C [16%] = 7.04 / 131.67 (*m*-Mes^{A}), 7.01 / 132.2 (*m*-Mes^{B}), 3.36 / 33.6 (CH^{P}), 2.37 / 24.4 (*o*-CH$_3$^{MesA}), 2.34 / n.o. (*p*-CH$_3$^{MesA}, *p*-CH$_3$^{MesB}), 2.27 / 23.7 (*o*-CH$_3$^{MesB}), 2.04 / 20.2 (CH$_2$^{B}), 1.68 / 20.2 (CH$_2$^{B}), 1.406 / 21.6 (CH$_3$^{P}).

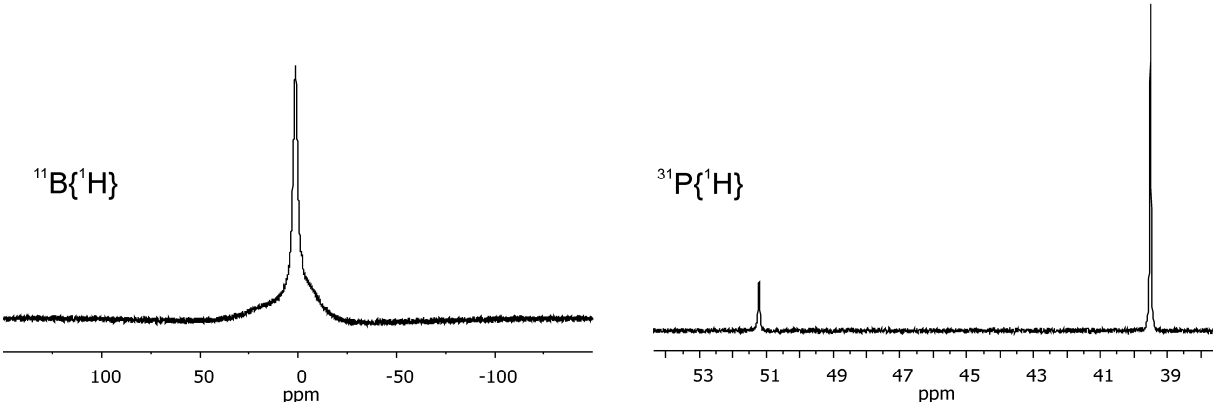
^{1}H / ^{13}C GHMBC (500 MHz / 126 MHz, CD_2Cl_2, 299 K): δ ^{1}H / δ ^{13}C [84%] = 7.02 / 144.0, 131.69, 120.3, 24.6, 21.19, 21.18 (*m*-Mes^{A} / *o*-Mes^{A}, *m*-Mes^{A}, *i*-Mes^{A}, *o*-CH_3^{MesA}, *p*-CH_3^{MesA}), 7.00 / 143.6, 132.5, 120.3, 23.3, 21.19, 21.18 (*m*-Mes^{B} / *o*-Mes^{B}, *m*-Mes^{B}, *i*-Mes^{B}, *o*-CH_3^{MesB}, *p*-CH_3^{MesB}), 4.14 / 120.4, 120.3, 22.3 (CH^{P} / *i*-Mes^{B}, *i*-Mes^{A}, CH_3^{P}), 2.38 / 144.0 (*o*-CH_3^{MesA} / *o*-Mes^{A}), 2.325 / 144.6, 131.69, 120.3 (*p*-CH_3^{MesA} / *p*-Mes^{A}; *m*-Mes^{A}; *i*-Mes^{A}), 2.318 / 144.3, 132.5, 120.4 (*p*-CH_3^{MesB} / *p*-Mes^{B}; *m*-Mes^{B}; *i*-Mes^{B}), 1.82 / 31.1, 22.3 (CH_2^{B} / CH^{P}, CH_3^{P}), 1.414 / 31.1, 21.1 (CH_3^{P} / CH^{P}, CH_2^{B}), 1.30 / 31.1, 22.3 (CH_2^{B} / CH^{P}, CH_3^{P}).

^{1}H / ^{13}C GHMBC (500 MHz / 126 MHz, CD_2Cl_2, 299 K): δ ^{1}H / δ ^{13}C [16%] = 7.04 / 144.1, 131.67, 121.1, 24.4 (*m*-Mes^{A} / *o*-Mes^{A}, *m*-Mes^{A}, *i*-Mes^{A}, *o*-CH_3^{MesA}), 7.01 / 143.3, 142.9, 132.2, 121.5, 23.7 (*m*-Mes^{B} / *p*-Mes^{B}, *o*-Mes^{B}, *m*-Mes^{B}, *i*-Mes^{B}, *o*-CH_3^{MesB}), 3.36 / 121.5, 121.1, 21.6 (CH^{P} / *i*-Mes^{B}, *i*-Mes^{A}, CH_3^{P}), 2.37 / 131.67, 121.1 (*o*-CH_3^{MesA} / *m*-Mes^{A}, *i*-Mes^{A}), 2.34 / 121.5, 121.1 (*p*-$CH_3^{MesA,B}$ / *i*-Mes^{B}; *i*-Mes^{A}), 2.27 / 142.9, 132.2, 121.5 (*o*-CH_3^{MesB} / *o*-Mes^{B}; *m*-Mes^{B}; *i*-Mes^{B}), 2.04 / 33.6, 21.6 (CH_2^{B} / CH^{P}, CH_3^{P}), 1.68 / 33.6, 21.6 (CH_2^{B} / CH^{P}, CH_3^{P}), 1.406 / 33.6, 20.2 (CH_3^{P} / CH^{P}, CH_2^{B}).

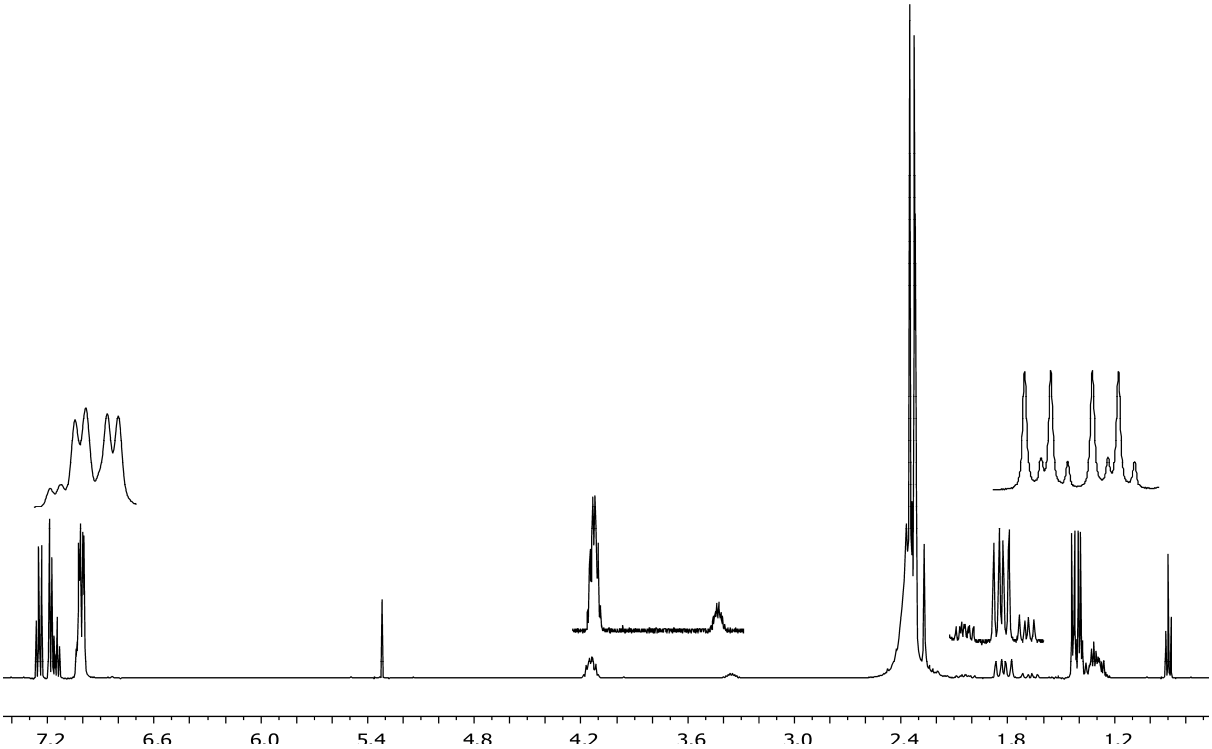
^{1}H / ^{1}H GCOSY (500 MHz / 500 MHz, CD_2Cl_2, 299 K): δ ^{1}H / δ ^{1}H [84%] = 4.14 / 1.82, 1.414, 1.30 (CH^{P} / CH_2^{B}, CH_3^{P}, CH_2^{B}), 1.82 / 4.14, 1.30 (CH_2^{B} / CH^{P}, CH_2^{B}), 1.414 / 4.14 (CH_3^{P} / CH^{P}), 1.30 / 4.14, 1.82 (CH_2^{B} / CH^{P}, CH_2^{B}).

^{1}H / ^{1}H GCOSY (500 MHz / 500 MHz, CD_2Cl_2, 299 K): δ ^{1}H / δ ^{1}H [16%] = 3.36 / 2.04, 1.406 (CH^{P} / CH_2^{B}, CH_3^{P}), 2.04 / 3.36, 1.68 (CH_2^{B} / CH^{P}, CH_2^{B}), 1.68 / 2.04 (CH_2^{B} / CH_2^{B}), 1.406 / 3.36 (CH_3^{P} / CH^{P}).

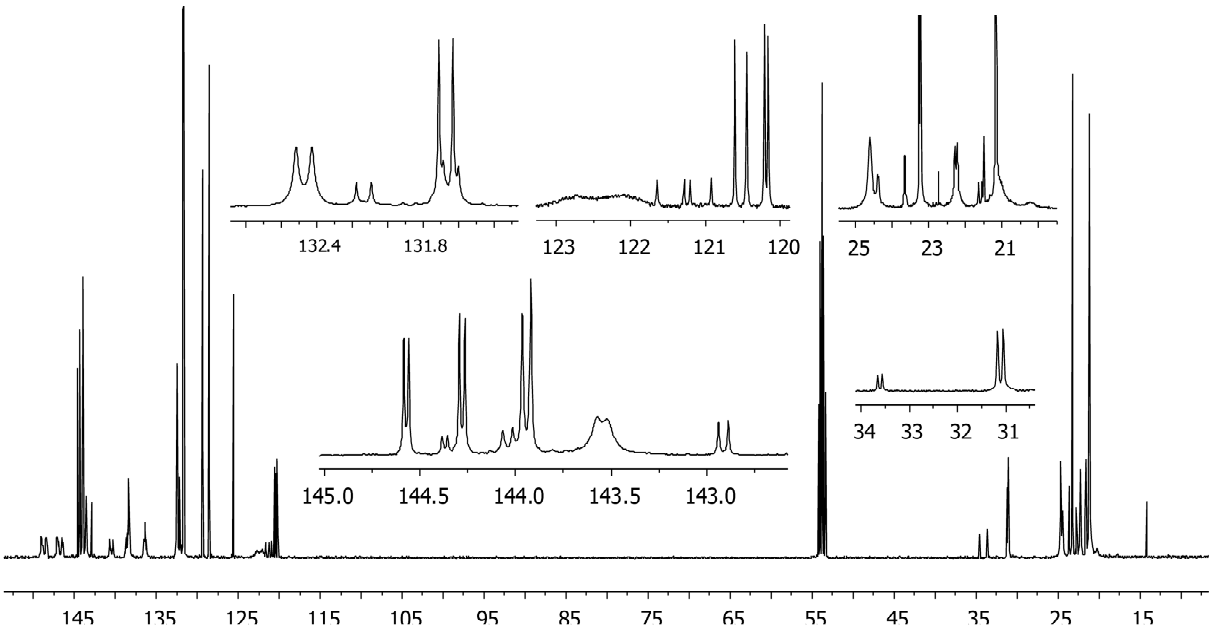
^{1}H{^{1}H} TOCSY (500 MHz, CD_2Cl_2, 299 K): δ $^{1}H_{irr}$ / δ $^{1}H_{res}$ [traces, 84%]= 4.14 / 1.82, 1.414, 1.30 (CH^{P} / CH_2^{B}, CH_3^{P}, CH_2^{B}), 1.82 / 4.14, 1.414, 1.30 (CH_2^{B} / CH^{P}, CH_3^{P}, CH_2^{B}), 1.414 / 4.14, 1.82, 1.30 (CH_3^{P} / CH^{P}, CH_2^{B}, CH_2^{B}), 1.30 / 4.14, 1.83, 1.414 (CH_2^{B} / CH^{P}, CH_2^{B}, CH_3^{P}).



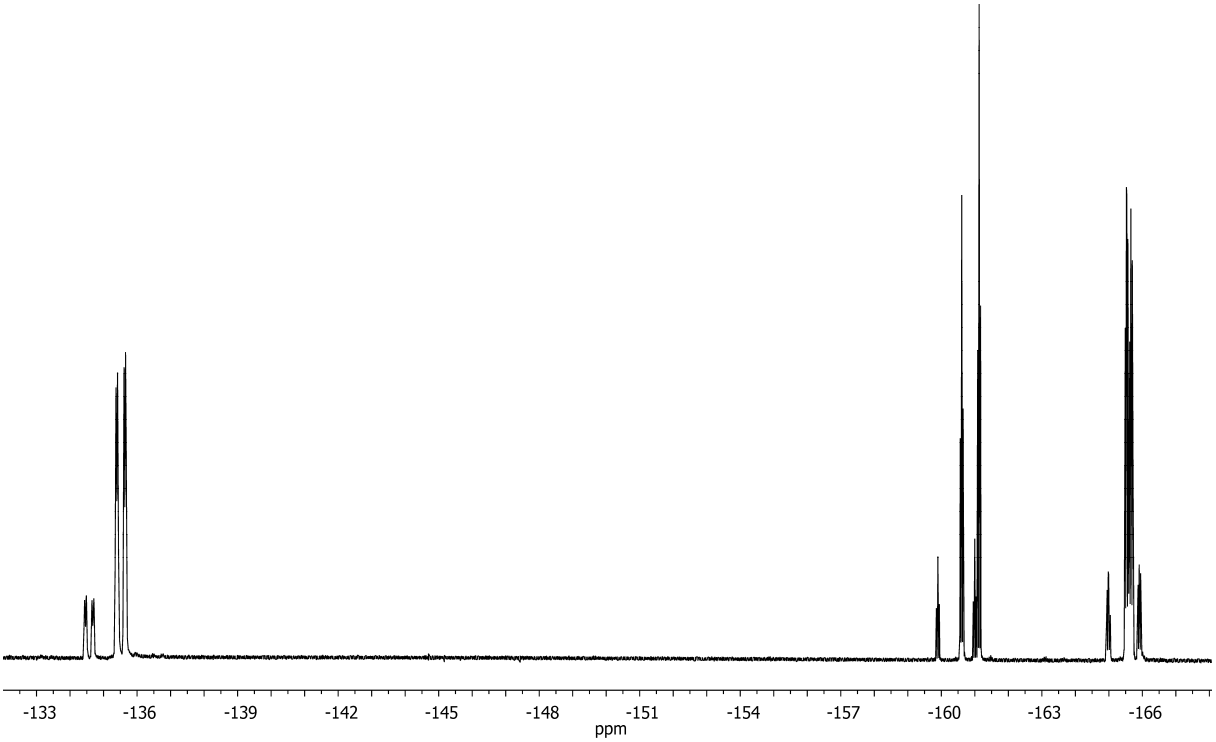
^{11}B{^{1}H} NMR (160 MHz, CD_2Cl_2, 299 K) and **^{31}P{^{1}H} NMR** (202 MHz, CD_2Cl_2, 299 K) spectra of **4b**.



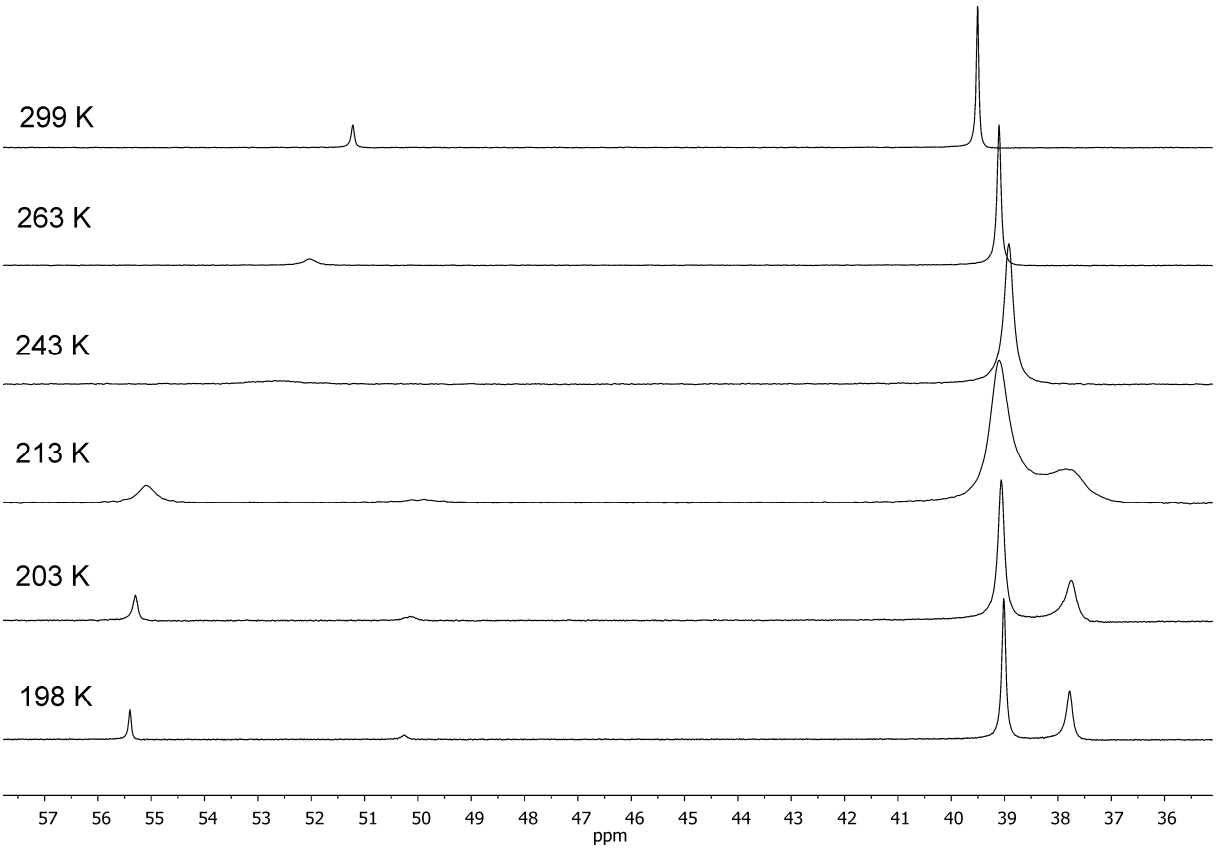
^{1}H NMR (500 MHz, CD_2Cl_2, 299 K) spectrum of **4b** [toluene, pentane].



^{13}C{^{1}H} NMR (126 MHz, CD_2Cl_2, 299 K) spectrumof **4b** [toluene, pentane].

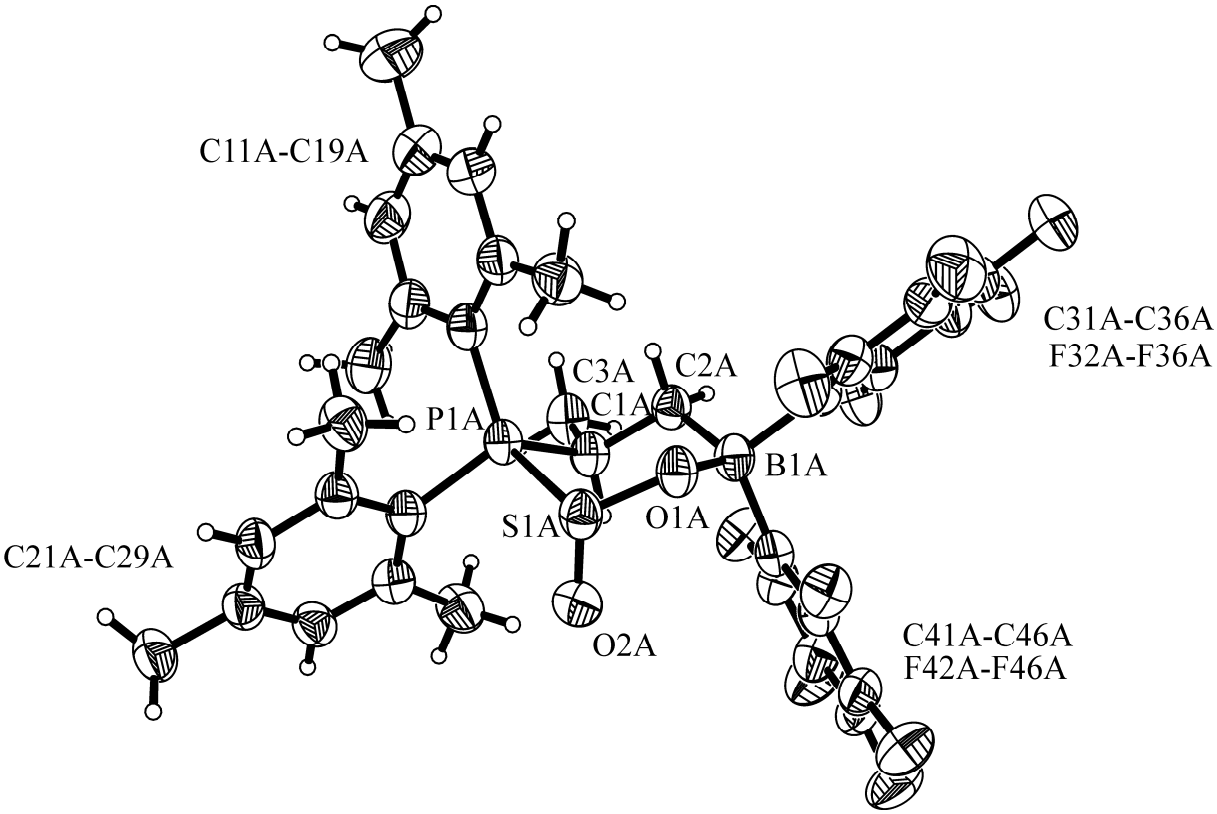


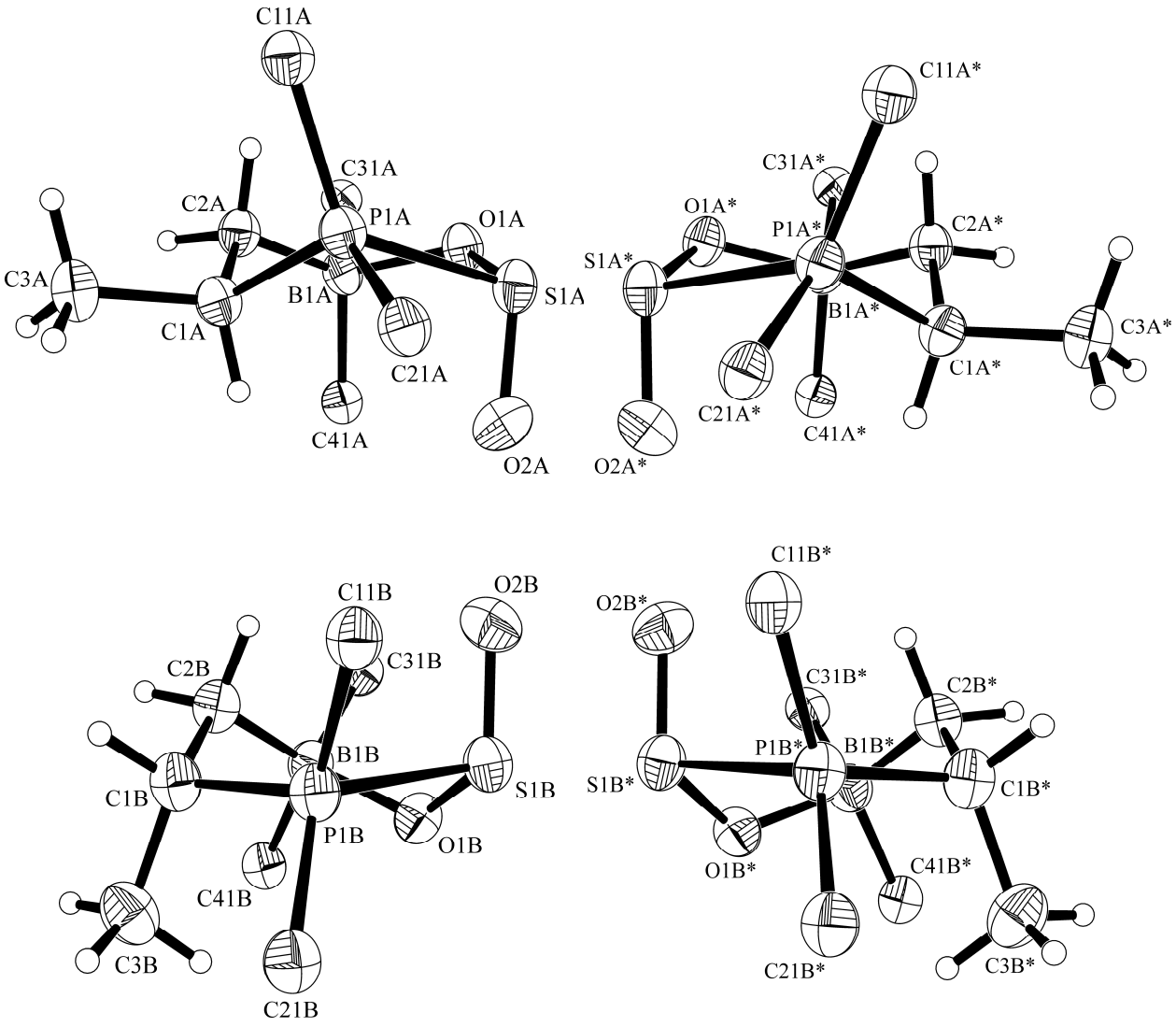
^{19}F NMR (470 MHz, CD_2Cl_2, 299 K) spectrum of **4b**.



^{31}P{^{1}H} NMR (202 MHz, CD_2Cl_2, VT) spectra of compound **4b**.

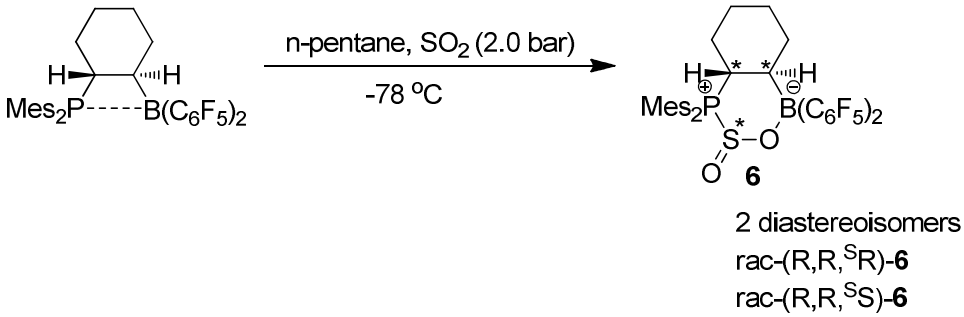
X-ray crystal structure analysis of 4b: formula $C_{33}H_{28}BF_{10}O_2PS$, M = 720.39, colourless crystal, 0.20 x 0.13 x 0.05 mm, a = 13.2898(3), b = 13.3521(6), c = 22.5790(9) Å, α = 73.392(3), β = 73.073(3), γ = 83.328(4)°, V = 3670.7(2) Å^3, ρ_{calc} = 1.304 gcm^{-3}, μ = 1.903 mm^{-1}, empirical absorption correction (0.702 ≤ T ≤ 0.910), Z = 4, triclinic, space group $P\bar{1}$ (No. 2), λ = 1.54178 Å, T = 223(2) K, ω and φ scans, 53257 reflections collected (±h, ±k, ±l), 12647 independent (R_{int} = 0.043) and 10730 observed reflections [I>2σ(I)], 877 refined parameters, R = 0.049, wR^2 = 0.145, max. (min.) residual electron density 0.35 (-0.32) e.Å^{-3}, hydrogen atoms calculated and refined as riding atoms.





Conformers of compound rac-R,S-**4b** found in the unit cell

Preperation of compound 6



Procedure A: Di(mesityl)cyclohexenylphosphane (120 mg, 0.34 mmol) and $HB(C_6F_5)_2$ (119 mg, 0.34 mmol) were weighed together, dissolved in toluene (2.5 mL) and stirred for 30 min at r.t. to get a yellow solution of **5**. The solution was cooled to -78 °C and SO_2 gas was pressed (2.0 bar) over the solution which resulted in disappearance of the yellow colour. After 3 minutes the gas pressure was released and the reaction flask flushed with argon. The solution was covered with precooled (-30 °C) *n*-pentane. The slow diffusion at -35 °C gave the compound **6** (136 mg, 52 %) as colourless crystals.

Procedure B: Di(mesityl)cyclohexenylphosphane (250 mg, 0.71 mmol) and $HB(C_6F_5)_2$ (247 mg, 0.71 mmol) were weighed together, dissolved in *n*-pentane (15 mL) and stirred for 30 min at r.t. to get a yellow solution of **5**. The solution was cooled to -78 °C and SO_2 gas was pressed (2.0 bar) over the solution which resulted in the formation of a precipitate. After 5 minutes the gas pressure was released and the reaction flask flushed with argon. The solvent was removed via a filter cannula and the residue was dried under vacuum at -78 °C. The colourless residue was dissolved in precooled CH_2Cl_2 and the solution was covered with precooled (-30 °C) *n*-pentane. The slow diffusion at -35 °C gave the compound **6** (310 mg, 57 %) as colourless crystals.

Melting point (DSC): 123.2 °C (decomposition observed without a melting point).

Elemental analysis: Calc. for $C_{36}H_{32}PBSO_2F_{10}$: C: 56.86, H: 4.24; Found: C: 56.30, H: 4.06.

The NMR resonances were not assigned to each diastereoisomer [1:1.3 (^{31}P)]:

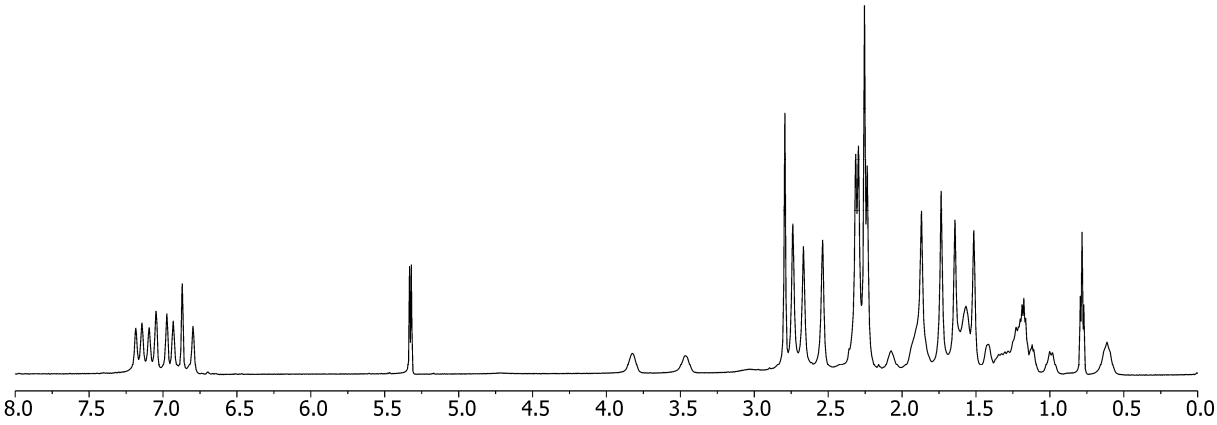
^{1}H NMR (600 MHz, CD_2Cl_2, 193 K) [all resonances are broad] δ = 7.18/6.97, 7.14/6.93, 7.09/6.80, 7.05/6.87 (each br s, each 1H, *m,m'*-Mes)[1], 3.82, 3.47 (each br., each 1H, PCH), 2.79/2.24(p)/1.64, 2.74/2.30(p)/1.51, 2.67/2.31(p)/1.87, 2.54/2.25(p)/1.74 (each s, each 3H, CH_3^{Mes})[1], 2.25/1.23, 2.07/0.62, 1.92/0.61, 1.88/1.35, 1.60/1.22, 1.58/1.77, 1.56/1.28, 1.42/0.99 (each br, each 1H, CH_2)[2], 2.31, 1.85 (each br, each 1H, BH)[2], [[1] from the gcosy NMR experiment; [2] from the ghsqc NMR experiment].

$^{13}C\{^1H\}$ NMR (151 MHz, CD_2Cl_2, 193 K) not listed [all resonaces are broad; see figure below]

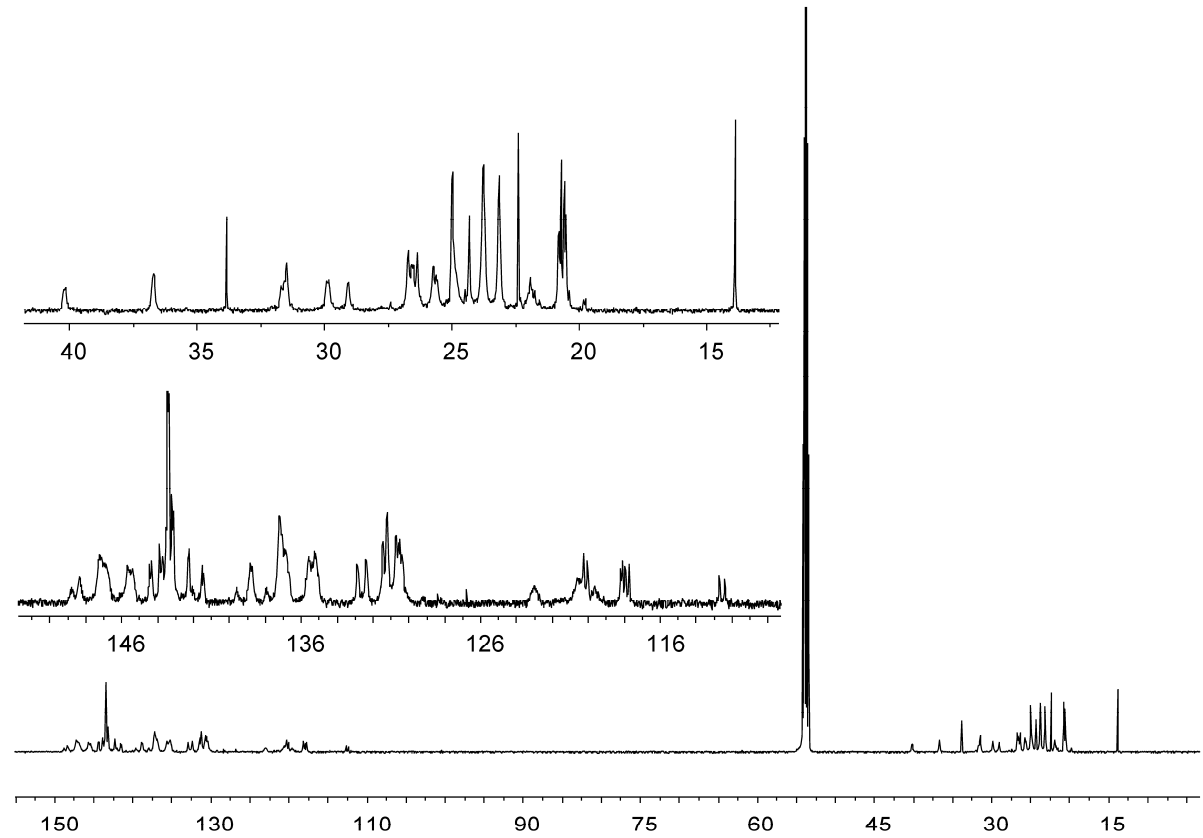
$^{11}B\{^1H\}$ NMR (192 MHz, CD_2Cl_2, 308 K): δ = 1.8 ($\nu_{1/2} \approx 500$ Hz)

$^{31}P\{^1H\}$ NMR (243 MHz, CD_2Cl_2, 193 K): δ = 60.5 ($\nu_{1/2} \approx 30$ Hz, [42%]), 41.1 ($\nu_{1/2} \approx 40$ Hz, [58%]).

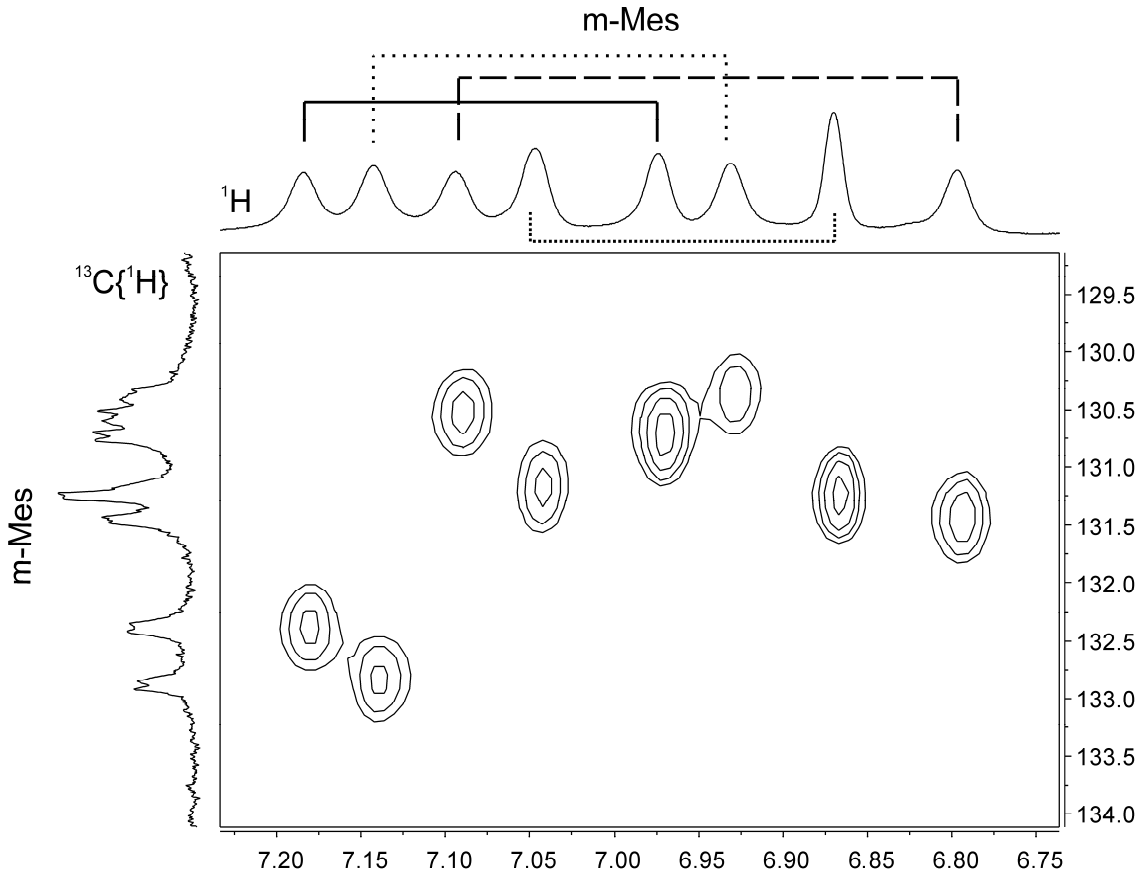
^{19}F NMR (564 MHz, CD_2Cl_2, 193 K): δ = −128.6, −130.8, −131.7, −132.3, −132.47, −132.53, − 136.3, −139.0 (each br, each 1F, *o*-C_6F_5), −158.1, −159.3, −159.7, −160.1 (each br, each 1F, *p*-C_6F_5), −163.6 (1F), −163.9 (1F), −164.5 (5F), −164.9 (1F) (each br, m-C_6F_5).



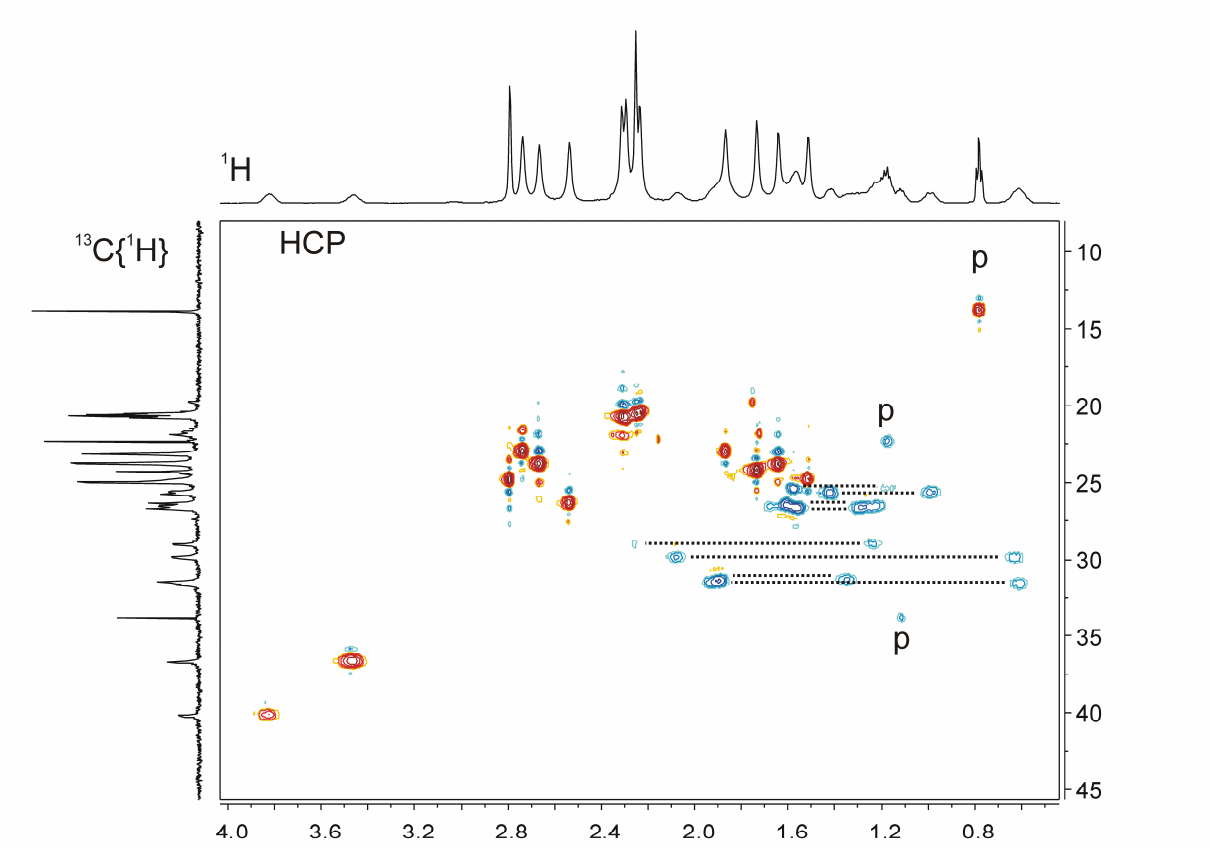
^1H NMR (600 MHz, 193 K, CD_2Cl_2)



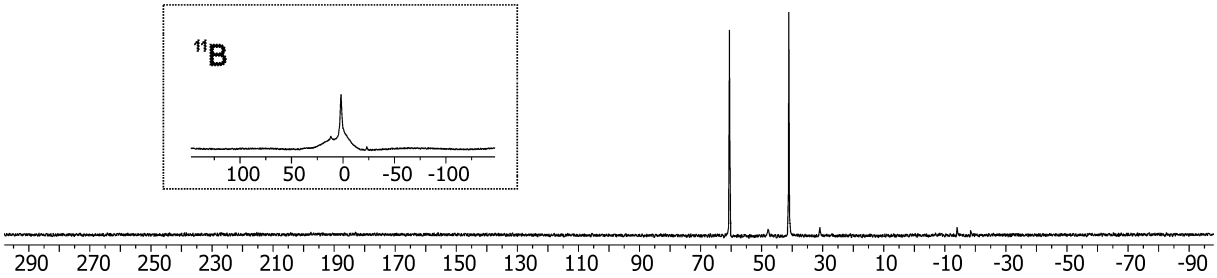
$^{13}C\{^1H\}$ NMR (151 MHz, CD_2Cl_2, 193 K)



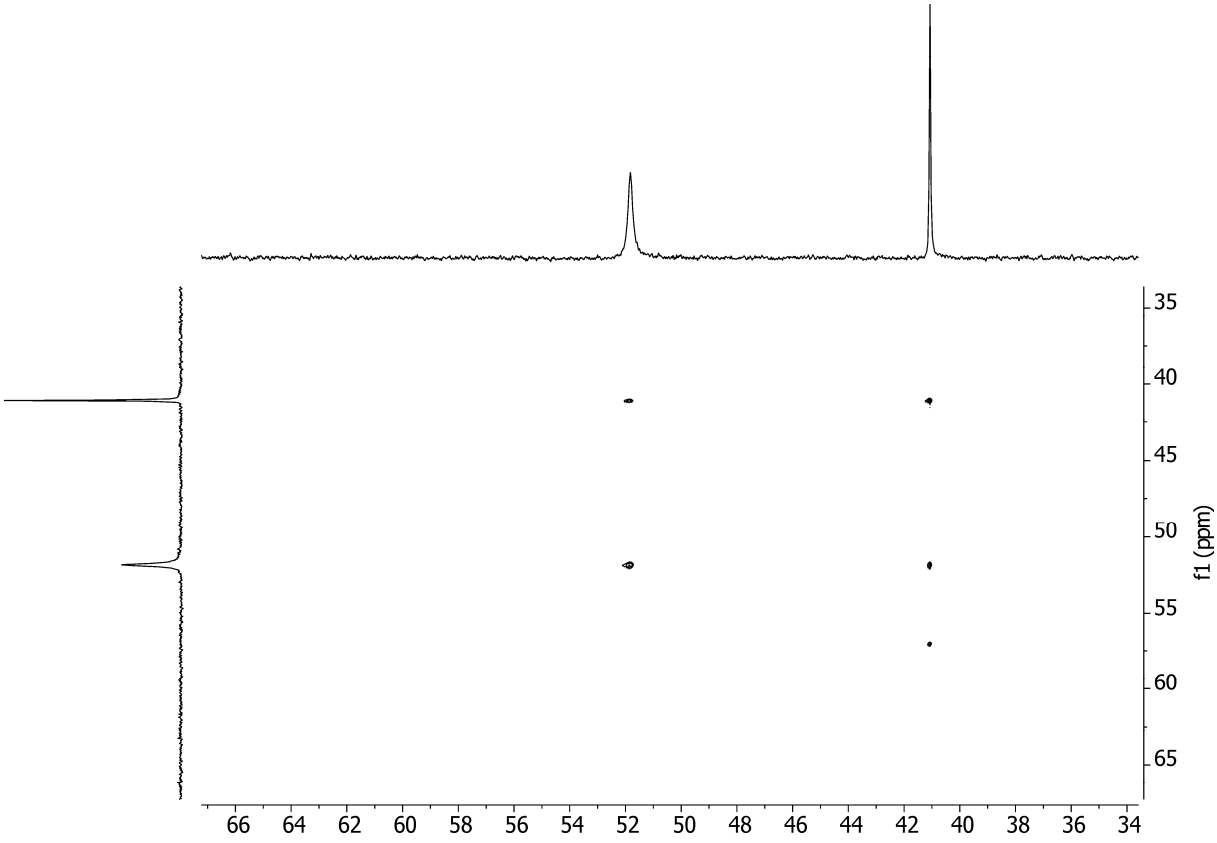
^{1}H/^{13}C GHSQC (600 MHz / 151 MHz, CD_2Cl_2, 193 K)



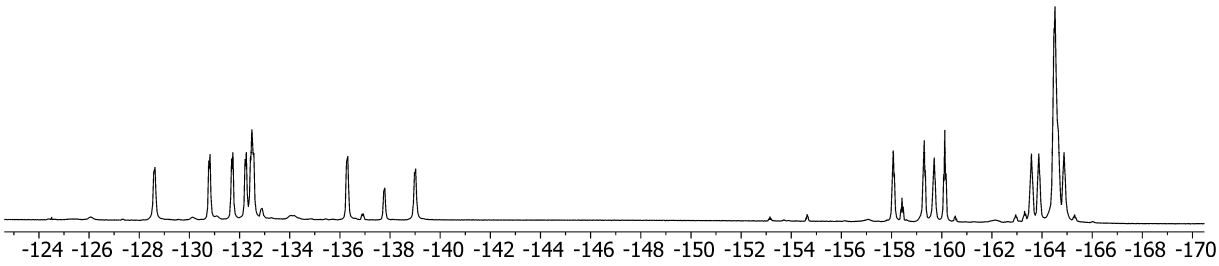
^{1}H/^{13}C GHSQC (600 MHz / 151 MHz, CD_2Cl_2, 193 K) [p: pentane; ··· CH_2 groups (blue cross peaks); red cross peaks for CH and CH_3 groups]



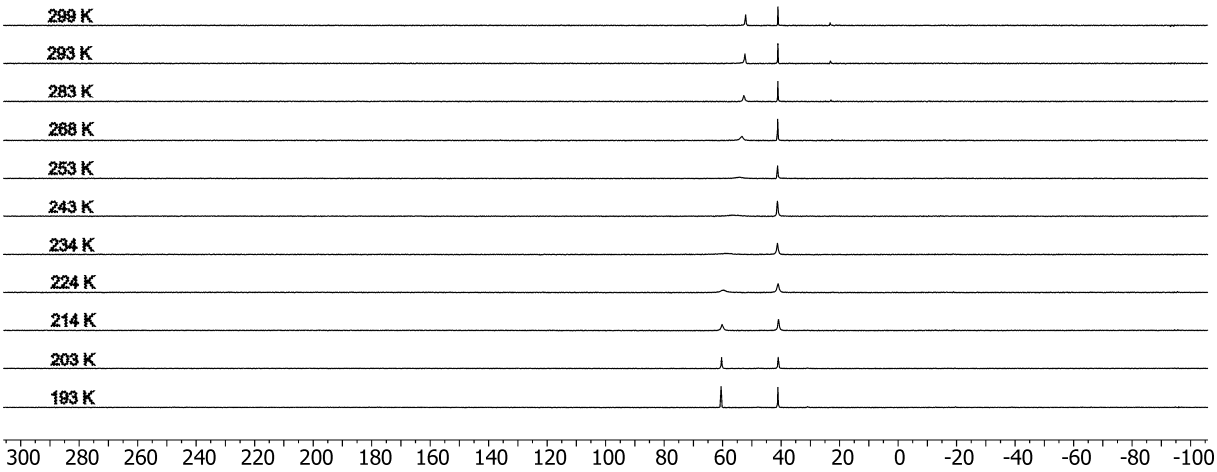
$^{31}P\{^{1}H\}$ NMR (243 MHz, 193 K, CD_2Cl_2) and **$^{11}B\{^{1}H\}$ NMR** (192 MHz, 308 K, CD_2Cl_2)



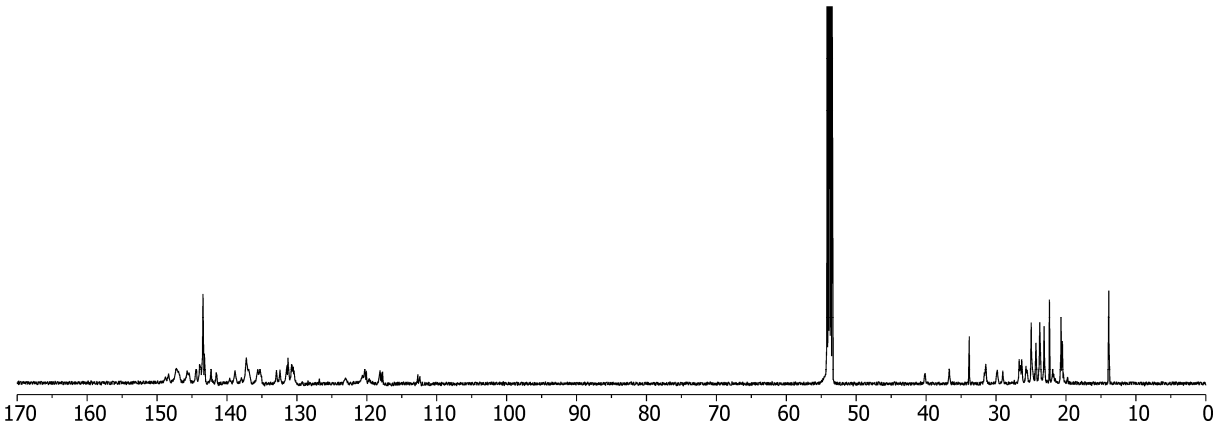
^{31}P, ^{31}P NOESY NMR (243 MHz, 308 K, CD_2Cl_2)



^{19}F NMR (564 MHz, 193 K, CD_2Cl_2)

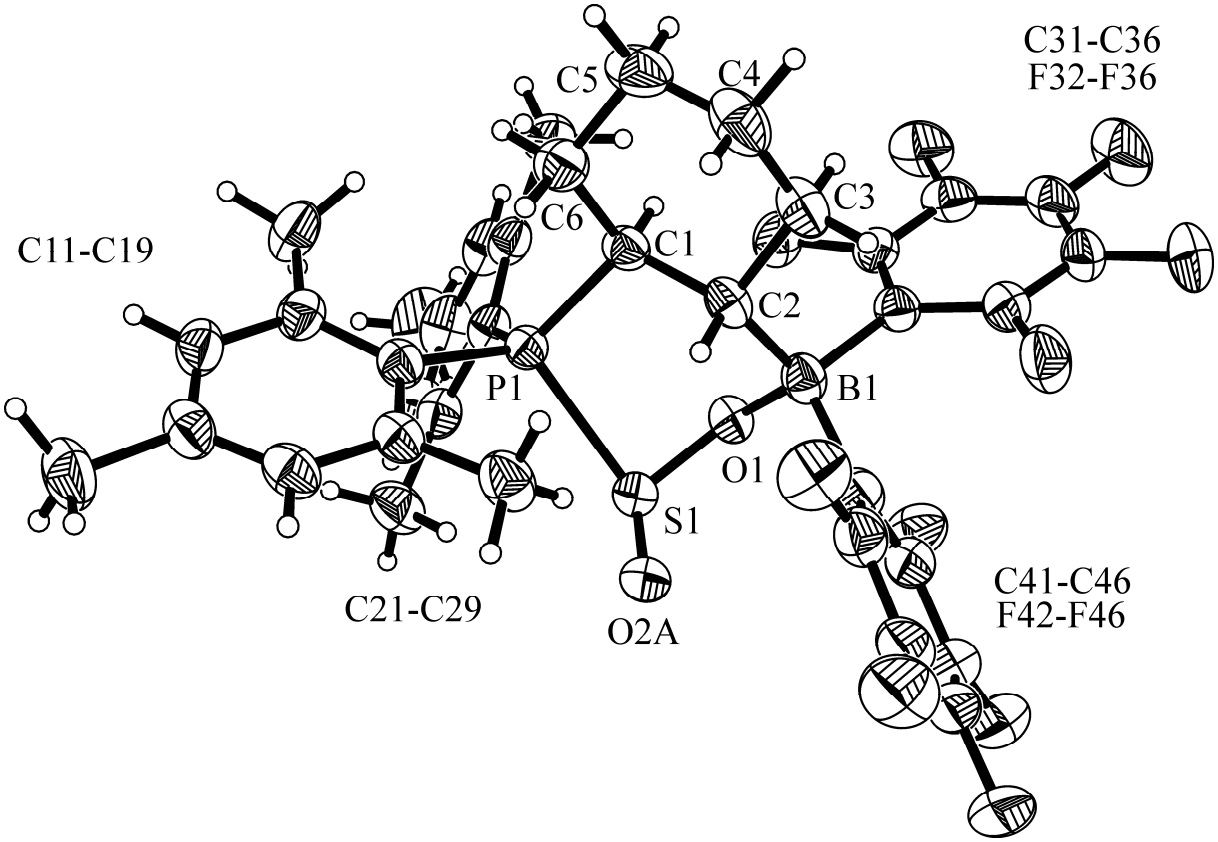


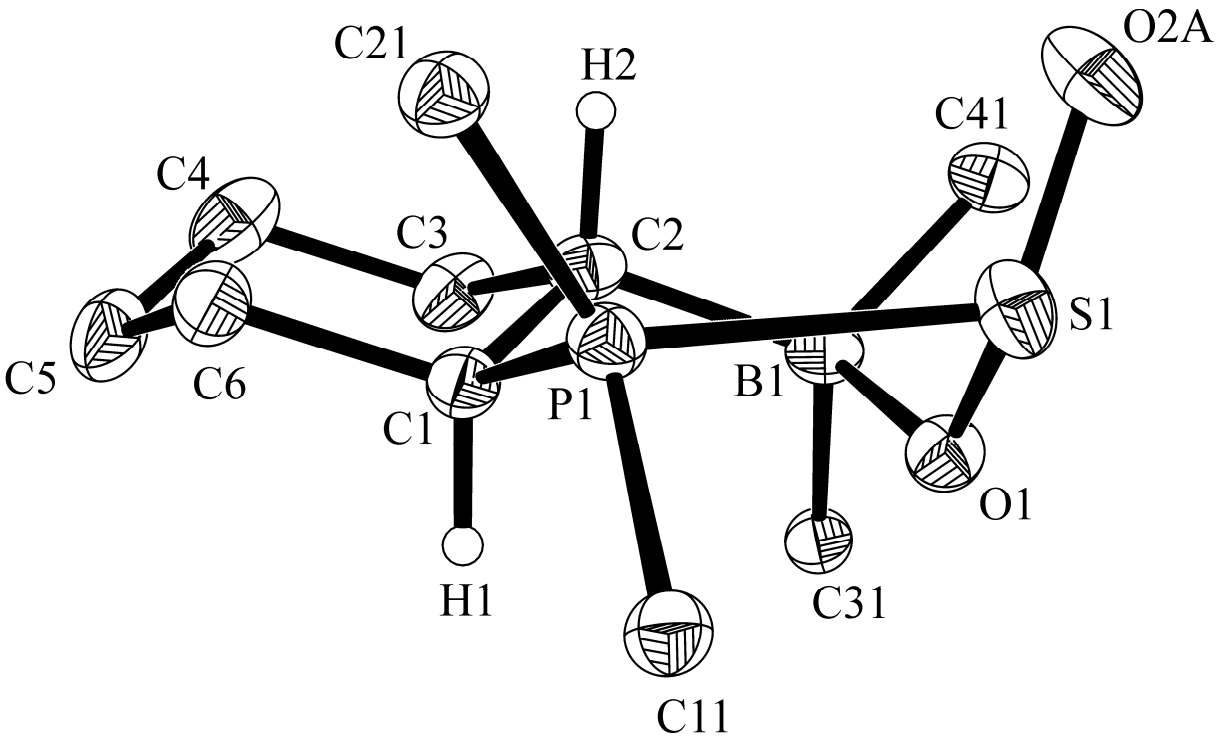
^{31}P{^{1}H} NMR (243 MHz, VT, CD_2Cl_2) of compound **6**.



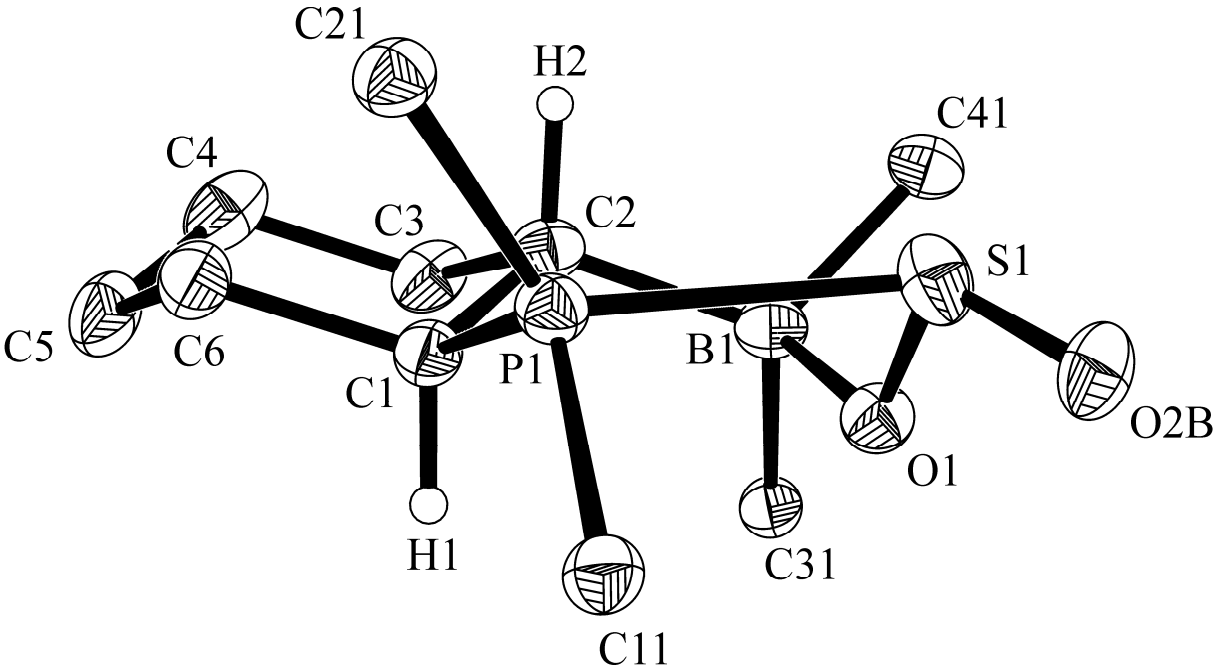
^{13}C{^{1}H} NMR (151 MHz, 193 K, CD_2Cl_2)

X-ray crystal structure analysis of 6: formula $C_{36}H_{32}BF_{10}O_2PS$, M = 760.46, colourless crystal, 0.28 x 0.15 x 0.06 mm, a = 10.5993(4), b = 11.8650(4), c = 14.4165(9) Å, α = 92.700(3), β = 95.322(2), γ = 111.030(13)°, V = 1678.66(13) Å^3, ρ_{calc} = 1.504 gcm^{-3}, μ = 2.113 mm^{-1}, empirical absorption correction (0.589 ≤ T ≤ 0.883), Z = 2, triclinic, space group $P\bar{1}$ (No. 2), λ = 1.54178 Å, T = 223(2) K, ω and φ scans, 19387 reflections collected (±h, ±k, ±l), 5692 independent (R_{int} = 0.048) and 4822 observed reflections [I>2σ(I)], 476 refined parameters, R = 0.043, wR^2 = 0.116 max. (min.) residual electron density 0.24 (-0.29) e.Å^{-3}, hydrogen atoms calculated and refined as riding atoms.


C31-C36
F32-F36
C5
C4
C6
C3
C1
C11-C19
C2
P1
B1
O1
S1
C41-C46
F42-F46
C21-C29
O2A



(75%)



(25%)

Supplemental Materials Section- Solid State NMR

Experimental

Solid State NMR measurements were carried out on BRUKER DSX 500, BRUKER Avance DSX 400 and BRUKER Avance III 300 spectrometers corresponding to magnetic flux densities of 11.7, 9.4 and 7.1 T, respectively. The spectrometers were equipped with 4 mm NMR double and triple resonance probes operating at MAS rotation frequencies between 10 and 14 kHz.

$^{31}P\{^{1}H\}$ CPMAS experiments were performed at 7.1 and 9.4 T. Typical acquisition parameters were: 90° pulse lengths of 4.2-5.5 µs for ^{1}H, contact time 5 ms; recycle delay 5 s. Chemical shifts are reported relative to a 85 % H_3PO_4 solution. The ^{11}B MAS-NMR signal was acquired following excitation with 30° pulses of approx. 0.5 µs length and repetition times within the range of 4- 20 s. Chemical shifts are reported relative to a $BF_3{\cdot}Et_2O$ standard. All spectra were acquired with TPPM-15 proton decoupling[1] during the data acquisition applying decoupling pulses of approx. 7 µs length (~10/12 π pulses). Line shape analysis was done by using the DMFIT software (version 2011)[2].

^{11}B triple-quantum (TQ) MAS NMR spectra[3] were obtained at 7.1 T and 11.7 T, at a spinning frequency of 14.0 kHz, using a three-pulse z-filtering sequence[4] with proton decoupling during the triple-quantum evolution and data acquisition (the TPPM-15 decoupling scheme was used). The optimized lengths of the strong preparation and reconversion pulses were 4.0-4.8 µs and 1.6- 2.0 µs, respectively (nutation frequency ω_1~125 kHz for a liquid sample). The single quantum signal was detected by a soft pulse of 10 µs length in all cases (nutation frequency ω_1~30 kHz for a liquid sample). The increment for the evolution time was adjusted to 1/(14000) s and recycle delays of 2-10 s were used.

$^{31}P\{^{1}H\}$ MAS NMR spectra were acquired at 9.4 T with a rotation frequency of 14.0 kHz. In both cases a 90 degree pulse of 5.0 µs length and relaxation delays of 1000 to 8500 s were applied to ensure quantitative conditions.

$^{11}B\{^{31}P\}$ REDOR experiments were conducted at 7.1 T using radio frequency power levels corresponding to 180° pulse lengths of 6.5 µs, for ^{11}B and 8.0-8.5 µs for ^{31}P. The phases of the ^{31}P π pulses were alternated according to the XY4 phase cycling scheme[5]. Spinning speeds of 14.0 kHz were used. For creating a reproducible magnetization corresponding to steady-state conditions in each experiment, a saturation comb consisting of 15 90° pulses was

applied. ^{1}H decoupling was achieved by using the TPPM-15 decoupling scheme during the evolution and data acquisition period with nutation frequencies of 40-50 kHz .

Ab initio calculations of NMR parameters

All calculations were carried out using the program packages TURBOMOLE (version 6.0 and 6.3)[6] and GAUSSIAN (version GAUSSIAN09)[7]. The geometry optimizations of the proton positions have been performed on a DFT meta-GGA (TPSS[8]) level of theory (starting with the crystal structure) applying the D3(BJ)[9] dispersion correction and Ahlrich's def2-TZVP basis set[10]. The geometry optimization was performed within the TURBOMOLE program suite. In all TURBOMOLE SCF calculations an energy convergence criterion of 10^{-7} E_h and in all geometry optimizations an energy convergence criterion of $5*10^{-7}$ E_h was chosen. The integration grid was set to m4[11] and the RI approximation[12] was used.

For the calculations of nuclear electric quadrupole coupling tensors in case of the B-O-(O)S-P conformers the positions of the heavy atoms were taken from the crystal structure, whereas the positions of the hydrogen atoms were optimized on the DFT TPSS level with Ahlrich's def2-TZVP basis set and the D3(BJ) dispersion correction. In case of the B-S(O)-O-P conformers, the fully optimized geometries were used (see DFT section in this work). The calculations of the electric field gradients were performed on a GGA DFT level (functional B97-D[13]) using the program package GAUSSIAN09. The def2-TZVP basis set obtained from the EMSL data base was modified in such a way that tighter basis functions on the boron atom (extracted from the cc-pCVTZ[14] basis set, for details see ref. [15]) were included for having a more accurate description of the region near the boron nucleus. The GAUSSIAN output files were analysed by using the program EFGShield, version 2.2[16], for determination of C_Q and η values and visualizing the orientation of the electric field gradient tensor in the molecular geometry by using the DIAMOND software[17].

The magnetic shielding calculations were performed within the GIAO (gauge independent atomic orbitals) framework[18]. Magnetic shieldings were calculated on the B3-LYP[19] level of theory with the def2-TZVP basis set using the TURBOMOLE program package. Chemical shifts are referenced to $BF_3{\cdot}Et_2O$ by using B_2H_6 ($\delta(B_2H_6)$= 16.6 ppm vs. $BF_3{\cdot}Et_2O$)[20] as an external standard ($\sigma^{B3\text{-}LYP}(B_2H_6)$= 84.23 ppm) in case of boron and to phosphoric acid ($\sigma^{B3\text{-}LYP}$= 274.31 ppm) in case of phosphorus.

Discussion of ^{11}B MAS NMR data

As our previous studies have also shown[15], ^{11}B MAS NMR is an extremely versatile tool for the structural characterization of FLPs since the ^{11}B quadrupolar coupling parameters turn out to be extremely sensitive experimental probes for the local surroundings of the boron nuclei. The line shape simulation for the ^{11}B MAS NMR spectrum of **4a** reveals two resonances at about 1 ppm with quadrupolar coupling constants C_Q of 1.6 and 1.9 ± 0.1 MHz and nearly identical asymmetry parameters η of about 0.5 indicating a boron site with an unsymmetrical ligation pattern that is significantly distorted from trigonal geometry. In accordance with the integrated peak ratios of approx. 3:1 for these resonances, we assign them to the two ring conformers.

In case of **6** (see Figure S2 bottom), one dominant resonance at 0.9 ppm and a minor peak at 2.5 ppm assigned to an impurity are observed. The main resonance exhibits a C_Q value of 1.9 ± 0.1 MHz and an asymmetry parameter η of 0.5 in close agreement with the results for **4a**. Since only one peak is observed, we conclude that both diastereomers possess similar quadrupolar coupling parameters as it is also indicated by our DFT calculations of electric field gradients (EFG) for the B-O-(O)S-P diastereomers based on the crystal structure (B97-D, def2-TZVP (mod.), see Experimental section) which yield ^{11}B quadrupolar coupling parameters that are in good agreement with those observed experimentally (see Table S1). The principal component of the EFG, V_{zz}, is aligned along the B···O bond vector in case of the B-O-(O)S-P conformers (see Figures S13 and S14). In contrast, analogous EFG tensor calculations for the two B-S(O)-O-P conformers yield significantly smaller C_Q values (around 1 MHz, see Table S2) and therefore the presence of such boron-sulfur bonded SO_2 addition products can be excluded in both cases.

$^{11}B\{^{31}P\}$ REDOR data analysis

For the B···P distance determination from the REDOR data, we use the fact that at short evolution times ($\Delta S/S_0 < 0.25$) these curves are well approximated by the expression [22]

$$\Delta S/S_o = 1.066 \times (D \times NT_r)^2. \qquad \{1\}$$

Here NT_r, the number of rotor cycles times the rotor period, is the dipolar recoupling time (which is systematically varied in the experiment) and D is the dipolar coupling constant

$$D = (\mu_o/8\pi^2)\, h\, \gamma_B\, \gamma_P \times d^{-3} \qquad \{2\}$$

Here γ_B and γ_P are the gyromagnetic ratios of the nuclei ^{11}B and ^{31}P and d is their internuclear distance to be determined. Using this initial curvature approach for the data in the region $\Delta S/S_0 < 0.25$ yields in case of **6** a calibration factor $f = D^2(exp.)/ D^2(calc.) = 0.88$. Applying this calibration factor to the experimental curvature determined via equ. {1} for compound **4a** application of equ {2} yields a boron-phosphorus distance of 3.72 Å ± 0.20 Å.

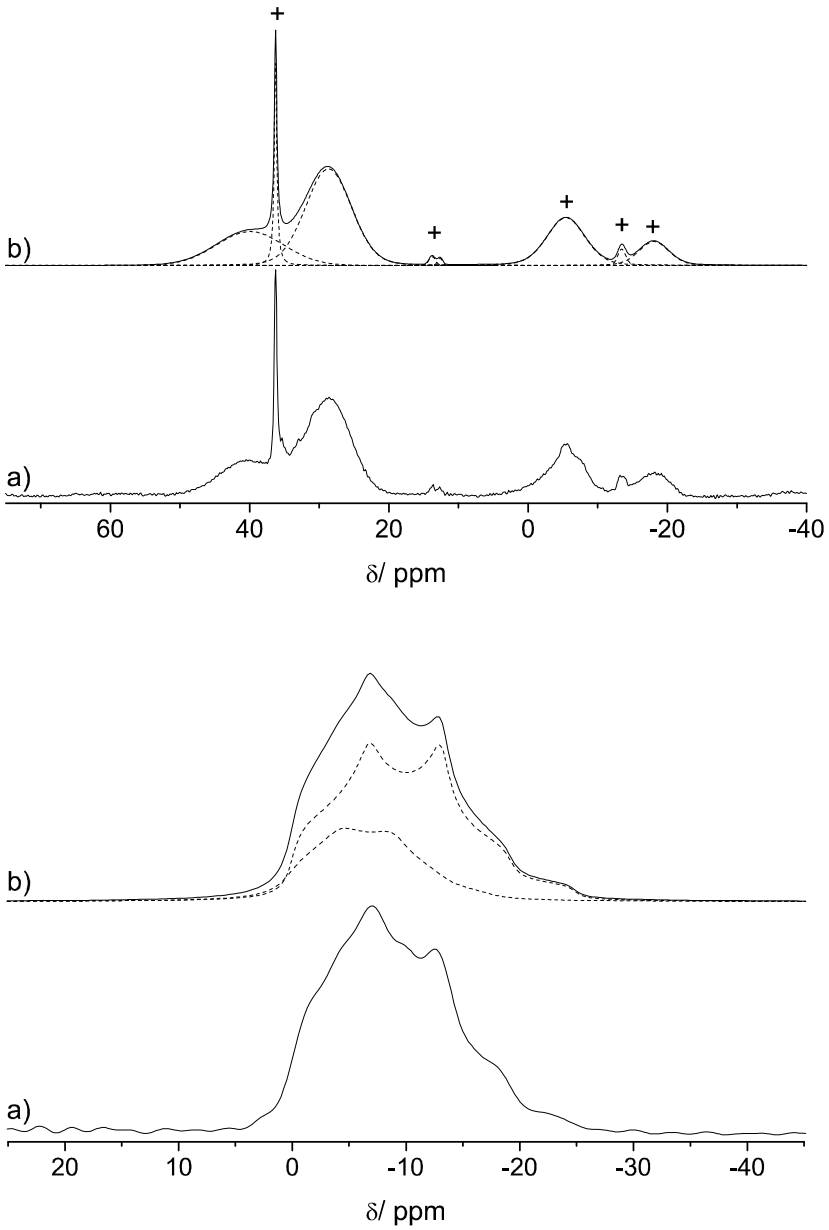


Figure S1: Top: $^{31}P\{^{1}H\}$ CPMAS NMR spectrum of **4a** (a) and corresponding line shape simulation (b) including the peak deconvolution (dashed lines) acquired at 7.1 T with a spinning frequency of 10 kHz applying the TPPM-15 ^{1}H decoupling scheme. + marks impurities. Bottom: $^{11}B\{^{1}H\}$ MAS NMR spectrum (a, using TPPM-15 decoupling) acquired at 7.1 T with a rotation frequency of 14 kHz and a relaxation delay of 4 s. Additionally, the corresponding line shape simulation is shown (b, straight line) including the peak deconvolution (b, dashed lines).

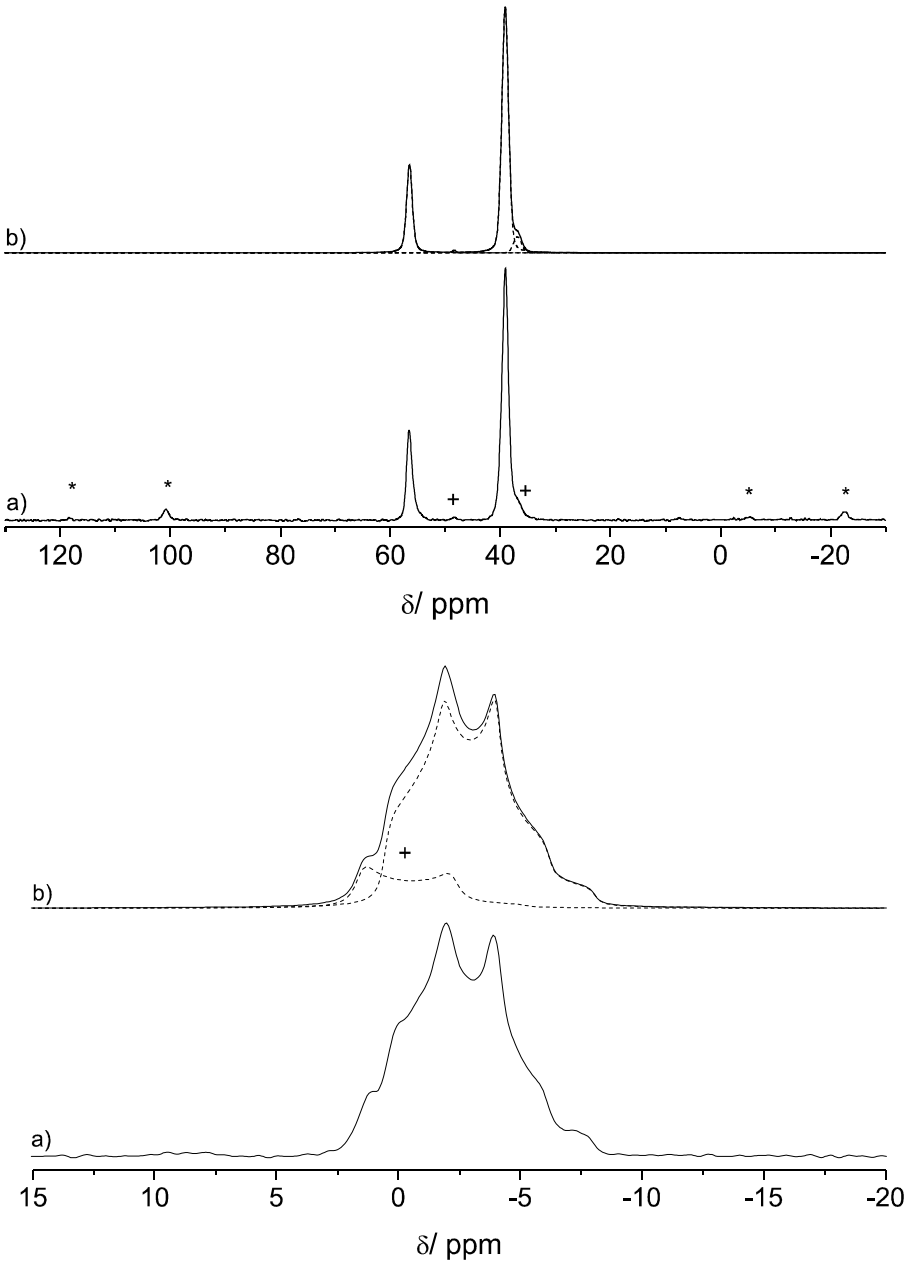


Figure S2: Top: $^{31}P\{^{1}H\}$ CPMAS NMR spectrum of **6** (a) and corresponding line shape simulation (b) including the peak deconvolution (dashed lines) acquired at 9.4 T with a spinning frequency of 10 kHz applying the TPPM-15 ^{1}H decoupling scheme. + marks an impurity. Bottom: $^{11}B\{^{1}H\}$ MAS NMR spectrum (a, using TPPM-15 decoupling) acquired at 11.7 T with a rotation frequency of 14 kHz and a relaxation delay of 20 s. Additionally, the corresponding line shape simulation is shown (b, straight line) including the peak deconvolution (b, dashed lines). + marks an impurity in both cases.

	δ_{CS}^{iso}/ ppm ±0.5	C_Q/ MHz ±10%	η ±0.1	δ_{CS}^{iso}/ ppm (calc.)	C_Q/ MHz (calc.)	η (calc.)
2a	3.3[a]	1.80[a]	0.60[a]	7.7	2.23	0.26
4a	1.0[b]; 1.0[b]; 0.7[c]; -0.8[c]	1.62[b];1.92[b]; 1.86[c]; 1.96[c]	0.46[b]; 0.48[b]; 0.46[c]; 0.47[c]	1.6[d]; 2.2[e]	2.21[d]; 2.15[e]	0.35[d]; 0.37[e]
5	8.6[a]	2.10[a]	0.43[a]	7.3[a]	2.14[a]	0.39[a]
6	2.5[b] (+); 0.9[b]	1.80[b] (+); 1.88[b]	0.01[b] (+); 0.50[b]	-2.6[f]; 0.4[g]	1.95[f]; 2.02[g]	0.43[f]; 0.44[g]

Table S1: Experimentally and theoretically determined ^{11}B NMR parameters for the B-O-(O)S-P conformers of **4a** and **6** (for comparison the unreacted FLPs **2a** and **5** are also included). Chemical shifts are calculated on a B3-LYP/def2-TZVP, electric field gradients on a B97-D/def2-TZVP (mod.) level of theory (for the full AO basis set see ref. [15]). [a]: See ref. [15]. [b:] Determined from line shape analysis of ^{11}B MAS NMR data. [c]: Determined by line shape simulation of 1D slices along F2 from MQMAS spectra. [d]: Fully geometry optimized structure is used (axial orientation of the exocyclic oxygen, see DFT part). [e]: Fully geometry optimized structure is used (equatorial orientation of the exocyclic oxygen, see DFT part). [f]: Geometry taken from the crystal structure, only protons were optimized on a TPSS-D3(BJ)/def2-TZVP level of theory (axial orientation of the exocyclic oxygen). [g]: Geometry taken from the crystal structure, only protons were optimized on a TPSS-D3(BJ)/def2-TZVP level of theory (equatorial orientation of the exocyclic oxygen). + marks an impurity.

	δ_{CS}^{iso}/ ppm (calc.)	C_Q/ MHz (calc.)	η (calc.)
4a	1.6[a]; 2.2[b]; -4.4[c]; -5.4[d]	2.21[a]; 2.15[b]; 1.16[c]: 1.00[d]	0.35[a]; 0.37[b]; 0.71[c]; 0.56[d]
6	-0.4[a]; -0.6[b]; -2.8[c]; -1.5[d]	2.12[a]; 1.90[b]; 1.05[c]; 1.25[d]	0.34[a]; 0.36[b]; 0.74[c]; 0.57[d]

Table S2: Theoretically determined ^{11}B NMR parameters for the fully geometry optimized structures of **4a** and **6** (for more details see DFT part). Chemical shifts are calculated on a B3-LYP/def2-TZVP, electric field gradients on a B97-D/def2-TZVP (mod.) level of theory. [a]: Fully geometry optimized structure of the B-O-(O)S-P product is used with an axial orientation of the exocyclic oxygen at the sulfur stereocenter. [b]: Fully geometry optimized structure of the B-O-(O)S-P product is used with an equatorial orientation of the exocyclic oxygen at the sulfur stereocenter. [c]: Fully geometry optimized structure of the B-S(O)-O-P product is used with an axial orientation of the exocyclic oxygen at the sulfur stereocenter. [d]: Fully geometry optimized structure of the B-S(O)-O-P product is used with an equatorial orientation of the exocyclic oxygen at the sulfur stereocenter.

	δ_{CS}^{iso}/ ppm ±0.5	|Δσ|/ ppm	η_σ	intensity (approx.)	δ_{CS}^{iso}/ ppm (calc.)
2a	21.7[a]	69.9[a]	0.92[a]	-	30.6[a]
4a	28.7; 39.9	-	-	3 : 1	40.0[b]; 39.6[c]; 59.1[d]; 71.9[e]
5	23.1[a]	78.2[a]	0.40[a]	-	32.0[a]
6	39.1; 56.5	62.3; 49.6	0.71; 0.68	5 : 1	46.2[f]; 38.4[g] 55.4[b]; 76.8[c]; 72.6[d]; 62.7[e]

Table S3: Experimentally and theoretically determined ^{31}P NMR parameters. Chemical shifts are calculated on a B3-LYP/def2-TZVP level of theory and are referenced to phosphoric acid. [a]: For more details see ref. [15]. [b]: Fully geometry optimized structure of the B-O-(O)S-P product is used with an axial orientation of the oxygen at the sulfur stereocenter (see DFT part). [c]: Fully geometry optimized structure of the B-O-(O)S-P product is used with an equatorial orientation of the oxygen at the sulfur stereocenter (see DFT part). [d] Fully geometry optimized structure of the B-S(O)-O-P product is used with an axial orientation of the oxygen at the sulfur stereocenter (see DFT part). [e]: Fully geometry optimized structure of the B-S(O)-O-P product is used with an equatorial orientation of the oxygen at the sulfur stereocenter (see DFT part). [f]: Geometry of the B-O-(O)S-P product (axial orientation of the exocyclic oxygen) taken from the crystal structure, only protons were optimized on a TPSS-D3(BJ)/def2-TZVP level of theory. [g]: Geometry of the B-O-(O)S-P product (equatorial orientation of the exocyclic oxygen) taken from the crystal structure, only protons were optimized on a TPSS-D3(BJ)/def2-TZVP level of theory.

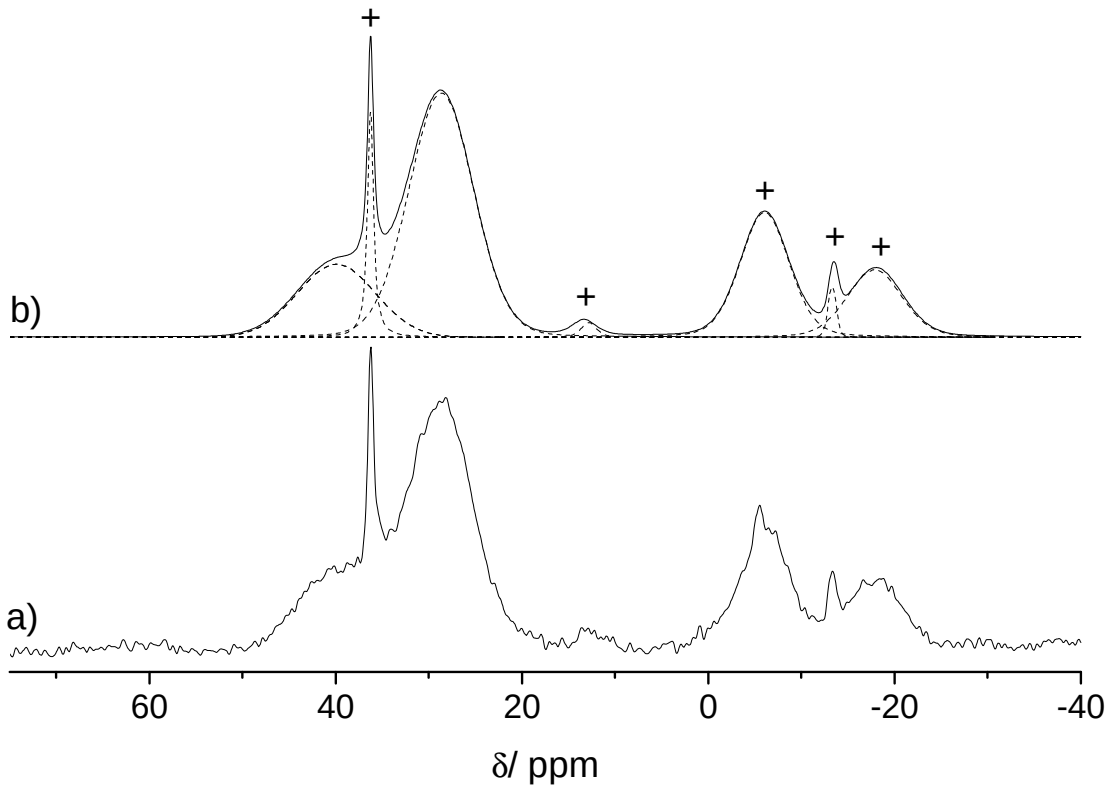


Figure S3: $^{31}P\{^{1}H\}$ MAS NMR spectrum of **4a** (a) and corresponding line shape simulation (straight line) with peak deconvolution (dashed lines) (b). The spectrum was acquired at 9.4 T with a spinning frequency of 14 kHz under TPPM-15 ^{1}H decoupling using a relaxation delay of 1000 s. For the resonances at 39.9 and 28.7 ppm an intensity ratio of approximately 1:3 is observed. + marks impurities.

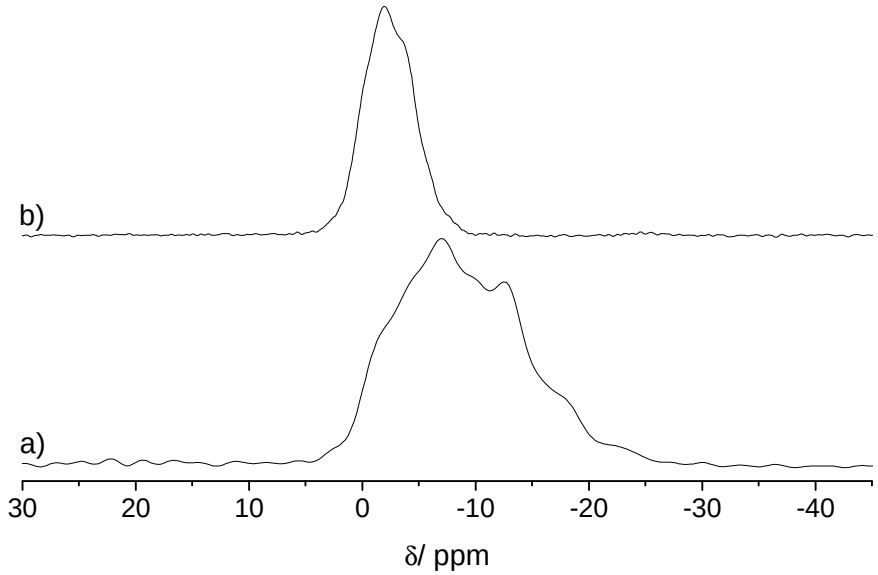


Figure S4: $^{11}B\{^{1}H\}$ MAS NMR spectra of **4a** acquired at 7.1 T (a) and 11.7 T (b) using the TPPM-15 decoupling scheme and a rotation frequency of 14 kHz.

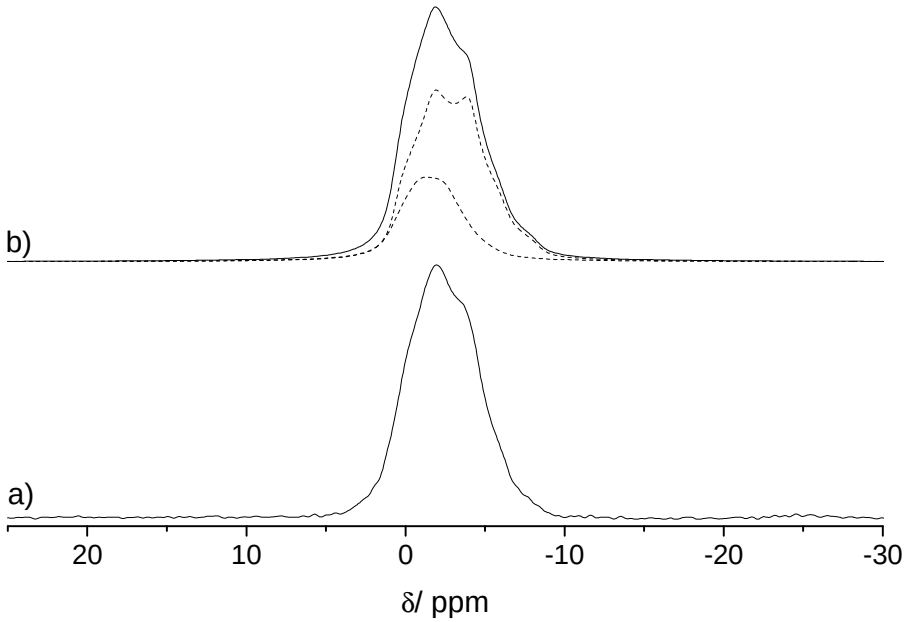


Figure S5: $^{11}B\{^{1}H\}$ MAS NMR spectrum of **4a** acquired at 11.7 T (a) using the TPPM-15 decoupling scheme and a rotation frequency of 14 kHz. Additionally, the line shape simulation (based on the fitting parameters given in Table S1) and corresponding peak deconvolution is shown (b).

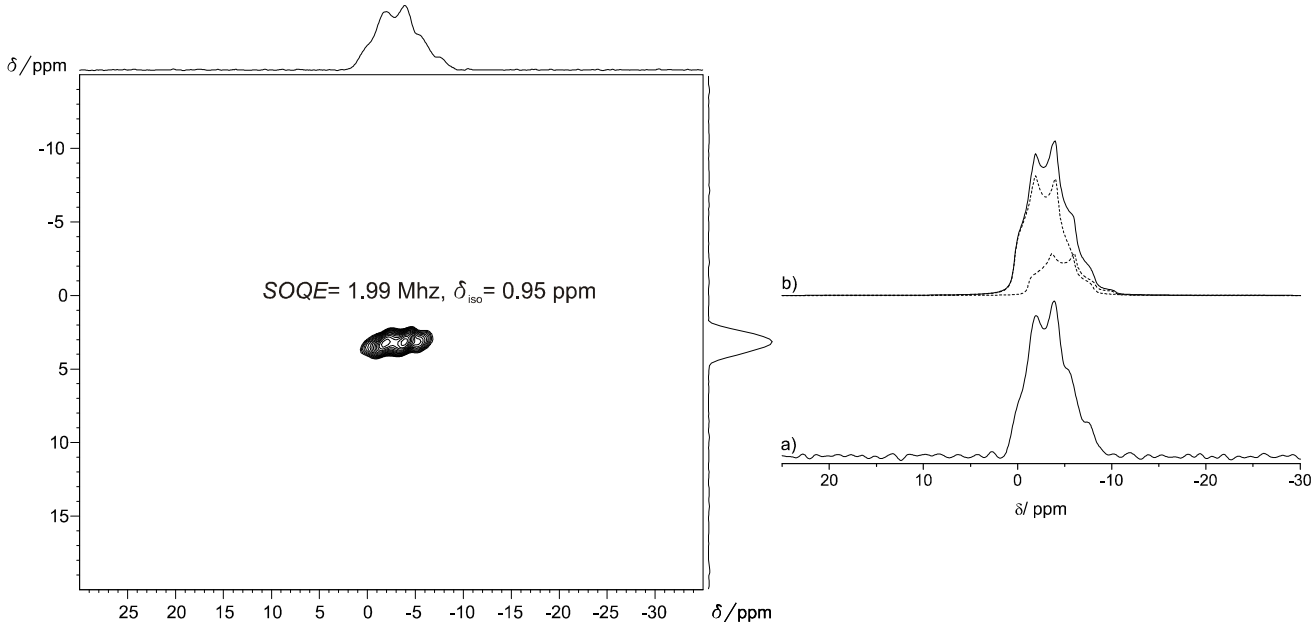


Figure S6: ^{11}B TQMAS of compound **4a** (left) and corresponding 1D slice along F2 (right, a) and line shape simulation (right, b) acquired at 11.7 T with a rotation frequency of 14 kHz. TPPM-15 ^{1}H decoupling was applied during triple quantum evolution and signal detection. The following simulation parameters were obtained: δ_{iso}= -0.8 ppm, C_Q= 1.96 MHz, η= 0.47 and δ_{iso}= 0.7 ppm, C_Q= 1.86 MHz, η= 0.46.

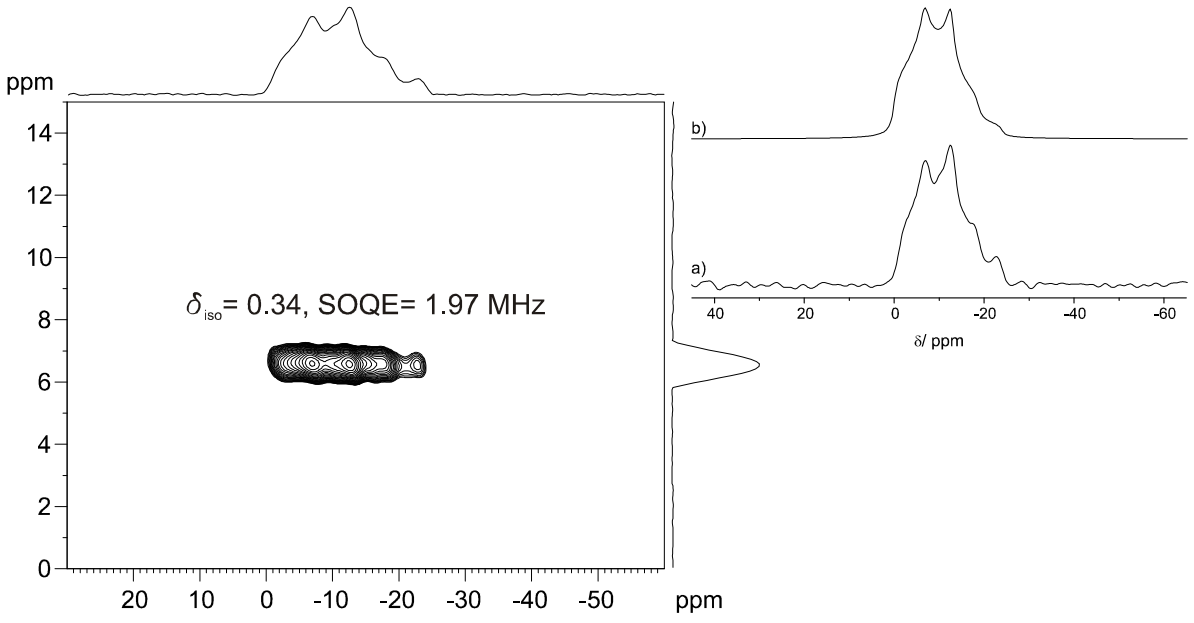


Figure S7: ^{11}B TQMAS spectrum (left) of **6** measured at 7.1 T using a rotation frequency of 14 kHz. TPPM-15 ^{1}H decoupling was applied during the triple quantum evolution and signal detection period. Additionally, the 1D spectral projection along F2 is shown on the right (a) with the corresponding peak deconvolution (b) based on the following simulation parameters: δ_{iso}= 0.9 ppm, C_Q= 1.88 MHz and η= 0.5.

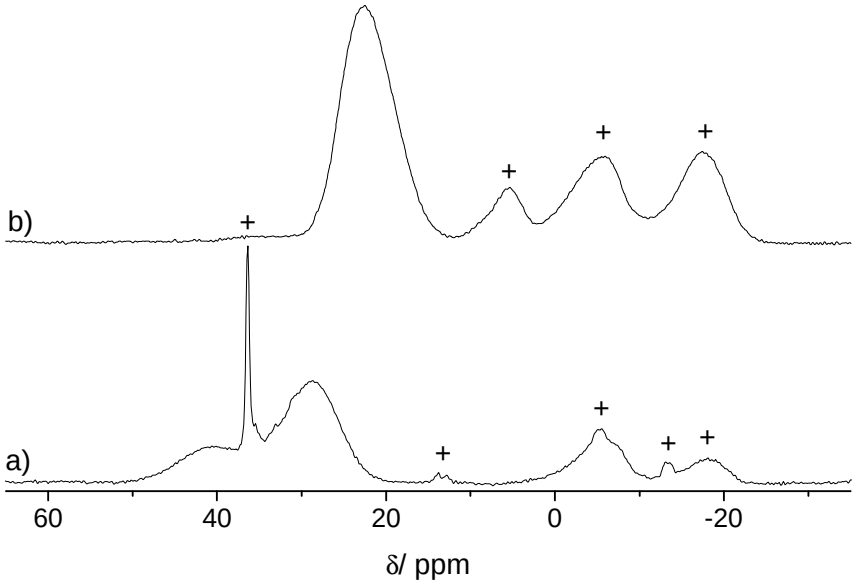


Figure S8: $^{31}P\{^{1}H\}$ CPMAS spectra of **4a** (a) and **2a** (b) acquired at 7.1 T applying the TPPM-15 decoupling scheme and a spinning frequency of 10 kHz. + marks impurities.

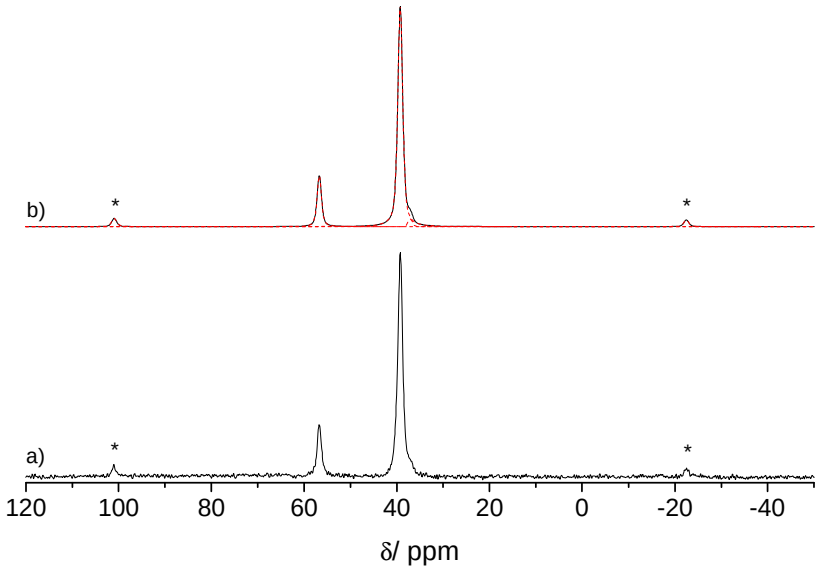


Figure S9: $^{31}P\{^{1}H\}$ MAS NMR spectrum of **6** (a) and the corresponding line shape simulation (straight black line) with peak deconvolution (dashed red lines) (b). The spectrum was acquired at 9.4 T with a spinning frequency of 10 kHz under TPPM-15 ^{1}H decoupling using a relaxation delay of 8500 s. For the resonances at 56.5 and 39.1 ppm an intensity ratio of approximately 1:5 is observed (which changed over a time period of 25 days to 1:10 due to re-equilibration processes of the conformers).

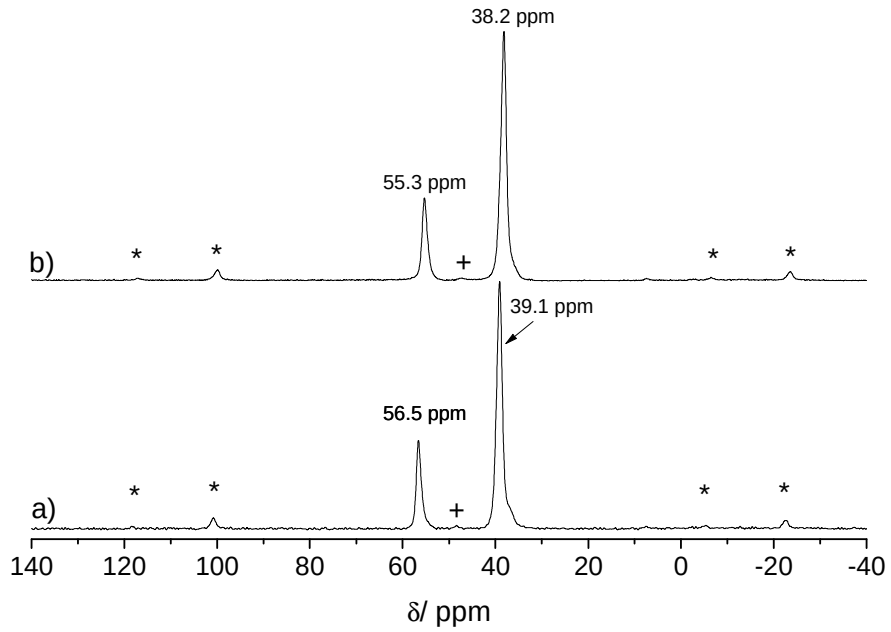


Figure S10: $^{31}P\{^{1}H\}$ CPMAS NMR spectra of **6** at r.t. (a) and at 200 K (b). The spectra were acquired at 9.4 T with a spinning frequency of 10 kHz under TPPM-15 ^{1}H decoupling using a relaxation delay of 5 s. + marks impurities. Beside the expected temperature dependence of the chemical shift values, no evidence for a fluxional behavior could be observed.

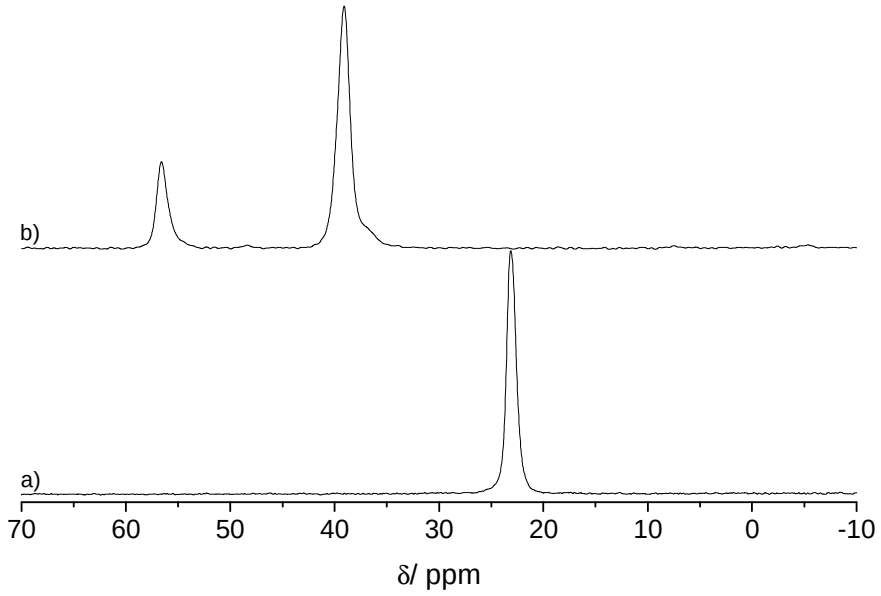


Figure S11: $^{31}P\{^{1}H\}$ CPMAS NMR spectra of the unreacted FLP **5** (a) and of **6** (b). The spectra were acquired at 9.4 T with a spinning frequency of 10 kHz under TPPM-15 ^{1}H decoupling using a relaxation delay of 5 s.

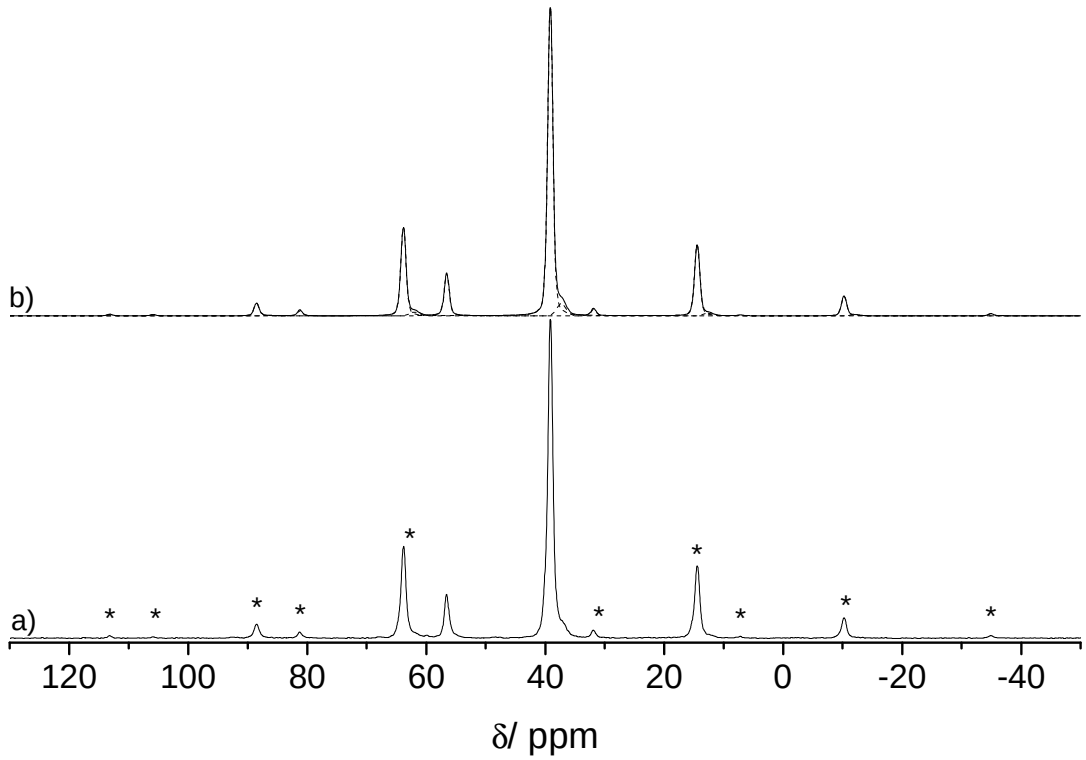


Figure S12: $^{31}P\{^{1}H\}$ CP MAS NMR spectrum of **6** (a) and the corresponding lineshape simulation (straight black line) with peak deconvolution (dashed red lines) (b). The spectrum was acquired at 9.4 T with a spinning frequency of 4 kHz under TPPM-15 ^{1}H decoupling using a relaxation delay of 5 s. The extracted CSA parameters are given in Table S2.

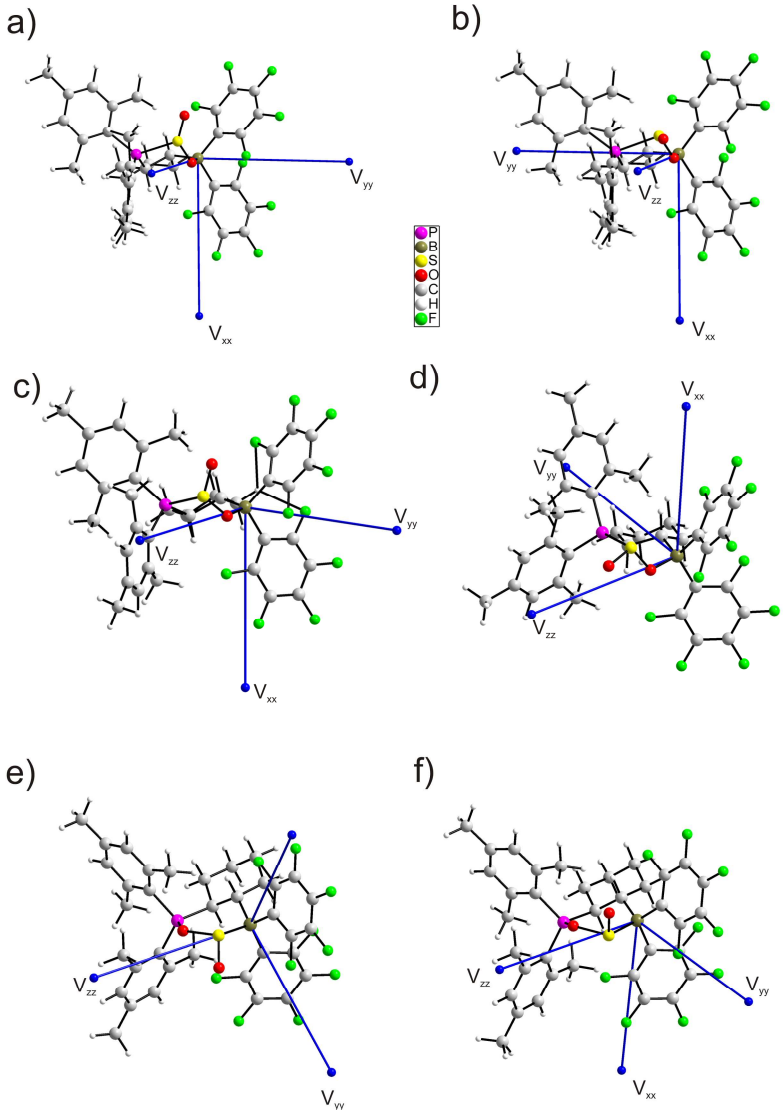


Figure S13: Calculated ^{11}B EFG tensor orientation (B97-D/def2-TZVP (mod.)) in the molecular axis frame for the B-O-(O)S-P diastereomers of **6** based on the crystal structure with the exocyclic oxygen in axial (a) and equatorial position (b) and for the B-O-(O)S-P diastereomers based on the geometry-optimized structures with the exocyclic oxygen in axial (c) and equatorial position (d) and for the B-S(O)-O-P diastereomers based on the geometry-optimized structures with the exocyclic oxygen in axial (e) and equatorial position (f). The largest principal component, V_{zz}, points along the B···O bond vector in case of B-O-(O)S-P diastereomers and along the B···S bond vector in case of B-S(O)-O-P diastereomers.

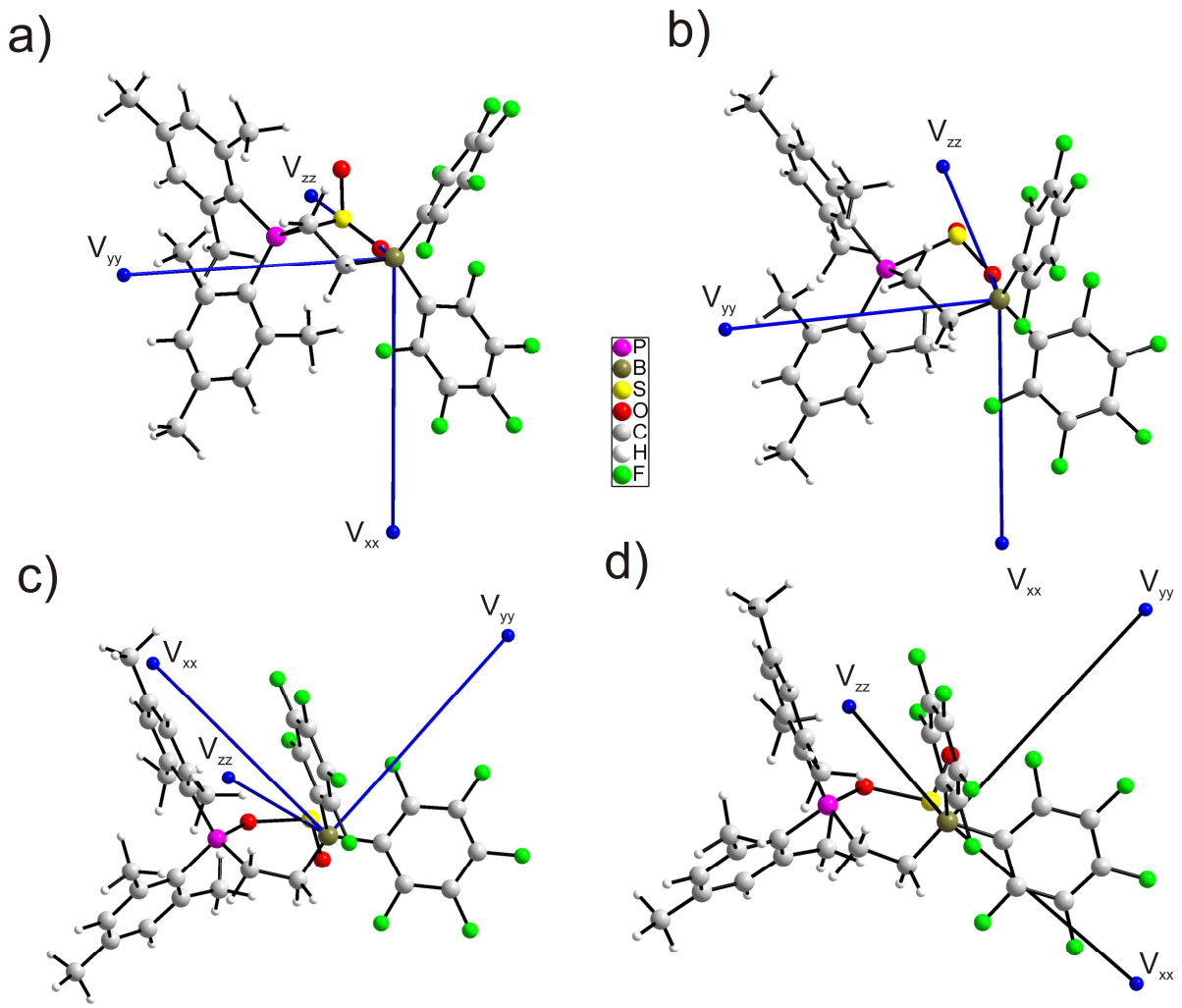


Figure S14: Calculated ^{11}B EFG tensor orientation (B97-D/def2-TZVP (mod.)) in the molecular axis frame for the B-O-(O)S-P confomers of **4a** based on the geometry-optimized structures with the exocyclic oxygen in axial (a) and equatorial position (b) and for the B-S(O)-O-P conformers based on the geometry-optimized structures with the exocyclic oxygen in axial (c) and equatorial position (d). The largest principal component, V_{zz}, points along the B···O bond vector in case of B-O-(O)S-P diastereomers and along the B···S bond vector in case of B-S(O)-O-P diastereomers.

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DFT-calculations for the reactions of the FLPs 2 and 5 with SO_2:

All calculations have been performed with the TURBOMOLE 6.3 suite of programs[1]. The structures have been fully optimized starting from the X-ray structure wherever available applying the meta-GGA functional TPSS[2] together the D3-dispersion correction with Becke-Johnson damping (denoted as (BJ))[3,4]. For the pre-optimization, the large Gaussian-AO basis set def2-TZVP[5] and the resolution of the identity (RI) approximation[6,7] have been used, for the final optimization the even larger basis set def2-QZVPP[5] was used. Subsequent single point calculations have been carried out at the more sophisticated B2PLYP-D3(BJ) level[8], but only with the def2-TZVP basis set due to the size of the systems under consideration. In all calculations the numerical quadrature grid *m4* has been used for the integration of the exchange-correlation contribution. The final level of theory can therefore be abbreviated as B2PLYP-D3(BJ)/def2-TZVP//TPSS-D3(BJ)/def2-QZVPP and provides an estimated accuracy of 1 kcal/mol.

The thermodynamic corrections are based on harmonic vibrational frequencies calculated at the PM6-D3H level[9,11] with the MOPAC suite of programms[10]. Low-lying frequencies (effectively those below 100 cm^{-1}) are treated in a quasi-free-rotor approximation in order to avoid errors in the entropy calculation (see ref.[11]). Enthalpies are denoted as ΔH, free enthalpies as ΔG, electronic energies as ΔE (i.e., not including ZPVE).

The frequencies for the thermodynamic corrections were also calculated on PBE-D3(BJ)/SVP level which yielded comparable enthalpic corrections, but due to numerical problems with artificial imaginary modes, the corresponding free enthalpy values are not sufficiently reliable and could not be used.

All (free) solvation enthalpies have been calculated with the COSMO-RS program[12-16] (solvent bromobenzene, at 298 K) and applying the gas phase optimized structures. For a thorough discussion of this procedure and the performance of current solvation models in general see ref. 11 and 17.

All energy or enthalpy values are given in kcal/mol and are to be understood as reaction energies for the formation of products **4** and **6** respectively, and their various isomers. The considered isomers differ in the orientation of the exocyclic O-atom (axial or equatorial), but also in the orientation in which SO_2 has added to the FLPs (B-SO-O-P and B-O-SO-P).

In addition to these 6-membered-ring structures, we also investigated the 5-membered-ring product which results from activation of the SO_2-sulfur by both, the boron and the phosphorus of the FLP. The corresponding energies can be found in the following tables. As these structures are considerably less stabilized they were not observed in the experiment.

Tab. 1: Electronic reaction energies for the formation of **4.**

Product	TPSS-D3(BJ)/ def2-TZVP	TPSS-D3(BJ)/ def2-QZVPP	B2PLYP-D3(BJ)/ def2-TZVP
5-ring	-7.14	-6.13	-3.37
6-B-O-SO-P, $O_{exocycl.}$ Eq	-17.35	-16.70	-14.72
6-B-O-SO-P, $O_{exocycl.}$ Ax	-17.18	-16.44	-14.92
6-B-SO-O-P, $O_{exocycl.}$ Eq	-14.89	-14.07	-13.51
6-B-SO-O-P, $O_{exocycl.}$ Ax	-17.76	-16.92	-17.12

Tab. 2: Thermodynamic corrections and reaction enthalpies and free enthalpies for the formation of **4** (gas phase, at 298 K).

product	correction to		B2PLYP-D3(BJ)	
	ΔH	ΔG	ΔH	ΔG
5-ring	1.63	15.73	-1.74	12.36
6-B-O-SO-P, $O_{exocycl.}$ Eq	1.00	13.52	-13.72	-1.20
6-B-O-SO-P, $O_{exocycl.}$ Ax	1.12	14.19	-13.80	-0.73
6-B-SO-O-P, $O_{exocycl.}$ Eq	1.55	15.59	-11.96	2.08
6-B-SO-O-P, $O_{exocycl.}$ Ax	1.45	14.98	-15.67	-2.14

Tab. 3: Thermodynamic corrections and reaction enthalpies and free enthalpies for the formation of **4** (in bromobenzene, at 298 K).

product	correction to		B2PLYP-D3(BJ)	
	ΔH	ΔG	ΔH	ΔG
5-ring	-0.45	-5.62	-2.19	6.74
6-B-O-SO-P, $O_{exocycl.}$ Eq	-1.72	-6.67	-15.44	-7.87
6-B-O-SO-P, $O_{exocycl.}$ Ax	-2.10	-6.99	-15.90	-7.72
6-B-SO-O-P, $O_{exocycl.}$ Eq	-0.43	-5.67	-12.39	-3.59
6-B-SO-O-P, $O_{exocycl.}$ Ax	0.55	-4.97	-15.12	-7.11

Tab. 4: Electronic reaction energies for the formation of **6.**

product	TPSS-D3(BJ)/		B2PLYP-D3(BJ)/
	def2-TZVP	def2-QZVPP	def2-TZVP
5-ring	-12.18	-11.21	-10.08
6-B-O-SO-P, $O_{exocycl.}$ Eq	-19.53	-18.40	-16.88
6-B-O-SO-P, $O_{exocycl.}$ Ax	-19.39	-18.24	-17.10
6-B-SO-O-P, $O_{exocycl.}$ Eq	-17.96	-16.79	-17.75
6-B-SO-O-P, $O_{exocycl.}$ Ax	-17.42	-16.19	-16.95

Tab. 5: Thermodynamic corrections and reaction enthalpies and free enthalpies for the formation of **6** (gas phase, at 298 K).

product	correction to		B2PLYP-D3(BJ)	
	ΔH	ΔG	ΔH	ΔG
5-ring	1.90	16.74	-8.18	6.66
6-B-O-SO-P, $O_{exocycl.}$ Eq	1.28	15.35	-15.60	-1.53
6-B-O-SO-P, $O_{exocycl.}$ Ax	1.28	15.35	-15.82	-1.75
6-B-SO-O-P, $O_{exocycl.}$ Eq	1.75	17.20	-16.00	-0.55
6-B-SO-O-P, $O_{exocycl.}$ Ax	1.81	17.05	-15.14	0.10

Tab. 6: Thermodynamic corrections and reaction enthalpies and free enthalpies for the formation of **6** (in bromobenzene, at 298 K).

product	correction to		B2PLYP-D3(BJ)	
	ΔH	ΔG	ΔH	ΔG
5-ring	1.69	-4.20	-6.49	2.46
6-B-O-SO-P, $O_{exocycl.}$ Eq	1.14	-4.64	-14.46	-6.17
6-B-O-SO-P, $O_{exocycl.}$ Ax	0.86	-4.93	-14.49	-6.68
6-B-SO-O-P, $O_{exocycl.}$ Eq	1.33	-4.56	-14.67	-5.11
6-B-SO-O-P, $O_{exocycl.}$ Ax	1.18	-4.58	-13.96	-4.48

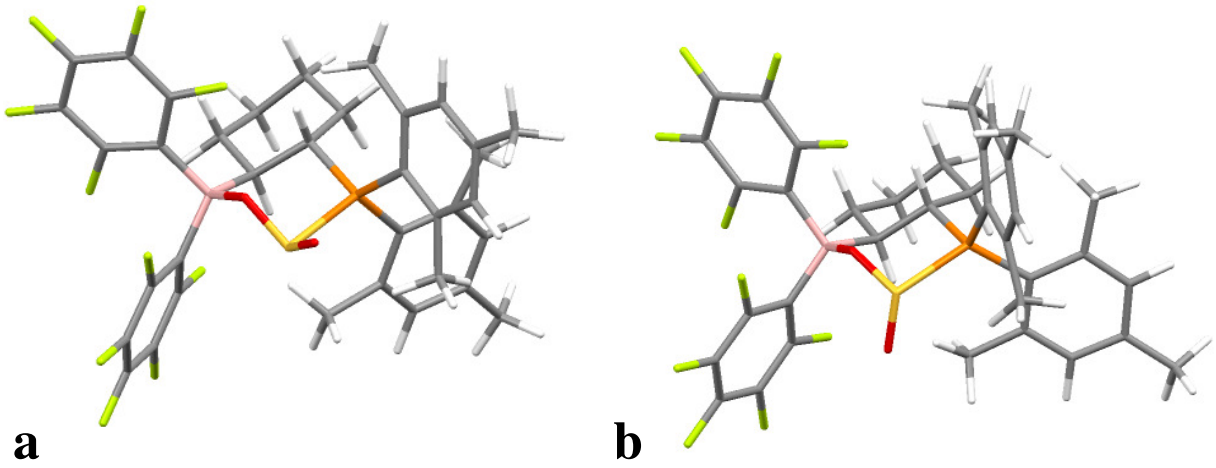

Fig. 1: The two different P-SO-O-B-isomers of compound **6** (colour code: C grey, P orange, B purple, S yellow, O red, F green; H white).

Additional structures in the investigation of the S-atom inversion in the P-SO-OB unit

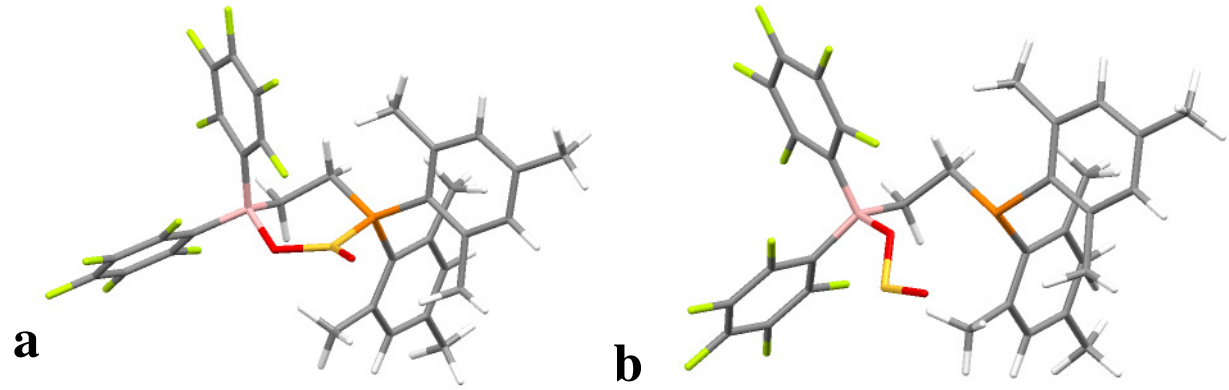

Fig.2 a) True transition state for the S-atom inversion. The corresponding (imaginary) vibrational transition mode has a frequency of 557 cm^{-1} and the electronic inversion barrier is +51.8 kcal/mol. b) The observed inversion process might occur by a mixed rotation/inversion geometric change but a corresponding TS has not been found. As a more realistic model we investigated a structure with broken P-S bond which is a true minimum. Its electronic energy relative to **4**-B-O-SO-P, O_{ax}. is +21.6 kcal/mol which is a good estimate for the P-S interaction energy. Both values are electronic energies calculated on TPSS-D3/def2-TZVP-level..

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Optimized Cartesian Coordinates (TPSS-D3(BJ)/def2-QZVPP, gas phase) in bohr

Isomers of compound 4a

B-O-SO-P, $O_{exocycl.}$ equatorial

-9.78872476461940	5.59364993764390	-5.89167886883913	f
6.15563045685360	-10.24590090492003	-4.50871875266618	h
6.69439910292723	-1.49238263687179	-5.52543867645706	h

6.75650514469989	-5.70369155991775	-4.59003703370741	h
4.39039471088763	0.59057719368676	-4.30664004528781	h
3.75755488396571	-11.60156932482832	-2.59674832220263	h
5.78163171424546	-0.84600100047744	-3.79207381841216	c
0.39460325288970	1.28481801936631	-3.92479997310183	h
5.31264661753345	-10.24282445769597	-2.62493297723613	c
-7.67713715158856	1.26008675139517	-4.36307047899347	f
5.37318754871751	-5.49004512590575	-3.08688894032586	c
2.90277964534486	4.55890150342208	-3.84230396918140	h
-9.54028692886342	9.82918302908211	-2.91493729793080	f
-8.58058581388398	5.50978510782937	-3.65503435865872	c
-3.69879901875944	-0.50696769472103	-3.81705747866727	h
4.09262643779982	7.56142093327320	-3.02424325008096	h
6.74637301066404	-10.91576330621307	-1.29078130297176	h
7.20758946965782	0.08481074248984	-2.61970920236776	h
4.41500153794776	-7.63987447195547	-1.89753991135318	c
4.60358834926564	-3.05405487691734	-2.42514430513032	c
-7.44206038201315	3.29525930749202	-2.81595951753754	c
-8.46740785664779	7.66146657660808	-2.14805853275949	c
3.20001587249477	5.86260014660915	-2.27056044659797	c
-0.54009917588075	1.33003277944747	-2.08528730327372	c
-1.13508029979812	3.27566283488557	-1.72228586399353	h
-5.98662143886674	-4.64602699291350	-2.68204727212406	f
-2.81603077805914	-0.50134033101171	-1.95279093210532	c
1.34384418873710	6.40534676914912	-1.54325457429274	h
-2.11931748245225	-2.42949181779209	-1.68842181568727	h
-9.83766645454287	-7.75146845983066	-1.73891233698275	f
2.62483992495198	-7.31146899725854	0.01300499564202	c
2.78155195773040	-2.78187534999404	-0.48961857404264	c
-6.14982058055811	3.05407007834500	-0.52054402297654	c
-7.23756828650124	7.52627345339350	0.16746564160360	c
4.84537278662367	4.74219022805898	-0.22698127640246	c
1.84520275921307	-8.95864645382380	0.95871497227092	h
7.34371542119157	7.90256733063278	-0.47289728788854	h

-7.57569456209146	-3.97815905164272	-0.78181581141437	c
1.68627345212015	0.36029597784517	0.37685916049245	p
-4.91450799158657	0.27674047053158	0.15834797076367	b
1.78676958026254	-4.92442090648325	0.75384152530763	c
-9.57117933390025	-5.63963625119704	-0.34201946793764	c
-6.13582737191984	5.25690409617038	0.92949811887742	c
-7.12957710348592	9.58415743188568	1.65982307575671	f
6.97855684366403	6.12257782388926	0.48364204644983	c
4.36437389147731	2.41067242315743	0.99652556402522	c
-7.19082106305901	-1.76370224266258	0.59434998159771	c
11.56664556484392	8.02828222070382	1.53410028892989	h
-1.98236843698152	-4.10758265809904	2.10455223851563	h
-11.30064324677636	-5.11082249035671	1.56227621796049	c
-5.04005960425058	5.31344144379755	3.25010371915195	f
6.12253211627194	-2.51120362750020	3.24841198300101	h
-0.14750923005255	-4.72109349628794	2.82997541593522	c
8.64247799127712	5.30798555644374	2.35983470467125	c
-13.23248928313185	-6.69222374362604	2.01751634793264	f
6.01074644546115	1.56500405126558	2.93792525886580	c
-0.41437561533068	-6.54953819404855	3.74632361583498	h
-3.57424809893762	0.27674818998929	2.83695055106838	o
-8.98908202084851	-1.31835523079564	2.48042201402766	c
-1.13785182995564	1.69855270744415	3.63603671901970	s
10.89033946556299	6.88370130538962	3.11358340599272	c
8.11504786573668	3.02307672655549	3.56192784691418	c
-11.00739341888890	-2.92241213068012	2.99192153977177	c
5.57957666880249	-0.86205408456106	4.37033843297859	c
12.44320221326366	5.70059093300676	3.78563312725240	h
0.40817314208593	-3.36029397723927	4.28334672154858	h
-8.81821071471558	0.78710476178245	3.92145889189948	f
3.59748015611774	-1.08245070042560	4.91436977964810	h
9.36127396863209	2.35223864347121	5.04980864968867	h
10.38259079415654	8.17710755254428	4.64923413326186	h
6.69742273998687	-0.86371910217073	6.10402226808687	h

-12.67510278096953	-2.38803218378557	4.83625515755749	f
-0.34333257414824	0.74343479592669	6.10745491728579	o

B-O-SO-P, $O_{exocycl.}$ axial

-7.86932712373731	-3.50928161916066	3.20074756192456	c
-8.20045713722103	-5.65883265899528	1.72258603160882	c
-6.67397964226805	-6.00662092032173	-0.38475938486948	c
-4.83602488457792	-4.21287567650311	-0.97074440935341	c
-4.40747404585586	-2.03436985362933	0.45486274732168	c
-6.01720731006332	-1.76560272308555	2.53692154569275	c
-3.45378373776579	-4.71926538228846	-3.07169883065914	f
-6.97943128222216	-8.07598873951411	-1.83700102863784	f
-2.28467670360961	0.14432963354089	-0.15236118870141	b
-0.82644092686089	0.35688997744862	2.46944480824510	o
1.74360741430915	1.47477318494989	3.27055715296064	s
2.16064575118431	4.11261567654319	2.48157289753809	o
-9.97507883844014	-7.37134961545799	2.32195565275539	f
-5.82583338603612	0.29725347644664	4.03176260759127	f
-9.34500376350528	-3.14268482550930	5.24032681839392	f
-0.22618386566482	-0.67857744991761	-2.28436904911902	c
2.13703835081976	1.03657246114946	-2.47811150372568	c
4.33697999903224	-0.06036648221152	-0.05328248455822	p
7.22135417595789	1.70098785563426	0.48188458239382	c
7.90133834219757	3.94209159999376	-0.81131846219857	c
10.20483398270866	5.08399437672309	-0.22418548301109	c
11.84191865744019	4.13007084255144	1.60994154119123	c
11.10167402221231	1.96043756499238	2.90927714885584	c
8.82543795320735	0.73464493149278	2.39965187581853	c
6.27427355982438	5.21020808179664	-2.77707155942874	c
14.28537568981523	5.45368744349450	2.22823237813017	c
8.16863542251058	-1.56606689875549	3.95236466165459	c
5.12219049718223	-3.32189369198715	-0.80320599491156	c
6.86381695084337	-3.81013088557319	-2.77212215045014	c
7.41602453625300	-6.31989909214044	-3.37358395333418	c

6.32239974406195	-8.34719785391617	-2.09214053763554	c
4.61939429807610	-7.81241525859580	-0.14911186061987	c
3.99287103724872	-5.34403028115779	0.53035581944659	c
6.98063048912337	-11.03648729365130	-2.75770096817728	c
8.18050990801495	-1.75498863119666	-4.24810698610343	c
2.12309547775184	-4.95287643021913	2.64102294444389	c
-3.72715022174362	2.80931596561691	-0.81894692959856	c
-4.95338046878714	3.03167180354184	-3.15164014806063	c
-6.26865450990726	5.16324682459777	-3.94524463826096	c
-6.43346933395808	7.23649306989113	-2.33911343171026	c
-5.30261332017804	7.10301124085969	0.02606198943851	c
-4.00837572378145	4.92165026718915	0.74571893060216	c
-7.39098044142752	5.23459859793439	-6.22942227080629	f
-4.95625430935386	1.04987682025560	-4.79012637141886	f
-7.68894980875887	9.32392113735887	-3.05476260482703	f
-5.48624850314246	9.08047529365863	1.61703643440015	f
-3.06731815619481	4.96053181188964	3.11599970372963	f
7.78921984202967	-11.16296132219211	-4.65208622222725	h
8.95368773999104	-2.52748037567890	-5.99760012902245	h
8.73313968192431	-6.69061359845882	-4.90523642651262	h
6.90963580392000	-0.20628293369708	-4.74737266352954	h
5.31435584422213	-12.25372697310832	-2.67021750502873	h
3.03288605543338	0.91142887666044	-4.33296835296300	h
5.81078234354256	3.94942132261275	-4.34487671707180	h
-1.12571475425794	-0.67419531135838	-4.13799727915250	h
7.26802727767456	6.83985991026922	-3.55659528977266	h
8.37193302511831	-11.79546583459296	-1.42487675714020	h
9.73627116767052	-0.93509171580663	-3.16117320288441	h
1.69048647030802	3.01270502552291	-2.09402196702376	h
4.50532664640242	5.87686738910792	-1.94742191872802	h
0.39584913660810	-2.63217716637265	-2.01265539648025	h
3.73384937986889	-9.36029638826860	0.86845219779197	h
10.72573604822819	6.79173343027360	-1.23834468279078	h
15.03311967829184	6.45193349678295	0.58305780189427	h

0.32111422575923	-4.22545624215234	1.94206697075017	h
8.49166217960940	-3.31792107249647	2.90488701937382	h
1.75565706881015	-6.73663749453006	3.60861298292781	h
15.71232683796190	4.11973036526286	2.89690964225606	h
2.81439118798066	-3.60404531071081	4.04736479462030	h
6.18483839070028	-1.55494714659702	4.53818001534911	h
12.31467381202312	1.20041995022928	4.38192465950063	h
13.98948844366321	6.85373760722089	3.72542061767487	h
9.32127638280211	-1.61399580268505	5.66230049622886	h

B-SO-O-P, $O_{exocycl.}$ equatorial

1.15894524011141	-3.76368404264613	0.95114499758943	c
2.25584710831275	-1.95496017141073	-0.62683171845982	c
3.27504287296330	-2.92901056752279	-2.86414277118330	c
3.24959186982581	-5.47585947156601	-3.51588953037853	c
2.13752852247285	-7.20198397843237	-1.87079262722869	c
1.08635630946186	-6.33486875839038	0.37389466856580	c
2.47350134787535	1.08272621893583	-0.20039016957515	b
0.77404718980347	2.66669227740443	-2.26762312690409	c
-1.74439904028239	1.34909196814869	-2.92726802783463	c
-3.83922990203402	1.20708167299707	-0.19974431959424	p
-5.37419166415291	-1.81331712494756	0.37172458161241	c
-5.17511161649519	-3.99821172889594	-1.17568437991612	c
-6.26121201222424	-6.24887820595308	-0.32641458385497	c
-7.54078320573488	-6.44772985798098	1.96582021375796	c
-7.77385168069342	-4.26896823995995	3.42278613898607	c
-6.71716042651441	-1.96634075712171	2.69626036622494	c
-3.88463446107356	-4.16015053178376	-3.72039315242479	c
-8.59222643730458	-8.93882300694385	2.85031038878947	c
-7.03472690833523	0.21487307528248	4.51144722715605	c
4.38052819763527	-1.33357402024308	-4.54181375009557	f
4.26295254728880	-6.28410424762806	-5.70423637894900	f
2.05712039365531	-9.66921148863281	-2.46137882280291	f
-0.01029964585890	-7.98705056631209	1.96643727842471	f

0.10427372061789	-3.10187732281726	3.16913291745234	f
5.40306700596813	2.02370370081447	0.11068365752903	c
6.40127288011679	4.26277844319369	-0.88092234624574	c
8.90581793050146	5.00815401896347	-0.57295111334234	c
10.54687972533914	3.49378812530478	0.81164399366043	c
9.64652558058185	1.26280068279247	1.87434005114799	c
7.12959583307698	0.59297016809123	1.52542718938706	c
11.21121437599372	-0.20625849723342	3.23393384950458	f
12.96444927671387	4.18309647305002	1.13272008381666	f
9.75198217967623	7.17748060489831	-1.59605377275193	f
4.93378446109027	5.86445344967335	-2.24076303834401	f
6.38013582173563	-1.57439026035719	2.64495271220464	f
1.14475486981589	2.61273482386076	2.87438211140454	s
-2.30624182009203	1.73833574815893	2.25754614530531	o
1.69299843506721	1.40050925885747	5.32244178215974	o
-6.19229183703304	3.68739356507563	-0.62995683271618	c
-8.14882682274399	3.28607260750431	-2.41392623273185	c
-9.96885741310953	5.15740142519896	-2.78570218554812	c
-9.92971144025959	7.42867630042893	-1.45469605071802	c
-7.96555621810737	7.80740820646134	0.25999388166248	c
-6.08646559222786	6.00826800191784	0.71458703591459	c
-8.37955956412668	0.91140543910908	-3.97583481342724	c
-11.94680597598232	9.40141761237292	-1.83589529193107	c
-4.08294603938768	6.71684134924389	2.62158123923645	c
-12.88805986288190	9.16905618712710	-3.65801108650663	h
-9.74234294217038	1.20081559377393	-5.49679328038440	h
-11.44823696134800	4.82196284211430	-4.17013728824144	h
-6.58347104423280	0.38288924323583	-4.84813301696274	h
-11.15580875821240	11.30689263501480	-1.74003922615253	h
-2.77661811284864	2.36223165127409	-4.40563402308100	h
-4.41150135549571	-2.63051258428650	-4.99741087685398	h
1.82074894281987	2.84529376507148	-4.03830723610008	h
-4.40933652374004	-5.93568663830964	-4.62820067006960	h
-13.39033913607908	9.25595755010989	-0.35827409621400	h

-9.00640886265785	-0.69452698120021	-2.83869140843927	h
-1.34611683578600	-0.54467952962920	-3.60099587114914	h
-1.82671626219031	-4.15759962655377	-3.53378366998274	h
0.40759790217365	4.60997693780697	-1.64432769273804	h
-7.86645941460693	9.58098845991353	1.29013976683001	h
-6.09067435681760	-7.91055154618392	-1.51981987010695	h
-9.14953825213064	-10.12775959435063	1.25688730191749	h
-2.17625351573567	6.58686578815182	1.84435115305166	h
-7.40752258444791	2.00140261839553	3.55007110015119	h
-4.39390126628228	8.66069821653855	3.23695699878347	h
-10.22691265872850	-8.66955035693800	4.08210415347016	h
-4.13224898388395	5.49027932471314	4.27991632269962	h
-5.32912082945583	0.46225110274485	5.64806670827844	h
-8.79576891507142	-4.34895176014969	5.20200920445298	h
-7.15833923618109	-9.97352938648943	3.92811786650208	h
-8.61630621793585	-0.17014441885614	5.77920250231095	h

B-SO-O-P, $O_{exocycl.}$ axial

-6.24430196303709	7.53212193153573	-4.73433220152699	f
9.46080804839918	-9.38931740885018	-4.56608775197190	h
6.64259132996227	-1.20418543384499	-5.86230727476070	h
8.23166297936733	-4.95133728930931	-4.81367131416307	h
3.57633716006821	-0.28042795328608	-4.96535020052836	h
7.79393738021839	-11.49373878008821	-2.55540267323776	h
5.40719457633432	-0.90265207482087	-4.23859179898118	c
-0.23658294266278	-2.14892421696242	-4.22639597139679	h
8.67781424210254	-9.63077420311800	-2.67164387441019	c
-6.81116912073982	2.54858176527479	-3.87828907115174	f
6.86280264204594	-5.25844513116743	-3.31384788796337	c
1.81238678663933	2.97183810487303	-4.82249750641443	h
-3.59933116069623	10.46823026743180	-1.39076921040977	f
-5.24433114933308	6.48773452610594	-2.64336726255504	c
-4.84031349776764	-1.94423992558871	-3.63350884631417	h
1.95409436195747	6.24713581545467	-4.26633507006732	h

10.25583208330011	-9.60995880462781	-1.33070594418612	h
6.18309376787280	0.64388469341026	-3.11115241245537	h
6.81620737118975	-7.56803991156339	-2.05123102759179	c
5.18705416033294	-3.30990977870743	-2.72639588434508	c
-5.49565799341015	3.91516043283991	-2.15622598052698	c
-3.90609837963710	7.98884877988684	-0.94543261377216	c
1.41323565997782	4.44063746562090	-3.43239413111306	c
-1.06263524074188	-0.99881638026790	-2.71920829883781	c
-1.25891027878219	0.91920149872542	-3.41439419136548	h
-8.47443960317373	-4.20902593612686	-2.15622816066166	f
-3.69006210863333	-1.99517114268391	-1.92092899602231	c
-0.62806051449350	4.49565874556801	-3.12821267655144	h
-3.57592885181029	-3.98193000316468	-1.35895260570010	h
-13.35551633284715	-4.83394209979731	-1.09737096667316	f
4.99389280786970	-7.89993727450470	-0.17842463566856	c
3.37539334101202	-3.66911243991647	-0.78542387248360	c
-4.49318863309785	2.70848115909567	-0.02834101225362	c
-2.87245371675178	6.88589137032906	1.20306951899636	c
2.83631108907709	4.08110866046816	-0.98225718057048	c
4.88741465700348	-9.69995894043474	0.80366497613420	h
4.00128207464441	7.93332119517541	-1.23294213867751	h
-9.47711283289256	-2.67644080299136	-0.37188708563940	c
1.20787190249822	-1.07392897284374	-0.13189347278595	p
-5.01354486263279	-0.32219180825038	0.30059364306945	b
3.25835358056597	-6.02600433584237	0.49663534164317	c
-12.03107958846403	-3.05194657157327	0.14252456991620	c
-3.19241504583722	4.30544959283742	1.61328021667216	c
-1.57495087670342	8.31771676147734	2.85603022823625	f
4.12833987200491	6.21440841188547	-0.11781120307985	c
2.96960617846618	1.82152883407522	0.46337034040621	c
-8.00421103341860	-0.84369922104293	0.83051118814181	c
7.41358067509672	9.79665828897264	1.42544666407517	h
-0.56569448626761	-6.46845666855780	1.94767040512589	h
-13.22845619962161	-1.57079870111333	1.95373260422482	c

-2.17728533452889	3.38271838102708	3.77660436260998	f
5.00302309063451	-2.24908748649299	3.33276254699919	h
1.39152726038267	-6.70339915339101	2.54531950756110	c
5.55595664268000	6.22814216593056	2.09359701469290	c
-15.68719585228246	-1.91457714819799	2.47185970239569	f
4.46998739418595	1.78238756191467	2.69642969425291	c
1.67184144863010	-8.67448340666714	3.08429541290295	h
-3.54549729980363	-1.72557222299202	3.45488909898550	s
-9.29766287355849	0.56648582163991	2.65547265971432	c
-0.17347834911878	-1.63124363510668	2.42700040615005	o
6.83092529754230	8.60195881843734	3.00556014410184	c
5.72685198084119	3.97599576974614	3.44282900610228	c
-11.84267703182215	0.26162794149989	3.23157228082430	c
4.77599933663297	-0.49476067113552	4.39303588201526	c
8.48815411092154	8.16976548872914	4.15803690305885	h
1.63616653112292	-5.53139293151386	4.22548993984996	h
-8.03105485421597	2.33803892995797	4.01658340575836	f
3.13063595371856	-0.71767491299086	5.61916360471389	h
6.86396885614959	3.90749225365197	5.15117140307538	h
5.52477083715258	9.70701354056146	4.17228479147384	h
6.44474810216338	-0.24512971893376	5.57999809525861	h
-12.96541534172836	1.69041882122034	5.01064496158412	f
-4.26494222025333	-4.43501029689168	3.37908188609100	o

5-membered ring compound

-12.82325704098385	5.02723977499386	-2.55174009168480	f
5.82371000654932	-10.29355287767845	-5.73257390174315	h
6.84577021532733	-1.29629805793798	-5.91016161765251	h
6.98462423947474	-5.47363393174571	-5.26123885717202	h
4.30588129432788	0.59730847690657	-4.87182399930274	h
4.52031140131240	-11.77179719213790	-3.02164942530003	h
5.73223748531624	-0.76293005706171	-4.25779450533927	c
0.19496887864891	0.51516242084456	-4.70965554573205	h
5.68372170708432	-10.19729902205678	-3.67273471998323	c

-10.12150737471247	1.00336368293231	-1.32239699186208	f
5.50414975488340	-5.42990406481298	-3.83801992610967	c
3.02004423633768	4.20330980685198	-4.24578167325515	h
-10.61452519206967	9.69849308857203	-2.93125694986562	f
-10.34754518309123	5.30935241384361	-2.05524002274823	c
-4.29748330401380	-0.34055924966902	-4.10804978275000	h
4.44532252753140	7.11708141216408	-3.48006236480074	h
7.59229308956848	-10.45782069985098	-2.91423560902769	h
6.97200474798676	0.21933330255018	-2.92885555885549	h
4.60231610766356	-7.69953609129524	-2.83547600495116	c
4.57544150370252	-3.08508658200504	-3.07747007958126	c
-8.87759080889629	3.23967234326097	-1.36504702392407	c
-9.23763321888194	7.68020743054788	-2.26090942110453	c
3.33234567774459	5.55625304104670	-2.71953789010328	c
-0.65485223006755	1.05669695201022	-2.90865459410912	c
-0.94295280734501	3.08930051981230	-2.87946230726673	h
-6.39465453565366	-4.60281655319624	-1.36601804893925	f
-3.14742989976061	-0.39953679511184	-2.38734054205598	c
1.49515099603635	6.30921836465731	-2.15407950845295	h
-2.68917215172569	-2.39370195633447	-2.10271225576588	h
-9.20021847567399	-7.55767296566236	1.61335017844064	f
2.70021257605534	-7.57029121980778	-1.02419241235108	c
2.63037193029489	-3.00509684629735	-1.22831171911629	c
-6.28442600544918	3.36419461428012	-0.80913327493528	c
-6.66323383413580	7.90636400042696	-1.80497142647360	c
4.68409272082633	4.40256586275146	-0.49407760201058	c
1.96034937205588	-9.30649583959497	-0.21512456242300	h
7.27608982211664	7.49631797680061	-0.40396711344677	h
-7.16116863887954	-3.61649034222531	0.87795108593887	c
1.39400746359962	0.09183656559501	-0.30170422064619	p
-4.80237271905084	0.75677516871509	-0.08207342327730	b
1.68654516972016	-5.27399053357942	-0.19337588039848	c
-8.64607832052604	-5.19298572220130	2.37175714699918	c
-5.26640278043626	5.78109316355963	-1.12885582230300	c

-5.52790629244993	10.16869200610000	-2.04905059237590	f
6.73657622099567	5.73180728670968	0.49752535586495	c
3.99161014221856	2.09288734164899	0.65599156251713	c
-6.52549622663047	-1.15123222166872	1.55523320209373	c
11.09955970833671	7.62502338525190	2.20289675485812	h
-2.23846319138339	-5.48388629134963	0.82072198692643	h
-9.58384361689406	-4.30351845455333	4.65976492784395	c
-2.75991277482170	6.20521683707373	-0.81943536355989	f
5.14545604626781	-2.85474271923763	3.12866836936590	h
-0.39188141427771	-5.37704895455878	1.74306941444821	c
8.09850716897179	4.89009001973056	2.59075732119290	c
-11.01588346203353	-5.79774253252876	6.12344049873409	f
5.31780682200717	1.22160516808384	2.81616442722913	c
-0.19379540319436	-7.06918063848374	2.90876428677074	h
-7.54657226768736	-0.34221723257381	3.85386427029857	c
-1.85555379744752	1.30427448539875	2.63934689554806	s
10.25812631430865	6.41438302399004	3.64779570770725	c
7.34962428925171	2.62918893624909	3.72213327273983	c
-9.03363943366910	-1.84170177641938	5.40934024424903	c
4.59665055163734	-1.16934403486029	4.19364067280341	c
11.72982357047737	5.19092144738803	4.42409271650992	h
-0.42363245874353	-3.73853818037215	2.98664115947057	h
2.56020904547411	-1.27183260424072	4.54186289177425	h
8.35369458429609	1.94429636136122	5.37729655172950	h
9.59418937454418	7.63729226609333	5.18148373696034	h
5.53721141523632	-1.23581856603144	6.02803696256036	h
-9.93701232465486	-0.95963269618409	7.61238061283401	f
-7.06055565330277	2.03861831911952	4.65888240915628	f
-0.87104748557562	3.82449793220835	3.17791729015031	o
-2.00771485406877	-0.47230669620555	4.75052571904023	o

Isomers of compound 6

B-O-SO-P, $O_{exocycl.}$ equatorial

3.26835413899122	5.22865147216693	-0.69462399461446	c
3.54665027055497	2.84163473266217	0.39298173184843	c
4.97855313187425	2.84452698105869	2.62100919018061	c
5.97596037386331	5.00589413144691	3.73696411407862	c
5.58536528579804	7.34089631060800	2.59492770683789	c
4.22562201749080	7.44564027669860	0.35134283675121	c
2.41361127323999	0.14332491497027	-0.68800933429236	b
4.73034486180257	-1.76298610127661	-1.50954726024205	c
4.58680127201443	-4.39357821922169	-1.34473516411521	c
6.53701740008390	-6.02442800988138	-2.02144135678604	c
8.78394472911430	-5.03694266659981	-2.95694314815535	c
9.01530680770689	-2.43291103083542	-3.21120040963241	c
7.01216137999277	-0.88005708589907	-2.50452965810085	c
2.43588870468362	-5.54812391466955	-0.54067056015458	f
6.25874161372725	-8.54609488631685	-1.80503357226955	f
10.68644322772311	-6.57432668637003	-3.63262380296882	f
11.16058615913243	-1.44281442208054	-4.15316114442522	f
7.38108946206416	1.62849094314697	-2.89210033817141	f
5.49313688806761	0.63907247186438	3.81231461058612	f
7.31965507418494	4.86504863371839	5.89051835218506	f
6.52043395952661	9.45724140959060	3.63437146590264	f
3.84793240555694	9.68916747981807	-0.79341733699183	f
2.03807745088693	5.53610620587971	-2.93114304387701	f
1.22547858021176	-1.25309196373688	1.65308079868732	o
-0.74594442821935	0.21272457063318	3.29683219967543	s
-1.52799395754654	-1.42275891237679	5.38685754995872	o
0.23645143610663	0.41845817717902	-2.93071475590390	c
-1.97661438248162	-1.52197046379714	-2.70894845286871	c
-3.67188932021889	-1.62395294071694	-5.08545791918503	c
-2.17238012470300	-1.88652985635331	-7.54725014601259	c
-0.28894774527978	0.28649021938881	-7.78543828957356	c
1.52653635934687	0.18361592829328	-5.54586194492678	c

-3.93892185641711	-0.64870889472628	0.09596743218558	p
-6.21120199184518	1.75431577543096	-0.87785977255993	c
-8.58861879907649	1.05748511878137	-1.90836970205136	c
-10.22428134650560	2.96416787266693	-2.70983767691865	c
-9.61857383371253	5.52566232268991	-2.52505003607949	c
-7.29725293097516	6.16379850139245	-1.46065031966690	c
-5.59122878014352	4.33814136288254	-0.60911249099157	c
-9.52060851584033	-1.63007946977611	-2.13874818495824	c
-11.43618454783172	7.52595495978867	-3.42167564096499	c
-3.22684916166203	5.24794920823139	0.68979026794246	c
-5.59972419799125	-3.09226801572274	1.81680311613935	c
-5.43538906956567	-5.72015244246079	1.34631123099678	c
-6.75024798180785	-7.37348282920614	2.92839589767944	c
-8.19068220997625	-6.55009098492352	4.97281358960294	c
-8.28499551873098	-3.95816016610101	5.43724648055861	c
-7.01934375379911	-2.21331760299532	3.92613380395436	c
-3.93204544175951	-6.89729232296217	-0.76852665070780	c
-9.58148894895459	-8.39089089287669	6.64055497596668	c
-7.27904263436510	0.53927334713814	4.63214987015458	c
-1.19409552679466	-3.38206684848887	-2.30403870558473	h
-5.01779469120628	-3.18435888599409	-4.92614155367186	h
-4.78372928745358	0.11734558759511	-5.19471836239679	h
-1.15064735311641	-3.69099620719283	-7.57010182107986	h
-3.50260341091106	-1.91948322814272	-9.13240641726763	h
-1.30583291028785	2.09451961103027	-7.81125453074833	h
0.76307181849742	0.15181105467772	-9.56234735449864	h
2.95368765637645	1.67121420130795	-5.68674473357640	h
2.54415311514265	-1.61823323295350	-5.63188102758328	h
-0.63406098272166	2.29441929500755	-2.90192458527655	h
-6.62270885875410	-9.38605832191324	2.54294114889464	h
-9.35135035819653	-3.25687287469552	7.04623643290331	h
-1.90242058876058	-6.70388404381573	-0.45035654370223	h
-4.37694768045178	-6.06262628838545	-2.60292805093097	h
-4.35692387259011	-8.91209017099303	-0.87954232110702	h

-11.62824437738609	-8.12903770674787	6.48035313954428	h
-9.08090837609766	-8.10851884801138	8.62669322597756	h
-9.14211753001007	-10.34123624024242	6.13111865748689	h
-8.74189458826564	1.47482155686376	3.50979570331404	h
-5.52782155270724	1.59822225067855	4.36044078977422	h
-7.78994914009633	0.69364875225795	6.62425575302618	h
-12.02977023473679	2.41508106020130	-3.52125290068098	h
-6.78502150791256	8.14289480860193	-1.27138706980599	h
-8.03786093630261	-2.95283032945992	-2.67324167502548	h
-11.01792814401404	-1.72825930341593	-3.55532382264052	h
-10.29357479788457	-2.29461531911526	-0.33915733627399	h
-13.11671368239459	7.58283427538233	-2.21481428804322	h
-12.07789657044705	7.13482543555201	-5.34746346685779	h
-10.56473805508033	9.39559116196731	-3.39178320810008	h
-2.83128063349258	7.20667687150577	0.18052185977672	h
-1.56253039555818	4.13314569151235	0.21415058310442	h
-3.45285157372230	5.16622667018228	2.74699097334412	h

B-O-SO-P, $O_{exocycl.}$ axial

4.18185395830139	-0.19591508768596	0.14763160069178	p
-2.37323644139202	0.28510858926527	0.33478590674931	b
1.39628075303431	0.90575435340195	-3.34748299788919	s
-0.79672615045424	-0.53056106880715	-2.07184585062768	o
0.99670452929645	3.64333932780304	-3.55719606540536	o
1.97395419018983	-0.91980185260775	2.79274913621042	c
1.39744080384942	-2.87901415327164	2.51995107548325	h
3.48834648590349	-0.64753996344445	5.27729840510983	c
5.09370450960113	-1.95693443098293	5.28129192578863	h
4.29870793844356	1.25506385183236	5.35352872397248	h
1.85404876373232	-1.03702018468329	7.62959965171031	c
1.10706281021913	-2.97158167011585	7.66262551752504	h
3.03113119536003	-0.80917423392276	9.31668776053851	h
-0.33702682241428	0.84390269289085	7.60333255089406	c

0.40827461817918	2.77906266974327	7.65574143214900	h
-1.52376872694932	0.60575871550936	9.28188206005296	h
-1.91089729395692	0.44557732009459	5.21543637542214	c
-3.52499940374279	1.73123298786284	5.19341902946179	h
-2.68663354807977	-1.47546443784447	5.27237314202724	h
-0.43064701249056	0.78641668140275	2.71242776100630	c
0.22860679388863	2.73873833295325	2.67113228402622	h
5.40255962114034	-2.87078756513669	-1.61867698928123	c
5.10762063710962	-5.44913903882041	-0.97383421179519	c
5.86222823012785	-7.28182116500856	-2.71659551089337	c
5.62980822319883	-9.25676807580225	-2.20392082401269	h
6.92135127678614	-6.67932388074416	-5.05192917357591	c
7.32045500088340	-4.13126210278911	-5.59489824651813	c
8.22796074424400	-3.60415873253101	-7.36005716881511	h
6.60465179005554	-2.21595223692188	-3.93321371280327	c
4.15465682143138	-6.40246450232164	1.54050071418538	c
2.09760712829861	-6.57374123057146	1.56101842978421	h
4.71706294134425	-5.18462056264872	3.10608970853179	h
4.93471294454082	-8.28010381812713	1.89372140385550	h
7.61252195127942	-8.70975618612391	-6.92282883725227	c
9.25356171954979	-8.16476051942409	-8.05158395770720	h
6.04165656488123	-9.04666553551312	-8.22958193204031	h
8.02583138534971	-10.49544236028025	-5.97298726104950	h
7.33261215769230	0.45708957502047	-4.62554857399325	c
9.07928398841479	0.99668887082915	-3.65443892879613	h
5.92809498010035	1.87952649478192	-4.10502969234521	h
7.65161511757219	0.60014525812330	-6.65789047183900	h
6.82938628250240	1.74337669736826	1.21847485881427	c
9.22695388672909	0.67357372485448	1.78013891331949	c
11.21435373743807	2.29388400429298	2.39904908037799	c
13.04107022829224	1.46180789937701	2.83484236710482	h
10.93730041003655	4.91498609013025	2.50591566250187	c
8.54450193835343	5.91140209200519	2.04761682907852	c
8.25028400653804	7.93933149849171	2.18332714673546	h

6.48405104803810	4.38601790356260	1.42260540129926	c
9.79208160785421	-2.12323472792402	1.82988324395485	c
8.26250313796491	-3.21046736956015	2.68302913710524	h
11.50169647140378	-2.45069291515604	2.93821528434410	h
10.10201016558248	-2.88942845153801	-0.06341438502605	h
13.15420799802611	6.60259759320078	3.09053933533163	c
14.22079911149103	7.01946508792486	1.36484495981784	h
14.45362240749596	5.69974067566721	4.41785524118775	h
12.53564309861122	8.40132399390633	3.89194155246781	h
3.95372683853842	5.64948856613426	1.11975868238036	c
3.03540205696373	5.85227081108678	2.96351345851178	h
2.66973383863382	4.62065350160877	-0.12085252417600	h
4.17469615032343	7.54284967382214	0.32892603505655	h
-4.22955887205942	-2.16778794089566	0.81283645325893	c
-3.60900213243586	-4.66131384752471	0.21672542318436	c
-1.32139564850435	-5.25163419310302	-0.80116774997124	f
-5.20409800473062	-6.71715813708423	0.61221087647454	c
-4.46530715500570	-9.07337478924449	-0.01863304298840	f
-7.57028678064784	-6.33518674557753	1.68289678116883	c
-9.13460307806739	-8.29197521421018	2.09043979604043	f
-8.28001213793721	-3.89346567494030	2.34519664524132	c
-10.55317562881122	-3.48614245956097	3.41089989510264	f
-6.61987394671613	-1.90043466158569	1.90957792820962	c
-7.45359348032458	0.40624518771053	2.65357441183948	f
-4.03117459337546	2.73742491459171	-0.59176470322970	c
-5.52896849130378	2.50242275768950	-2.75822796693880	c
-5.64076369113102	0.25746113095938	-3.99184384527689	f
-6.95846794749260	4.45041983942940	-3.78907683952125	c
-8.35059416915036	4.08642814304910	-5.88814952992045	f
-6.94556084718694	6.80639776193212	-2.62408188664433	c
-8.30824252740822	8.72453984145734	-3.57751682074495	f
-5.50406702377186	7.14352881962821	-0.45663946360293	c
-5.47403860277748	9.41344256763942	0.69917629189193	f
-4.10126499440340	5.13312876538127	0.50083094322974	c

-2.77264130109534	5.66784993662008	2.63831430747330	f

B-SO-O-P, $O_{exocycl.}$ aequatorial

5.23158396531809	5.43059940629872	-1.03689439967066	c
5.11676808150032	3.04526153956447	0.08684175987121	c
7.02303980825542	2.62131424424939	1.87131583862768	c
8.93610977913669	4.32393352160953	2.44219650877360	c
8.98955802107314	6.64819002381342	1.21555243933227	c
7.11092809352562	7.20277421625750	-0.53090305018133	c
2.89102235895563	0.94983225888891	-0.32377426828021	b
3.97317731056132	-1.95784216386771	-0.31084069867482	c
2.69683015636958	-3.99281195518288	0.76115605559204	c
3.51619140052737	-6.49055052257537	0.69338778049715	c
5.77346435579113	-7.05765050188409	-0.52230805511324	c
7.14211931048840	-5.10459726345744	-1.63065002857599	c
6.23203144039234	-2.63876782908666	-1.50840838164129	c
0.45996626285809	-3.58729733853404	1.97931521284205	f
2.14309318349941	-8.34559111198944	1.77128431987314	f
6.61556620955542	-9.44805938178132	-0.63128050997354	f
9.32922358184954	-5.62408347755959	-2.81653611625947	f
7.68846062534919	-0.86638960910565	-2.63899696065846	f
7.02965971963098	0.43682695055369	3.22530595683215	f
10.70961321860711	3.76642300394679	4.17743013085885	f
10.81041781026051	8.33741795611727	1.73220429856930	f
7.11203331885310	9.45806655158101	-1.71089997518752	f
3.46420964755119	6.19426100808723	-2.73741272850202	f
1.01305349220477	1.53243332960020	2.97023494150357	s
-2.26107780197434	1.32302018365303	1.78680771096666	o
1.21136849637862	4.26625017340705	3.54887490294364	o
1.08498152131128	1.39280448843432	-2.80727785607411	c
-1.22877482773605	-0.40593802682446	-3.09368162313868	c
-2.62525763365446	0.01994191991818	-5.63176532794818	c
-0.87565624936085	-0.29857903526137	-7.90948519862346	c
1.36211441607072	1.51125835364298	-7.68361713667898	c

2.74847971040278	1.03694024697282	-5.19356483929252	c
-3.52180327736574	-0.05247977895709	-0.50959328040154	p
-6.09329693806272	2.01985588260076	-1.50074911461467	c
-8.34148814997666	0.99787489316021	-2.55843458870550	c
-10.30169949459519	2.63111661629391	-3.22145007994693	c
-10.14726587446328	5.23944076807929	-2.88527969965649	c
-7.91028140323114	6.20701115230337	-1.89849847695696	c
-5.86629473972915	4.68200425685463	-1.20338721497996	c
-8.82444870772802	-1.77693469685194	-3.05252258063273	c
-12.32539739918930	6.94151695795581	-3.56518612867226	c
-3.58443023780854	6.05484331807959	-0.17566729037800	c
-4.87151128021660	-2.94736861668630	0.76519934034814	c
-4.55210057039336	-5.39773726096750	-0.25924840190528	c
-5.60193884030879	-7.45816907945443	1.01225889943674	c
-6.97023936194371	-7.20470124060891	3.24488200500227	c
-7.30081288370986	-4.77281099325189	4.20191490239259	c
-6.28643458078696	-2.63882694029462	3.03282415019081	c
-3.16564419613156	-6.01879452068264	-2.67672090482345	c
-8.08003742825579	-9.46756305312252	4.56830675160489	c
-6.77538905421792	-0.13410951205613	4.32304701230660	c
-0.51491747633715	-2.33825479935344	-3.00818898407304	h
-4.24759443103332	-1.25269445303517	-5.80191523033540	h
-3.39436172822196	1.94024013846082	-5.63503044260347	h
-0.18246789677106	-2.25211148994780	-7.99362203659298	h
-1.94933759396003	0.04065104042546	-9.64552582744177	h
0.68324010568006	3.46916822140102	-7.74968298122669	h
2.66227890943685	1.26438215263351	-9.27452260876628	h
4.39911096739840	2.26259142739656	-5.04475153766671	h
3.45861130240585	-0.91083876780842	-5.21200223707091	h
0.37712662685880	3.33062863463813	-2.83347306748156	h
-5.33336398269125	-9.32960422989599	0.21202437653667	h
-8.38425259986077	-4.50640533444036	5.92611102556789	h
-1.11714181247201	-6.01484564037956	-2.40050475470195	h
-3.59889579550648	-4.71678391163988	-4.21575334906032	h

-3.69340413813245	-7.91380974039467	-3.29626511138707	h
-10.14752689889550	-9.37876871540354	4.56940193009761	h
-7.46872603646713	-9.53847651196400	6.54207929139624	h
-7.51172200952189	-11.22489065007484	3.64919272324040	h
-7.18308071933742	1.38777564083678	2.99363857264568	h
-5.13773574366765	0.45071243422030	5.43495803297482	h
-8.38922852297948	-0.32978293050308	5.59364577923786	h
-11.99987171620450	1.82208245483870	-4.04604872489844	h
-7.71461685766674	8.23749769256903	-1.66630967226741	h
-7.17841136285126	-2.76657101539210	-3.79583726618566	h
-10.34264913793235	-1.95893463090302	-4.43834167295954	h
-9.40376710357125	-2.76596769626656	-1.33421307799971	h
-13.80166047495940	6.84387423113726	-2.11665659819238	h
-13.18422663940201	6.37587487500357	-5.35743440073316	h
-11.71931515578673	8.90802314499980	-3.71744693654355	h
-1.80856219165931	5.37134312348964	-0.95488218753013	h
-3.43205523787492	5.85914755002046	1.87202530970205	h
-3.74648801345383	8.06125244345106	-0.62569833789792	h

B-SO-O-P, $O_{exocycl.}$ axial

4.76291200280218	5.42687004513950	-0.76074197312054	c
4.69314432981589	2.99891154531760	0.29419188902326	c
6.70199493594925	2.50482115597506	1.95992679219135	c
8.66045888756493	4.18837296815149	2.44812296609716	c
8.66101040263445	6.54576859956869	1.28643942522833	c
6.68448813639713	7.16923597426048	-0.32686544497494	c
2.38774932634507	0.92951457561771	-0.10358392324300	b
3.34385719033334	-1.99019748508937	0.02732527432554	c
2.02016732061333	-3.93865858348005	1.20491300169575	c
2.79853846075954	-6.45290653623854	1.23797053902233	c
5.02877210279912	-7.12752746426943	0.02813722025838	c
6.42718836199305	-5.26294014966560	-1.18871365508982	c
5.56851313342423	-2.77822572941659	-1.16697492740369	c
-0.20085050592701	-3.45171980488451	2.38018461490371	f

1.39610814624310	-8.23195573563384	2.40194603103075	f
5.81325594750028	-9.54060635978228	0.01901341858178	f
8.58993172757657	-5.88254598854435	-2.37442178341486	f
7.05446713978362	-1.08118738655781	-2.38238604136724	f
6.82336861803355	0.28542903464739	3.20895756467592	f
10.54114138695665	3.56756752624283	4.03787633281939	f
10.52375646748918	8.20278070430319	1.73633452490010	f
6.63628615176784	9.45576944574548	-1.44022430235021	f
2.89828380197624	6.24737109620068	-2.32404673024618	f
0.59057876722683	2.21209224018777	2.88357829878259	s
-2.80058203741390	1.32392381330115	2.11476176326350	o
1.19147469733286	0.83250375456403	5.23931995030650	o
0.58069579882480	1.40958256553489	-2.58730014633721	c
-1.75406451824600	-0.37478752185042	-2.80575904399736	c
-3.16469609265180	0.01514839524790	-5.34097896629576	c
-1.43501790629074	-0.36495612300866	-7.62499424206537	c
0.80499878376402	1.44900093198741	-7.46643617078964	c
2.21964562946369	1.02940423929191	-4.98276980153772	c
-4.04604720047055	-0.00463668067874	-0.20340195636839	p
-6.61715274756972	2.05240251113194	-1.26044822932206	c
-8.84928840979279	1.03767141464601	-2.35057983562763	c
-10.78807251930064	2.67985690367891	-3.06739618194191	c
-10.62595802362656	5.28759949693094	-2.75683545831607	c
-8.40265262654013	6.25197472765139	-1.72889668081369	c
-6.39154622261479	4.71619561745989	-0.97751017602175	c
-9.35463498715888	-1.73790864461634	-2.81948316480929	c
-12.77816224557708	7.00131645306698	-3.48831533126144	c
-4.12218138385618	6.07348700657729	0.10298308969496	c
-5.44113858796892	-2.89593366055741	1.03479288284323	c
-5.12404747044960	-5.35355824825543	0.01866549053010	c
-6.23320481862679	-7.39771765615132	1.25886185142862	c
-7.64956849074569	-7.12784752447641	3.46352338453770	c
-7.97116260209374	-4.69572092077150	4.41179395054628	c
-6.89830874106859	-2.57240553670400	3.26821071802063	c

-3.68071667504663	-5.99138757058193	-2.36079342609764	c
-8.75332760985192	-9.39166895420122	4.78874305095771	c
-7.36780206762952	-0.06694045411069	4.56197590553837	c
-1.04821616042397	-2.30817929170934	-2.69461135631831	h
-4.79870948671729	-1.24507052015983	-5.47565803187020	h
-3.91776716873851	1.94151973472455	-5.37885510676203	h
-0.74404698711866	-2.32057205348385	-7.66465833059777	h
-2.52260425990559	-0.06926549266711	-9.36025971973255	h
0.12226513300800	3.40444254452984	-7.56800939748899	h
2.08649958880775	1.16829383849619	-9.06680809947309	h
3.86032415987687	2.27549456630629	-4.86804847812300	h
2.95252253337349	-0.90909644219193	-4.97369403283503	h
-0.11883490664558	3.35222908562468	-2.62959136652304	h
-5.97709622962154	-9.27044840095264	0.45695872539498	h
-9.09226058011788	-4.41736427455534	6.10949088843745	h
-1.63865691887144	-5.95358382462209	-2.04357758912908	h
-4.10191604439922	-4.71924222419159	-3.92869214537384	h
-4.16920217923761	-7.90281723260991	-2.96149019790066	h
-10.37743047662833	-8.86420478607237	5.94853693254437	h
-7.34210107709926	-10.25041715292361	6.03741261125602	h
-9.34536657282938	-10.83731830597396	3.43785113209405	h
-7.70694491242896	1.47340662638534	3.23402951901219	h
-5.74173817544774	0.46665132844130	5.71597278614853	h
-9.01755467465206	-0.23445643298430	5.79003307454669	h
-12.47679286695843	1.87370418876793	-3.91367226896925	h
-8.19837911902215	8.28331836817669	-1.50880852363358	h
-7.70809363298373	-2.75943025040270	-3.51509731224173	h
-10.84921663117720	-1.92043425073219	-4.23083468930562	h
-9.97817968452319	-2.69508137174115	-1.09846117248785	h
-14.02400201610536	7.32956172391202	-1.86679268108724	h
-13.92045932951796	6.17010830241841	-4.99386173940286	h
-12.08781124537584	8.84137776196644	-4.12156072643146	h
-2.34190031306994	5.42104981078926	-0.70011659801142	h
-3.98710065448030	5.81560690439396	2.14546291361927	h

-4.28845427582157	8.09122150013881	-0.29157735774579	h

5-membered ring compound

-11.27372944067137	7.82523945660360	-0.56541012620169	f
8.88660830327015	-9.53587347923609	-4.43059029837950	h
8.94977674310076	-0.81879650019805	-5.24580863391175	h
9.15222189448090	-4.82083520024271	-4.06577372542492	h
6.24011605531636	1.11086329287525	-5.00364402350360	h
6.28027820534708	-11.17071874765281	-3.09280667121635	h
7.44017615058451	-0.21216094744361	-3.97584070892105	c
0.50130556030075	0.08084039559722	-6.60908162347873	c
7.55591852670182	-9.56601449520779	-2.85133872474715	c
-9.57637305733716	3.11474962256276	-0.47522921776151	f
7.23850668001525	-4.82390246700614	-3.31969539028016	c
3.60480331292822	4.08308600856817	-5.76902008050499	h
-8.00976494421755	11.82064088601043	-0.98833423150258	f
-8.76891170833829	7.41222705670171	-0.67997979107669	c
-4.80328365738710	1.30657755143699	-5.54201254212279	c
5.07441569920210	7.05988464624215	-5.49423817857288	h
8.65078919733052	-9.89063924938131	-1.12360965729397	h
8.29828628289399	0.82801263993348	-2.41198257013893	h
6.11501630342734	-7.11798426900270	-2.66853569582849	c
5.99702392455332	-2.50913018831157	-3.08492348025585	c
-7.81102498610536	4.96184844514527	-0.60303014521731	c
-7.12404162100437	9.44751920986425	-0.90410020290358	c
3.77813506533640	5.74923502590578	-4.56700689886002	c
-0.29384559863526	1.31807398368491	-4.09559448157856	c
-0.24757041820364	3.36746915304274	-4.27610121434679	h
-6.67018435977608	-3.42990176715512	-2.66931249197367	f
-3.02974402508330	0.49827488961462	-3.35886545125084	c
1.92995407768612	6.66678250259988	-4.47684164150612	h
-3.00324140205805	-1.56257765460056	-3.34477953668037	h
-9.55537044944426	-6.47165596042446	0.06799940247969	f
3.61574186443757	-7.05704164079048	-1.85255447804578	c

3.48432199381843	-2.48167031433596	-2.12646799495739	c
-5.22915784051747	4.37715429737931	-0.71095897353163	c
-4.54705372349247	8.97531479274599	-1.08378100722010	c
4.76874048249937	5.11966197098222	-1.96700220948035	c
2.65484229058214	-8.81741607447337	-1.41172029905943	h
6.86255562151028	8.56945331313302	-1.93148564043046	h
-7.10168612717755	-2.71693793024633	-0.23871629218462	c
1.89872704507618	0.52889188357597	-1.51233311470019	p
-4.21324629355037	1.47304888773840	-0.68426540074660	b
2.26391708215404	-4.80365813231143	-1.59120477702098	c
-8.64299335791226	-4.34986641127488	1.13743319431475	c
-3.68283840190073	6.49512164259626	-1.00906922231503	c
-2.91738213378522	10.90900858454736	-1.36522326277336	f
6.43494933680095	6.85452301806068	-0.88538990233889	c
4.21288804860697	2.87783727626677	-0.62225611238149	c
-6.09551330395576	-0.48467370559768	0.74259543155500	c
10.22235467204944	9.55226882079203	1.15072603213613	h
-1.63190131164124	-5.28673136580064	-2.58127659002521	h
-9.25435759202277	-3.77873084732363	3.62550046197372	c
-1.15110883162675	6.21455710188460	-1.30587620056902	f
6.28243011277537	-1.53024184673947	2.36683879587732	h
-0.47976443990709	-5.03883565280084	-0.88045280971603	c
7.58106294516924	6.45804233099596	1.45440530877581	c
-10.73144736702631	-5.33444066252309	4.97599778700639	f
5.41886343951402	2.39480928574862	1.72468548233164	c
-0.77132462067201	-6.70140528861107	0.30716658738263	h
-6.79708724678282	0.00201259510959	3.24776551211679	c
-1.13201010536347	1.24647755435798	1.83099715617296	s
9.28891009380677	8.42262530536638	2.60551395048202	c
7.07462744298430	4.19391132185031	2.70285343934703	c
-8.32020552400320	-1.56429132342994	4.69542342237262	c
5.09119845526336	-0.04128534280980	3.17317430115438	c
10.73376660394658	7.55550526008098	3.79895982836768	h
-1.19256546136614	-3.41788315423107	0.16146342482117	h

3.15177480743471	-0.74786215871681	3.17964943360050	h
7.97925357397126	3.80858808224723	4.50553354494741	h
8.19322511594472	9.71720832598835	3.79396797783741	h
5.64709890862558	0.23303728323542	5.14005508116827	h
-8.89719719851524	-0.97914362744835	7.09824984404876	f
-5.93790594689422	2.12915039215721	4.38381312412289	f
-0.16898224730626	3.56216807904286	2.97262035055283	o
-1.22490494452911	-1.00590505003115	3.43987572956119	o
-1.30886353727482	0.82828307918034	-8.74399475489589	c
-4.03802542100407	0.13595205455218	-8.07511114957112	c
-4.76799665810757	3.37443045633439	-5.69492714420192	h
-4.21669663776570	-1.92604147698398	-7.95344762422172	h
-1.17423585915181	2.87328745900015	-9.06434046035277	h
0.48782348856966	-1.97595155253547	-6.37010198050114	h
-6.74615002425852	0.78165084461980	-5.07323933350618	h
-5.32301697758637	0.76558138259933	-9.57016409805869	h
-0.72460551145953	-0.09674175488874	-10.50043310920850	h
2.44306490680208	0.59912779120825	-7.10269722705152	h

Transition state of the inversion on S in molecule 4

0.000000	0.000000	0.000000	c
2.631163	0.000000	0.000000	c
3.918681	2.291641	0.000000	c
2.553643	4.544285	0.011492	c
-0.081276	4.655236	-0.008408	c
-1.281770	2.297511	0.003976	c
3.963307	6.689253	0.037579	f
6.465339	2.308851	0.004330	f
-1.789927	7.225405	0.016565	b
-3.013372	7.030602	2.720114	o
-4.628292	9.303981	3.816206	s
-7.030941	8.773731	5.217399	o
3.913241	-2.190921	-0.002030	f
-3.834762	2.169741	0.031511	f

-1.261479	-2.208974	0.007173	f
-0.210546	9.877292	-0.150633	c
-1.903777	12.257446	-0.343915	c
-3.391841	12.764154	2.734425	p
-6.210678	14.615860	3.236180	c
-7.912510	15.134441	1.232733	c
-10.015893	16.636553	1.729575	c
-10.532879	17.590815	4.137967	c
-8.904481	16.932270	6.101556	c
-6.753451	15.449983	5.724505	c
-7.605195	14.091632	-1.398727	c
-12.809217	19.236498	4.595336	c
-5.219525	14.746573	8.025846	c
-0.792790	14.232095	4.503850	c
-0.355598	16.822641	3.992814	c
1.621377	18.047689	5.245179	c
3.164048	16.805798	6.980990	c
2.699534	14.247478	7.433068	c
0.762380	12.912616	6.236450	c
5.283694	18.162712	8.314421	c
-1.932251	18.396555	2.196572	c
0.461988	10.159911	6.931389	c
-3.874692	7.128079	-2.295938	c
-2.961440	7.209484	-4.776622	c
-4.482094	7.177089	-6.922737	c
-7.094150	7.055319	-6.639399	c
-8.107147	6.943703	-4.217786	c
-6.502106	6.964788	-2.125569	c
-3.463122	7.262357	-9.253549	f
-0.427711	7.299021	-5.200390	f
-8.612216	7.039470	-8.675535	f
-10.631982	6.820436	-3.913408	f
-7.666832	6.806566	0.145441	f
5.387215	20.143223	7.735266	h

-0.838820	20.035475	1.572989	h
1.961100	20.033575	4.830519	h
-2.531334	17.366394	0.507225	h
7.105872	17.269291	7.900734	h
-0.783936	13.958685	-0.722632	h
-6.023414	14.974027	-2.403618	h
0.966924	9.891488	-1.848042	h
-9.317748	14.446498	-2.495244	h
5.022999	18.100306	10.368349	h
-3.651733	19.085531	3.121124	h
-3.329920	12.009317	-1.805347	h
-7.286797	12.048209	-1.359425	h
1.103301	10.095861	1.436951	h
3.897464	13.229080	8.758444	h
-11.316247	17.031565	0.187074	h
-12.478196	21.150755	3.869992	h
0.356906	8.912452	5.289385	h
-3.564039	15.966443	8.252968	h
2.080221	9.572805	8.074262	h
-13.235495	19.385389	6.611296	h
-1.253889	9.839334	8.046990	h
-4.567845	12.787402	7.943122	h
-9.336053	17.549795	8.014233	h
-14.474881	18.490181	3.621142	h
-6.398559	14.942997	9.710725	h

SO2-adduct of 2a

-10.33256408222769	5.24150764794825	-5.84502400613605	f
6.25975991102689	-9.85351233652080	-5.11833658920193	h
6.86326244126246	-1.07088331680406	-5.39967936911467	h
6.88565264435497	-5.32803881363114	-4.80817927470752	h
4.54410631634934	0.92688202470851	-4.03966515591043	h
3.84237504864365	-11.35822344510708	-3.34080920116118	h
5.93044788867154	-0.54956340500792	-3.63110936770411	c

0.51904426503107	1.07063464258023	-3.77084167270297	h
5.40537585558334	-10.00708761998116	-3.24264656577974	c
-8.38118596054627	0.90707645527340	-4.05085670447989	f
5.49564271252263	-5.22872519531802	-3.29492567312636	c
2.49690596206870	4.81829315692916	-3.49416418538964	h
-9.09170561258027	9.77043990468056	-3.65172309996403	f
-8.76149637694501	5.30184680653672	-3.84730717091431	c
-3.66015031916318	-0.58475399644867	-3.85281611305443	h
3.61192624619096	7.80735263262992	-2.50667377627966	h
6.83164908207058	-10.80161593448767	-1.96416062063611	h
7.34624744623767	0.29139982848367	-2.37676042921373	h
4.51463179600054	-7.46843488316070	-2.30411722610598	c
4.73388629305392	-2.84686262429615	-2.44045546652157	c
-7.73032557677105	3.09055699958681	-2.86857391917246	c
-8.13503397063477	7.60470991445603	-2.74002005228734	c
2.84043367363723	6.01086961399392	-1.84151525884849	c
-0.51212754048687	1.20099890702623	-1.98034155472277	c
-1.13064318819561	3.15259866189378	-1.73460569369657	h
-5.78459541253954	-5.03998113864559	-2.14045799644280	f
-2.79751563722846	-0.59870599944245	-1.96753728711224	c
1.01135439316909	6.40389863163048	-0.95607427584020	h
-2.14534293626734	-2.53861115818990	-1.67512404377372	h
-9.71587659862754	-8.01604251950989	-1.12374112641640	f
2.71240001593578	-7.28747335567373	-0.38565531313982	c
2.88911119618887	-2.70359736230866	-0.51212934384347	c
-6.09223654831952	3.00894412782844	-0.79741761294657	c
-6.49298690038768	7.63345232687444	-0.68818768218926	c
4.65605337216435	4.80932045949998	0.00077012362207	c
1.91964215945940	-9.00375622533232	0.42360588259233	h
7.10342977498443	8.00735010055322	-0.30723459349144	h
-7.51749575338408	-4.14360292284163	-0.48767171821726	c
1.59619753737456	0.29797663681848	0.66016088216615	p
-4.97054992720159	0.25411079888229	0.03241323853859	b
1.90346822767683	-4.95288215312171	0.53844557307762	c

-9.55603531124202	-5.74090613049651	-0.00274137993565	c
-5.51110067561717	5.36723571183118	0.23225773310942	c
-5.85639505392634	9.85019785577447	0.38567329077475	f
6.82672550326699	6.18331990745558	0.60201584883131	c
4.28468149443453	2.40206807804269	1.12580552374399	c
-7.24250145249196	-1.75779807879700	0.61168940802550	c
11.49271473458130	8.07029190682047	1.34663101733545	h
-1.83910950884733	-4.20844804897112	2.01628253743141	h
-11.44541135947310	-4.97364833944535	1.65695612039904	c
-3.91068328926985	5.58728738762583	2.22367269331347	f
6.08695202999608	-2.55582932430390	3.21671040212899	h
0.00616075547818	-4.90894084322489	2.66811315452899	c
8.64226414869807	5.31272987037692	2.30708103595668	c
-13.41388243236225	-6.49101187737772	2.14734769371547	f
6.06409000231139	1.53992392401264	2.95052696191365	c
-0.29336807587331	-6.80866522762488	3.42333079084465	h
-3.44796833329126	0.70193101977908	2.62497928774120	o
-9.19830622993917	-1.08846746592516	2.26363344799892	c
-3.86984906905988	-0.75596722943068	5.09179881468817	s
10.93882515474457	6.87304350832124	2.93891317633358	c
8.20418809127345	2.98794964966216	3.47070447124253	c
-11.26452811241619	-2.61574098321078	2.81240178660122	c
5.71626803231180	-0.89458145865335	4.39363452862029	c
12.54308109442633	5.67288229871857	3.45075374075170	h
0.64159759166242	-3.67614491747381	4.20266426591520	h
-9.10545552843051	1.17769042658009	3.47006108429055	f
3.77464980310434	-1.05792391063625	5.10026980907816	h
9.55350369103566	2.27943750900217	4.85213402294974	h
10.55488277075369	8.11997685412443	4.55146013103439	h
7.00152797301826	-0.94878916694528	6.01059743978704	h
-13.06773868996770	-1.85612144628387	4.43258467471815	f
-1.97095166704125	-0.01484733231250	6.95319992638062	o