# Reversible Formylborane/$SO_2$ Coupling at a Frustrated Lewis Pair Framework

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## *Supporting Information*

### Materials and Methods

General Information

All syntheses involving air- and moisture sensitive compounds were carried out using standard Schlenk-type glassware (or in a glovebox) under an atmosphere of argon. Solvents were dried and stored under an argon atmosphere. NMR spectra were recorded on a *Varian Inova 500* ($^1$H 500 MHz, $^{13}$C 126 MHz, $^{19}$F 470 MHz, $^{11}$B 160 MHz, $^{31}$P 202 MHz) and on a *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 shifts δ are given relative to TMS and referenced to the solvent signal. $^{19}$F NMR: chemical shifts δ are given relative to $CFCl_3$ (external reference, δ = 0), $^{11}$B NMR: chemical shifts δ are given relative to $BF_3{\cdot}Et_2O$ (external reference, δ = 0), $^{31}$P NMR: chemical shifts δ are given relative to $H_3PO_4$ (85% in $D_2O$) (external reference, δ = 0). NMR assignments were supported by additional 2D-NMR experiments. IR spectra were recorded on a *Varian 3100 FT-IR* (Excalibur Series). HRMS was recorded on GTC Waters Micromass (Manchester, UK). Elemental analyses: *Foss–Heraeus* CHNO-Rapid.

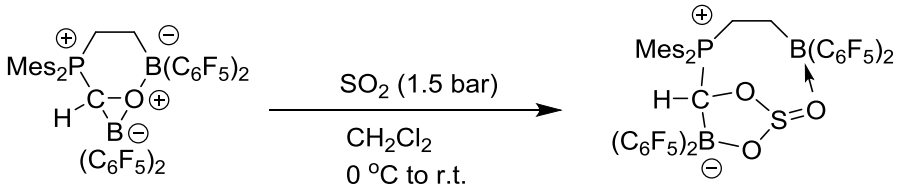
X-Ray diffraction: For compounds **9d** data sets were collected with a Nonius Kappa CCD diffractometer. Programs used: data collection, COLLECT (R. W. W. Hooft, Bruker AXS, 2008, Delft, The Netherlands); data reduction Denzo-SMN (Z. Otwinowski and W. Minor, *Methods Enzymol.* 1997, **276**, 307-326); absorption correction, Denzo (Z. Otwinowski, D. Borek, W. Majewski and 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). For compound **9c** data sets were collected with a D8 Venture Dual Source 100 CMOS diffractometer. Programs used: data collection: APEX2 V2014.5-0 (Bruker AXS Inc.,

2014); cell refinement: SAINT V8.34A (Bruker AXS Inc., 2013); data reduction: SAINT V8.34A (Bruker AXS Inc., 2013); absorption correction, SADABS V2014/2 (Bruker AXS Inc., 2014); structure solution SHELXT-2014 (Sheldrick, 2014); structure refinement SHELXL-2014 (Sheldrick, 2014) and graphics, XP (Bruker AXS Inc., 2014). *R*-values are given for observed reflections, and $wR^2$ values are given for all reflections. *Exceptions and special features*: For compound **9d** a 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. The quoted formula and derived parameters are not included the squeezed solvent molecules. CCDC deposition numbers are 1500866 and 1500867.

Materials

Bis(pentafluorophenyl)borane [D. J. Parks, W. E. Piers and G. P. A. Yap, *Organometallics* 1998, **17**, 5492-5503; D. J. Parks, R. E. von H. Spence and W. E. Piers, *Angew. Chem. Int. Ed.* 1995, **34**, 809-811], compound **2c** [M. Sajid, L.-M. Elmer, C. Rosorius, C. G. Daniliuc, S. Grimme, G. Kehr and G. Erker, *Angew. Chem. Int. Ed.* 2013, **52**, 2243-2246], and compound **2d** [K.-Y. Ye, G. Kehr, C. G. Daniliuc, L. Liu, S. Grimme and G. Erker, *Angew. Chem. Int. Ed.* 2016, **55**, 9216-9219] were synthesized according to the literature.

Preparation of compound **9c**




**2c** **9c**

Scheme S1

A solution of compound **2c** (203.2 mg, 0.20 mmol) in dichloromethane (20.0 mL) was degassed by freeze-pump-thaw cycles (×2). Then the cooled (0 °C) reaction mixture was exposed to $SO_2$ gas (1.5 bar). After the reaction mixture was stirred at room temperature for 4 days, all volatiles were removed in *vacuo* to give compound **9c** (148.7 mg, 0.14 mmol, 69%) as a white solid.

**IR (KBr)** [white solid]: $\tilde{\nu}$ ($cm^{-1}$) = 2959 (m), 2930 (m), 1647 (s), 1606 (m), 1519 (s), 1467 (s), 1384 (m), 1289 (s), 1246 (m), 1201 (w), 1093 (s), 1029 (m), 974 (s), 868 (m), 803 (m), 738 (m), 706 (m).
**Decomposition point** [white solid]: 129 °C

The NMR data of a solution of the obtained white solid in [$D_2$]-dichloromethane showed a mixture of compound **9c** (ca 78 mol%) and compound **2c** (ca 22 mol% ($^{31}$P)).

**$^1$H NMR (**500 MHz, [$D_2$]-dichloromethane, 193 K) [all resonances are broadened]: δ = 7.09, 6.88, 6.86, 6.51 (each br, each 1H, *m*-Mes), 6.67 (d, $^2J_{PH}$ = 10.0 Hz, 1H, OCH), 3.32, 2.92 (each br, each 1H, $PCH_2$), 2.98, 2.25, 2.18, 2.14, 2.13, 1.97 (each s, each 3H, $CH_3^{Mes}$), 1.13 (m, 2H, $BCH_2$).
**$^{13}$C{$^1$H} NMR** (126 MHz, [$D_2$]-dichloromethane, 193 K)[selected resonances]: δ = 116.7 (d, $^1J_{PC}$ = 74.6 Hz), 115.1 (d, $^1J_{PC}$ = 69.8 Hz)(*i*-Mes), 70.3 (br m, OCH), 21.4 ($PCH_2$)[a], 15.3 (br, $BCH_2$). [[a] from the $^1$H,$^{13}$C ghsqc experiment]
**$^{11}$B{$^1$H} NMR** (160 MHz, [$D_2$]-dichloromethane, 193 K): δ = no resonance observed
**$^{19}$F NMR** (470 MHz, [$D_2$]-dichloromethane, 193 K): δ = -128.0 (1F), -132.4 (1F), -135.6 (5F), -139.3 (1F)(each br m, *o*-$C_6F_5$), -155.4, -157.1, -157.6, -158.1 (each t, $^3J_{FF}$ = 20.8 Hz, each 1F, *p*-$C_6F_5$), -162.5 (1F), -162.9 (1F), -163.4 (1F), -163.5 (1F), -163.8 (2F), -164.1 (2F)(each br m, *m*-$C_6F_5$).
**$^{31}$P{$^1$H}** NMR (202 MHz, [$D_2$]-dichloromethane, 193 K): 30.4 ($\nu_{1/2}$ ~ 8 Hz).

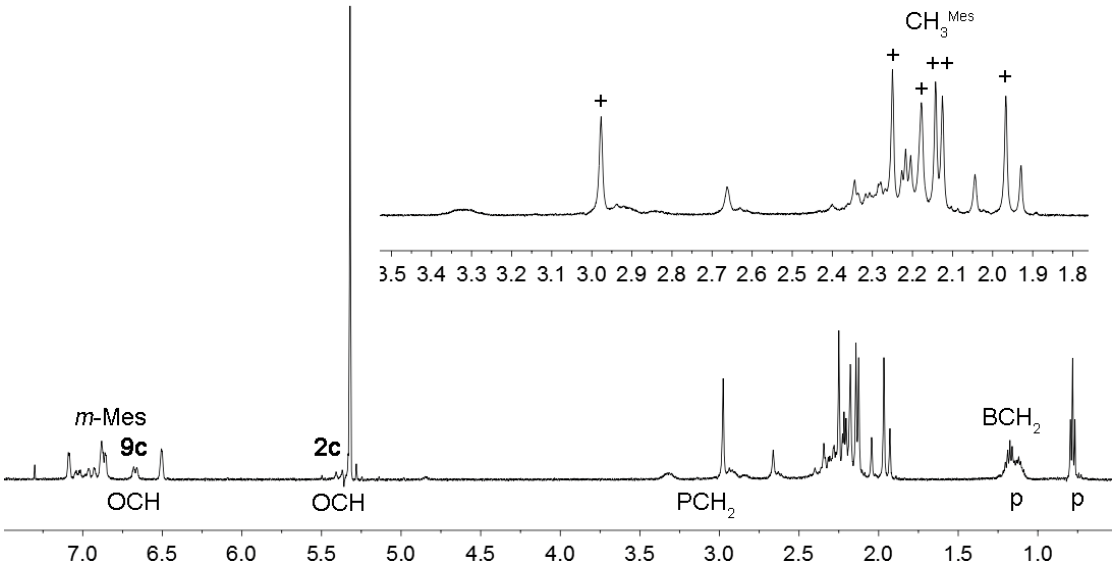



**Figure S1**: **$^1$H NMR** (500 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid. [p: pentane]

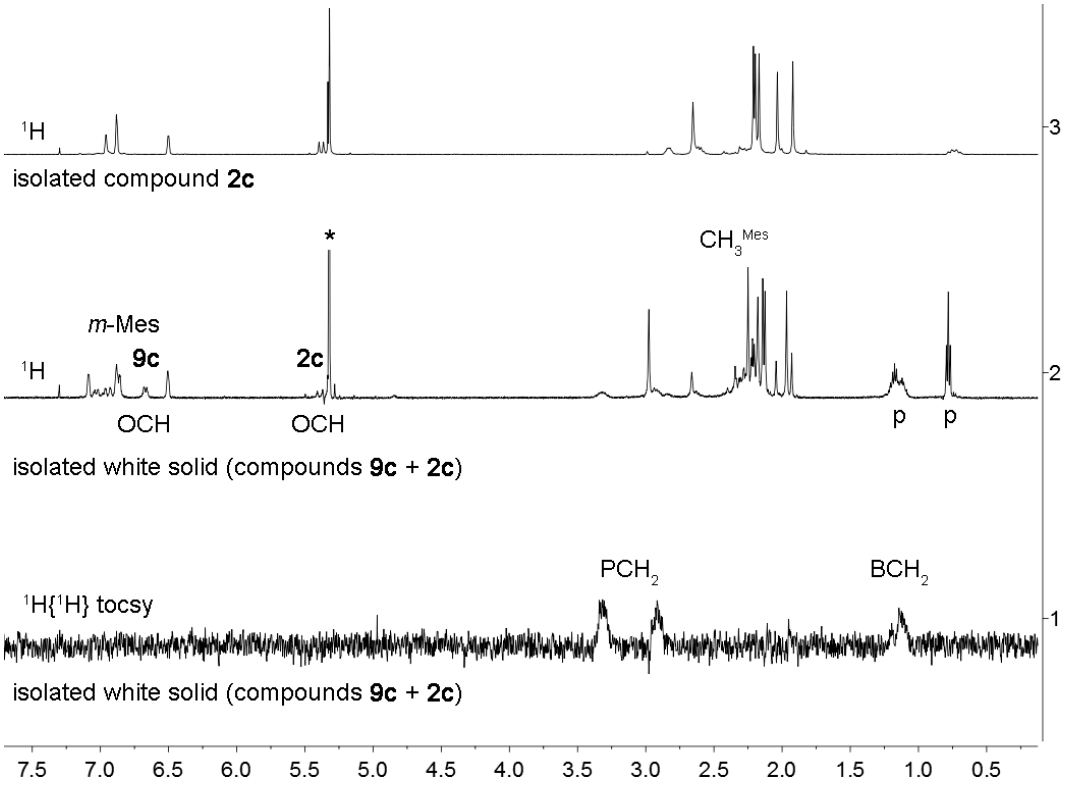



**Figure S2**: (1) **$^1$H{$^1$H} tocsy** and (2) **$^1$H NMR** (500 MHz, [$D_2$]-dichloromethane*, 193 K) spectra of the obtained white solid and (3) **$^1$H NMR** (600 MHz, [$D_2$]-dichloromethane*, 193 K) spectrum of isolated compound **2c**. [p: pentane]

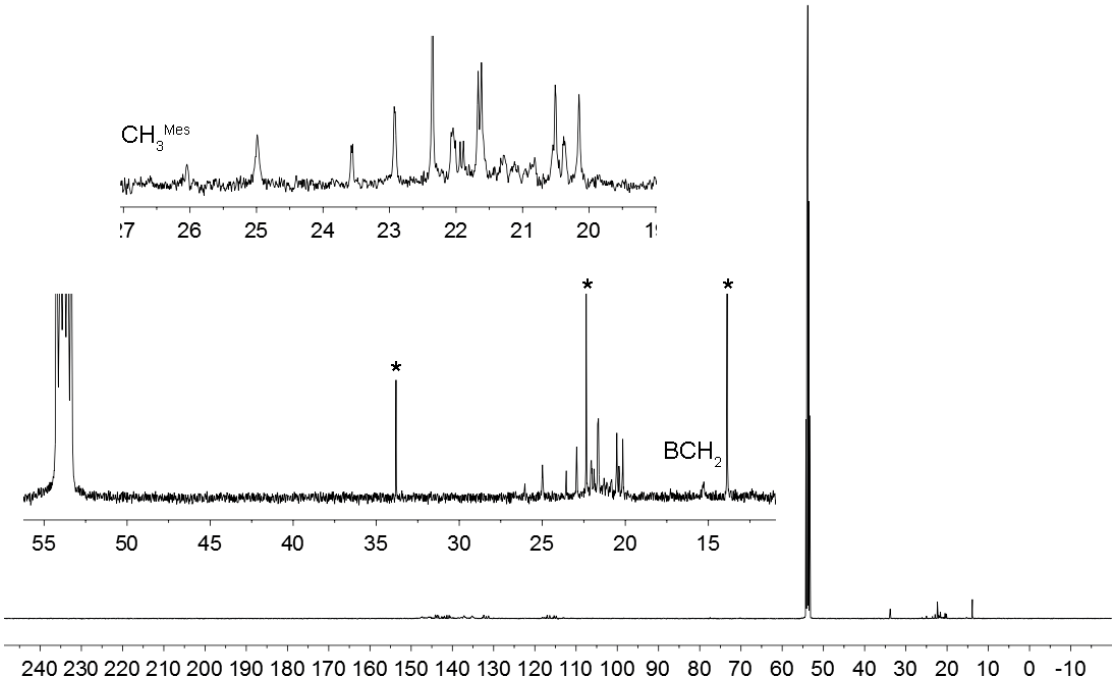



**Figure S3**: **$^{13}C\{^{1}H\}$ NMR** (126 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtained white solid (* pentane)

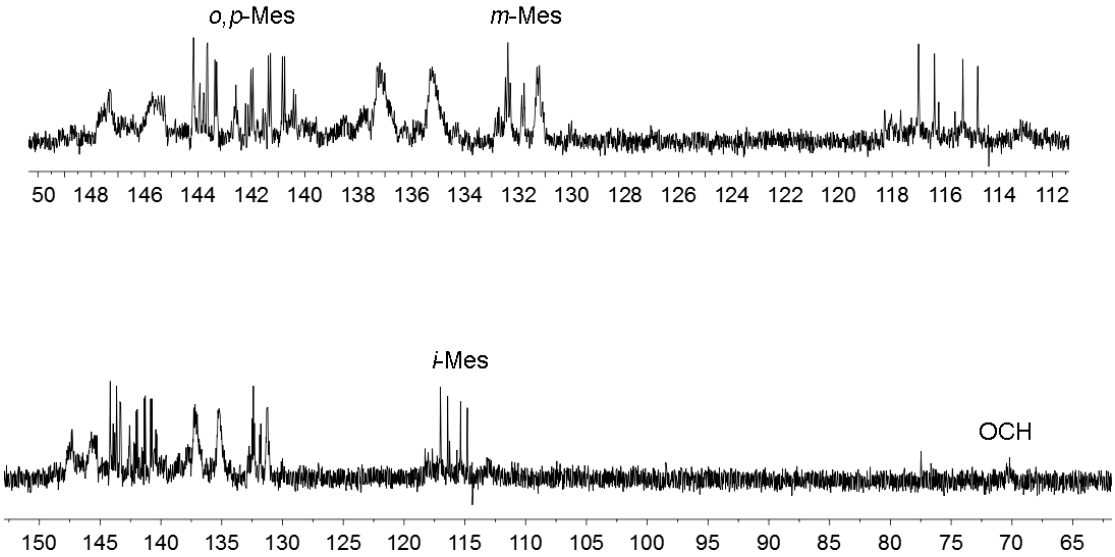



**Figure S4**: **$^{13}C\{^{1}H\}$ NMR** (126 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtained white solid

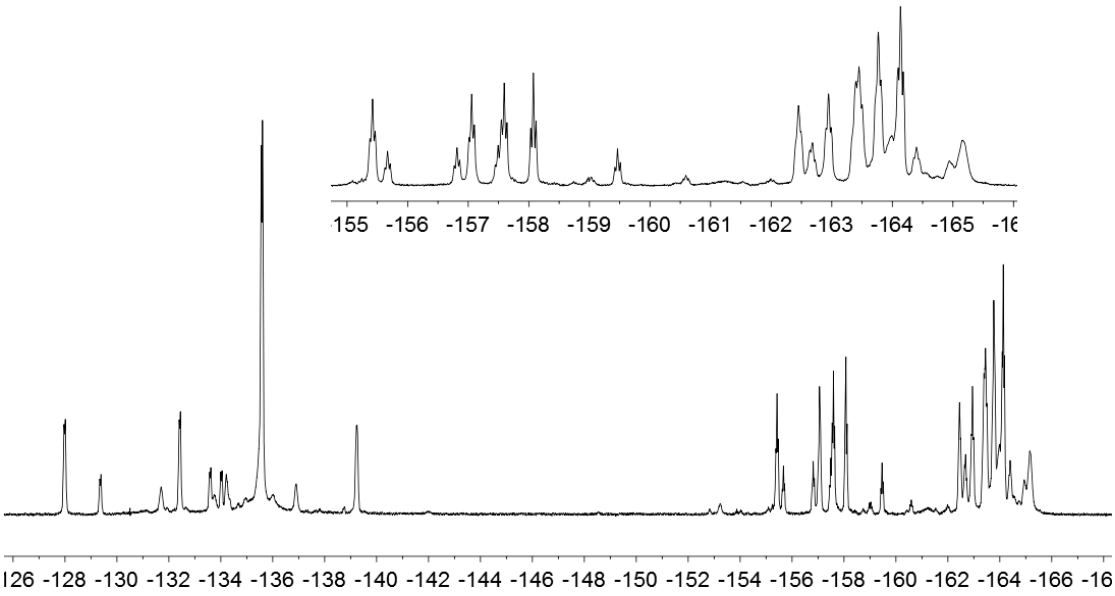



**Figure S5**: **$^{19}$F NMR** (470 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid

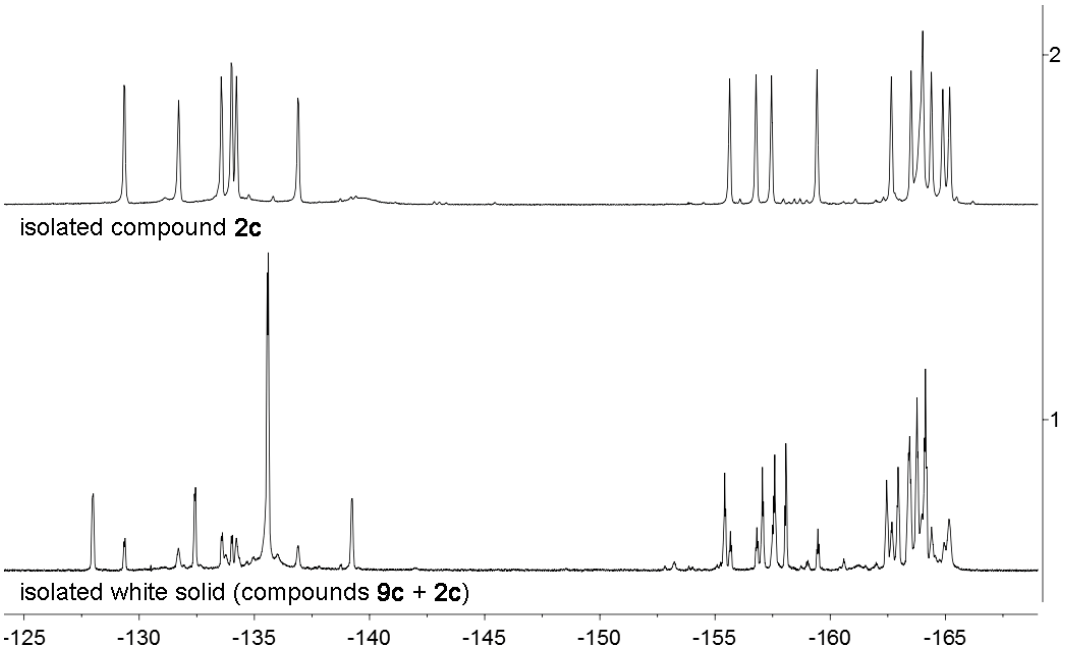



**Figure S6**: (1) **$^{19}$F NMR** (470 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid and (2) **$^{1}$H NMR** (564 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of isolated compound **2c**

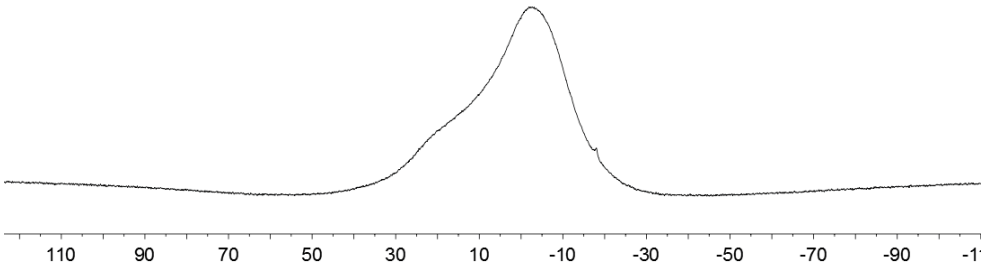



**Figure S7**: **$^{11}B\{^{1}H\}$ NMR** (160 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtained the white solid

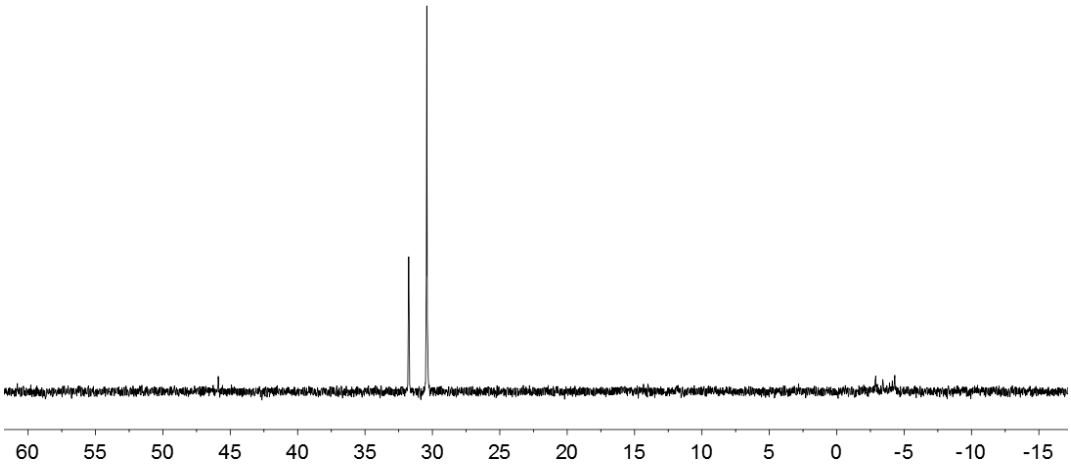



**Figure S8**: **$^{31}P\{^{1}H\}$ NMR** (202 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtained white solid.

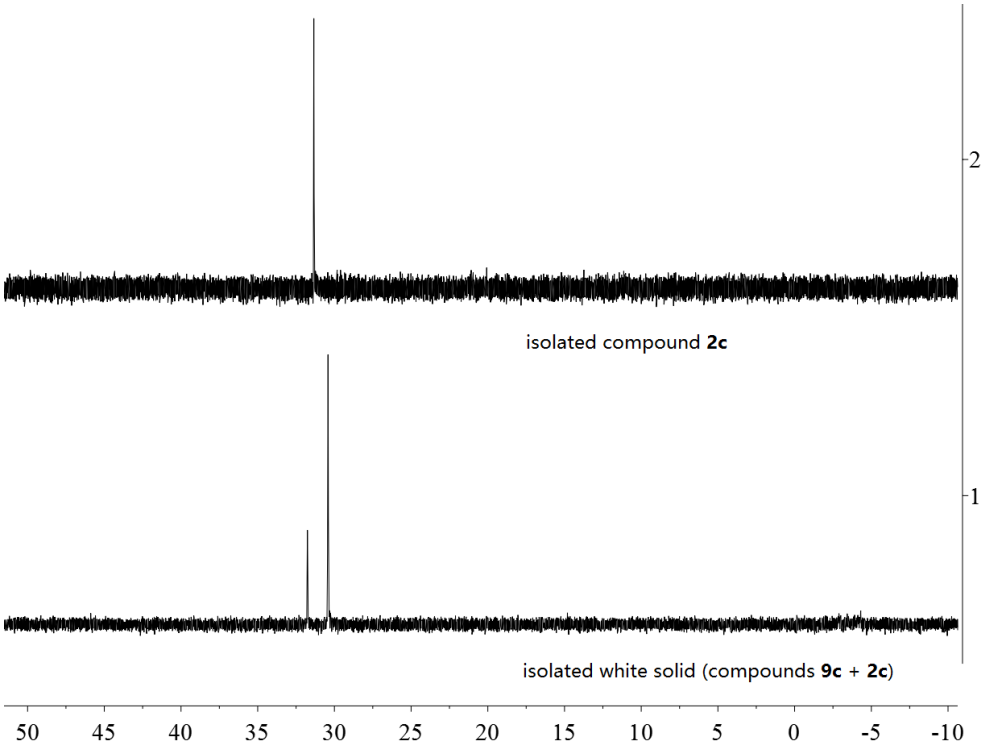
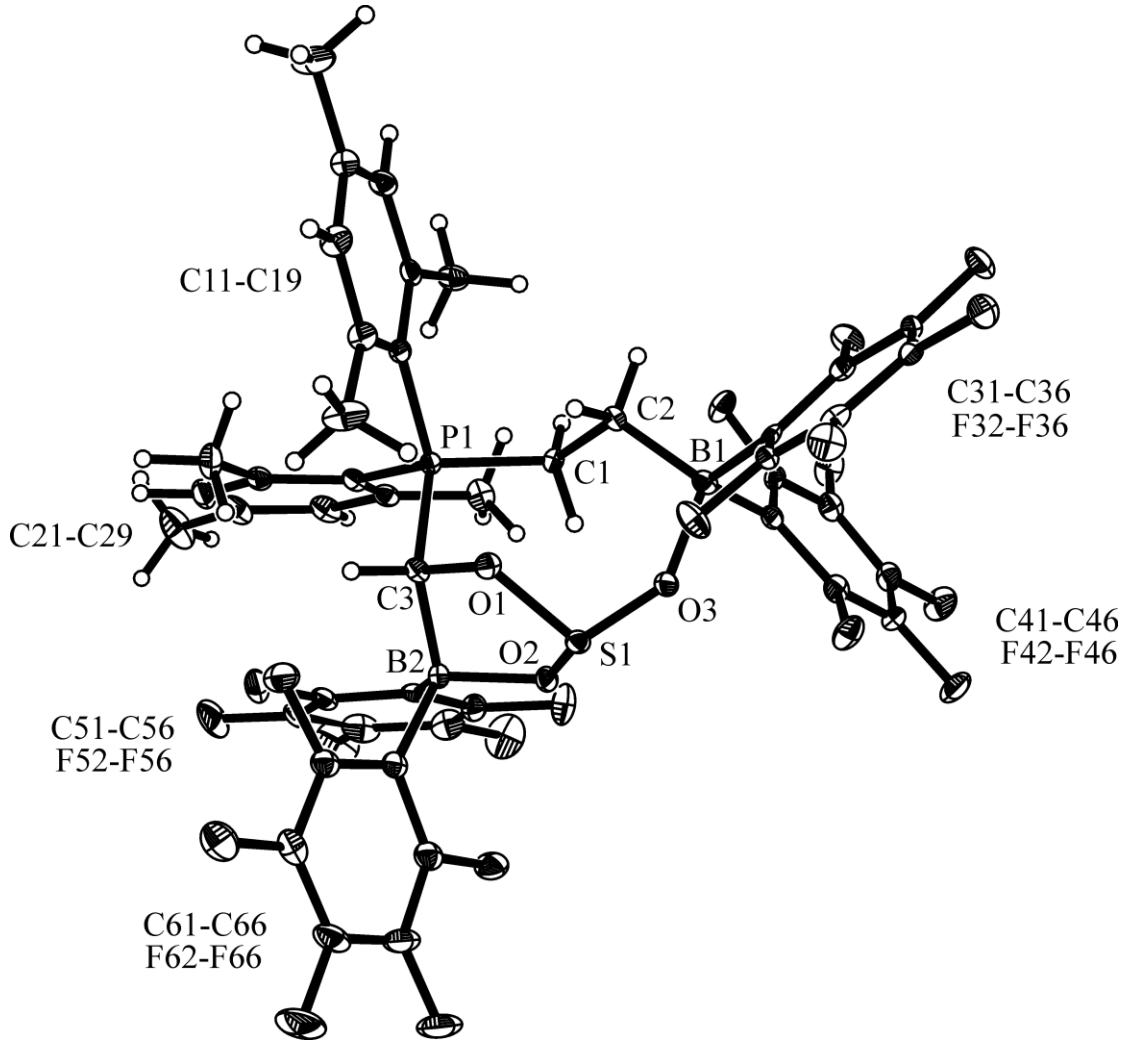


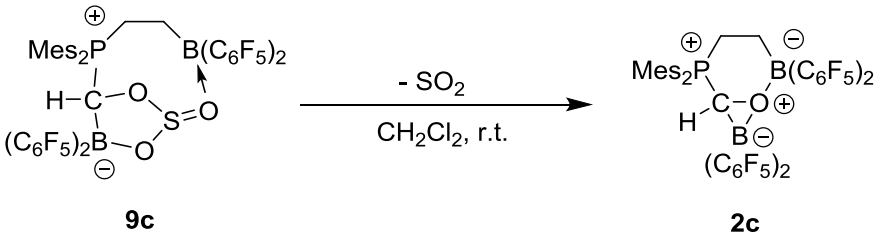

**Figure S9**: (1) **$^{31}P$ NMR** (202 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtained white solid and (2) **$^{31}P$ NMR** (243 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of isolated compound **2c**

Crystals suitable for the X-ray crystal structure analysis were obtained from a solution of the obtained white solid in $CH_2Cl_2$ (1 mL) and *n*-pentane (1 mL) at -30 $^oC$.

**Figure S10**: **X-ray crystal structure analysis of compound 9c:** A colorless prism-like specimen of $C_{46}H_{29}B_2Cl_2F_{20}O_3PS$, approximate dimensions 0.102 mm x 0.137 mm x 0.273 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. A total of 654 frames were collected. The total exposure time was 4.54 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 45435 reflections to a maximum θ angle of 25.35° (0.83 Å resolution), of which 8509 were independent (average redundancy 5.340, completeness = 99.9%, $R_{int}$ = 4.27%, $R_{sig}$ = 3.19%) and 6859 (80.61%) were greater than $2\sigma(F^2)$. The final cell constants of a = 10.6838(5) Å, b = 11.7958(5) Å, c = 20.5532(9) Å, α = 81.9990(10)°, β = 81.4810(10)°, γ = 65.8300(10)°, volume = 2328.18(18) $Å^3$, are based upon the refinement of the XYZ-centroids of 9897 reflections above 20 σ(I) with 4.451° < 2θ < 55.01°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.952. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9120 and 0.9660. The final anisotropic full-matrix least-squares refinement on $F^2$ with 682 variables converged at R1 = 3.70%, for the observed data and wR2 = 9.17% for all data. The goodness-of-fit was 1.020. The largest peak in the final difference electron density synthesis was 0.369 $e^-/Å^3$ and the largest hole was -0.573 $e^-/Å^3$ with an RMS deviation of 0.062 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.662 $g/cm^3$ and F(000), 1168 $e^-$.


C11-C19
C31-C36
F32-F36
P1
C2
B1
C1
C21-C29
C3
O1
O3
C41-C46
F42-F46
B2
O2
S1
C51-C56
F52-F56
C61-C66
F62-F66

$SO_2$ release of compound **9c** in solution (NMR scale)




**9c** **2c**

Scheme S2

A solution of the isolated white solid (see above: *Preparation of compound **9c***) (20.3 mg, 0.019 mmol) in [$D_2$]-dichloromethane (1.0 mL) was stirred at room temperature overnight. Then the reaction mixture was characterized by NMR experiments.
Comment: the NMR spectra showed the formation of compound **2c**.
[Compound **2c** see: M. Sajid, L.-M. Elmer, C. Rosorius, C. G. Daniliuc, S. Grimme, G. Kehr and G. Erker, *Angew. Chem. Int. Ed.* 2013, **52**, 2243-2246.]

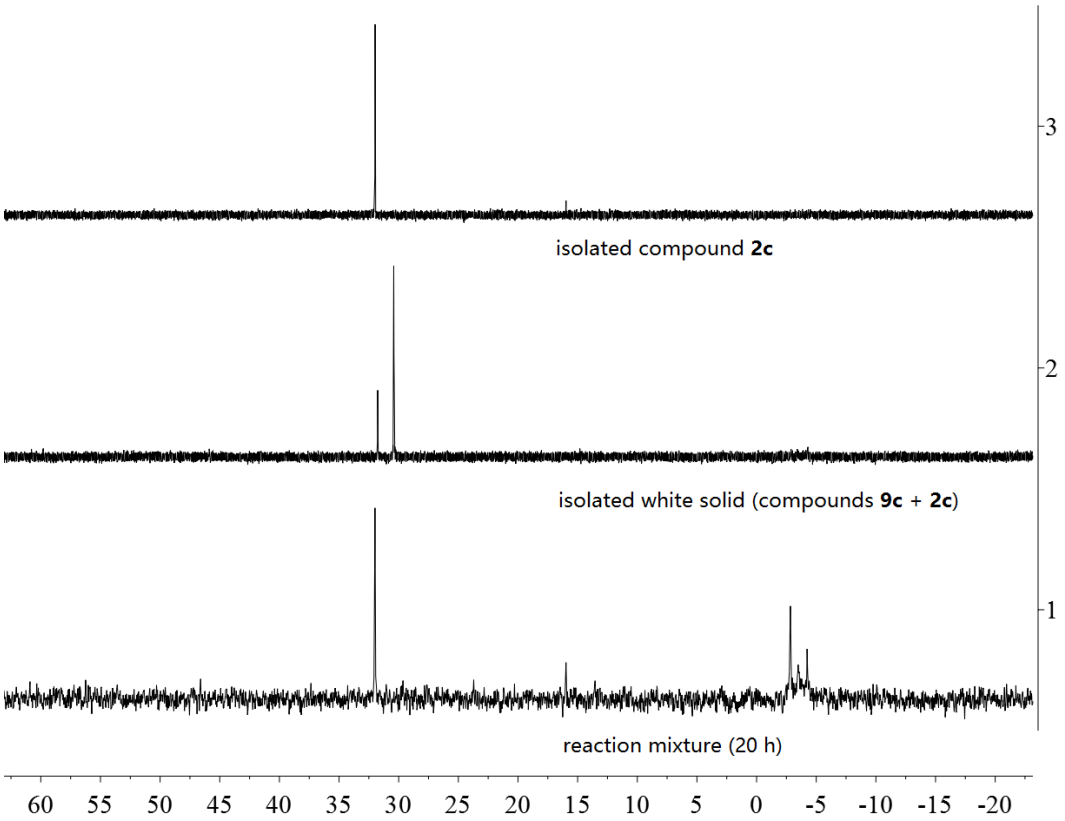
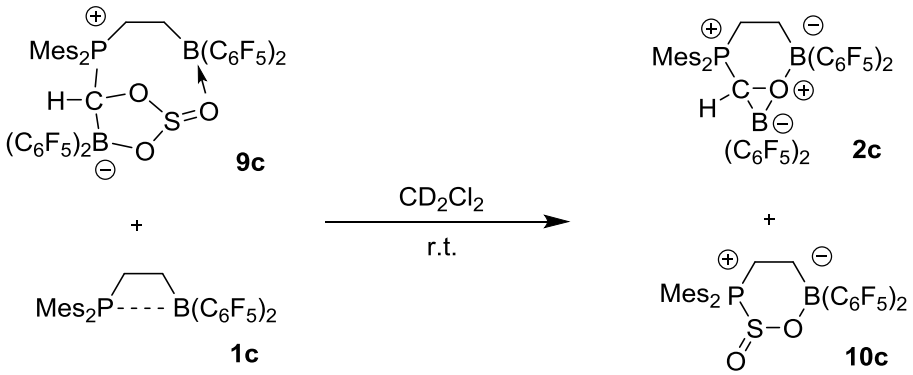



**Figure S11**: (1) **$^{31}$P NMR** (202 MHz, [$D_2$]-dichloromethane, 299 K) spectrum of the reaction mixture (20 h) [$\delta$ $^{31}$P = 32.0 ($\nu_{1/2}$ ~ 12 Hz)]; (2) **$^{31}$P NMR** (202 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid [$\delta$ $^{31}$P = 31.8 ($\nu_{1/2}$ ~ 8 Hz, compound **2c**) and 30.4 ($\nu_{1/2}$ ~ 8 Hz, compound **9c**)]; (3) **$^{31}$P NMR** (202 MHz, [$D_2$]-dichloromethane, 299 K) spectrum of isolated compound **2c** [$\delta$ $^{31}$P = 32.0 ($\nu_{1/2}$ ~ 8 Hz)].

Reaction of compound **9c** with compound **1c** (NMR scale)




Scheme S3

A suspension of bis(pentafluorophenyl)borane (11.9 mg, 0.04 mmol, 1.0 eq) in [$D_2$]-dichloromethane (0.5 mL) was added to a solution of dimesitylvinylphosphine (13.8 mg, 0.04 mmol, 1.0 eq) in [$D_2$]-dichloromethane (0.5 mL). After stirring for 20 min the the isolated white solid (see above: *Preparation of compound **9c***) (43.2 mg, 0.040 mmol) was added to the reaction mixture at room temperature. Then, 10 min later, the mixture was characterized by NMR experiments. After the measurement the solution was stirred at room temperature for further 20 hours. Then the reaction mixture was characterized by NMR experiments.

The $^{31}$P NMR spectrum of the mixture after 10 min at room temperature showed a mixture of compounds **1c** (ca. 47 mol%), **9c** (ca. 35 mol%), **2c** (ca. 12 mol%)**,** and **10c** (ca. 6 mol%).[admixed with some compounds not identified yet ca. Σ14%]
After 20 hours at room temperature the $^{31}$P NMR spectrum showed a mixture of compounds **1c** (ca. 19 mol%), **9c** (ca. 2 mol%), **2c** (ca. 40 mol%)**,** and **10c** (ca. 39 mol%).[admixed with some compounds not identified yet ca. Σ17%]

[Compound **1c** see: P. Spies, G. Erker, G. Kehr, K. Bergander, R. Fröhlich, S. Grimme and D. W. Stephan, *Chem. Commun*. 2007, 5072-5074; compound **2c** see: M. Sajid, L.-M. Elmer, C. Rosorius, C. G. Daniliuc, S. Grimme, G. Kehr and G. Erker, *Angew. Chem. Int. Ed*. 2013, **52**, 2243-2246 and compound **10c** see: M. Sajid, A. Klose, B. Birkmann, L. Liang, B, Schirmer, T. Wiegand, H. Eckert, A. J. Lough, R. Fröhlich, C. G. Daniliuc, S. Grimme, D. W. Stephan, G. Kehr and G. Erker, *Chem. Sci*. 2013, **4**, 213-219.

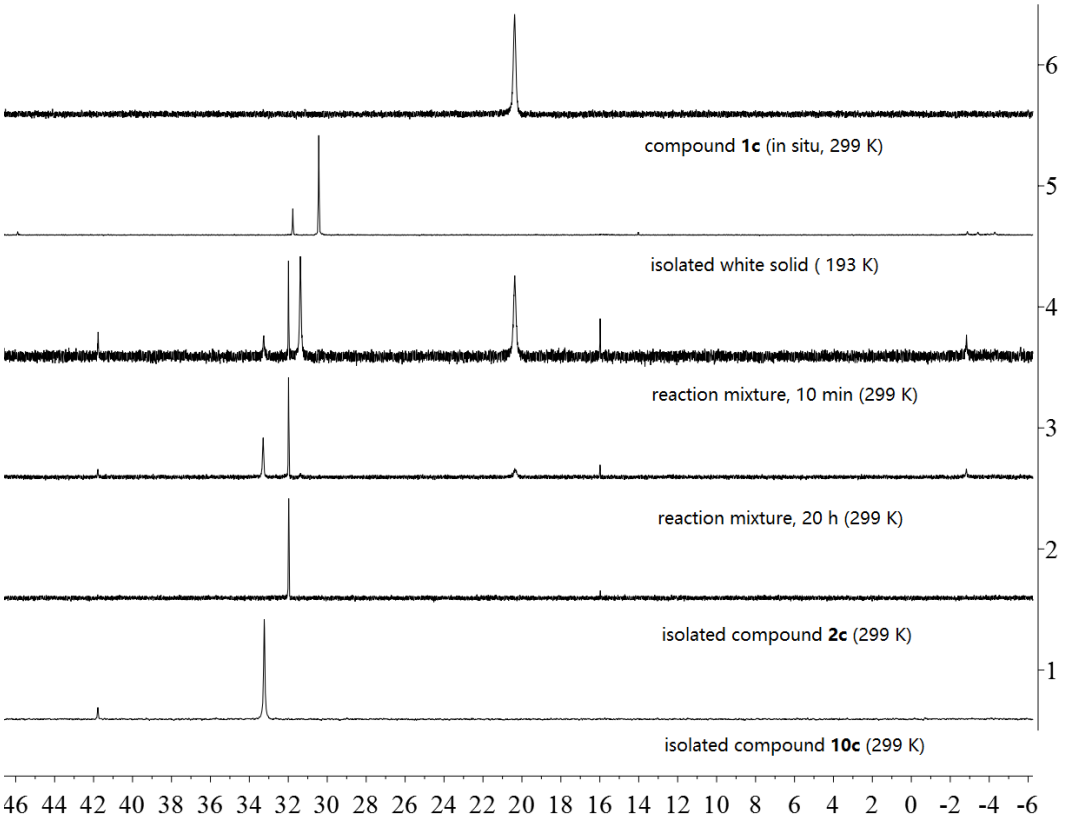
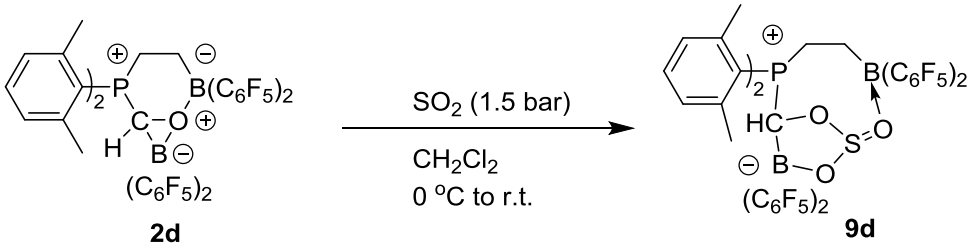



**Figure S12**: (1) **$^{31}$P NMR** (202 MHz, [$D_2$]-dichloromethane, 299 K) spectrum of isolated compound **10c** [$\delta^{31}$P = 33.2 ($\nu_{1/2}$ ~ 18 Hz)];
(2) **$^{31}$P NMR** (202 MHz, [$D_2$]-dichloromethane, 299 K) spectrum of isolated compound **2c** [$\delta^{31}$P = 32.0 ($\nu_{1/2}$ ~ 8 Hz)];
(3) **$^{31}$P NMR** (202 MHz, [$D_2$]-dichloromethane, 299 K) spectrum of the reaction mixture (20 h) [$\delta^{31}$P = 33.3 ($\nu_{1/2}$ ~ 18 Hz, **10c**) and 32.0 ($\nu_{1/2}$ ~ 8 Hz, **2c**)].
(4) **$^{31}$P NMR** (202 MHz, [$D_2$]-dichloromethane, 299 K) spectrum of the reaction mixture (10 min) [$\delta^{31}$P = 33.2 ($\nu_{1/2}$ ~ 18 Hz, **10c**), 32.0 ($\nu_{1/2}$ ~ 8 Hz, **2c**), 31.4 ($\nu_{1/2}$ ~ 18 Hz, **9c**), 20.4 ($\nu_{1/2}$ ~ 30 Hz, **1c**)].
(5) **$^{31}$P NMR** (202 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid [$\delta^{31}$P = 31.8 ($\nu_{1/2}$ ~ 8 Hz, **2c**) and 30.4 ($\nu_{1/2}$ ~ 8 Hz, **9c**)] (see above: *Preparation of compound **9c***);
(6) **$^{31}$P NMR** (202 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of compound **1c** (*in situ* generated) [$\delta^{31}$P = 20.4 ($\nu_{1/2}$ ~ 30 Hz)];

Preparation of compound **9d**




Scheme S4

Compound **2d** (320.7 mg, 0.32 mmol) was dissolved in dichloromethane (20.0 mL) at room temperature. The solution was degassed by freeze-pump-thaw cycles (×2). Then the cooled (0 °C) reaction mixture was carefully evacuated and exposed to $SO_2$ gas (1.5 bar). After the reaction mixture was stirred at room temperature for 4 days, all volatiles were removed in *vacuo* to give compound **9d** (284.5 mg, 0.27 mmol, 84%) as a white solid.

**IR (KBr)** [white solid]: $\tilde{\nu}$ ($cm^{-1}$) = 3065 (w), 2981 (m), 2937 (m), 1647 (s), 1519 (s), 1462 (s), 1388 (s), 1289 (s), 1246 (m), 1093 (s), 974 (s), 867 (m), 777 (s), 740 (m), 685 (s).
**Decomposition point** [white solid]: 109 °C

The NMR data of a solution of the obtained white solid in [$D_2$]-dichloromethane showed a mixture of compound **9d** (ca 78 mol%) and compound **2d** (ca 22 mol% ($^{31}$P)).

**$^1$H NMR (**500 MHz, [$D_2$]-dichloromethane, 193 K) [all resonances are broadened]: δ = 7.42 (t, $^3J_{HH}$ = 7.8 Hz), 7.28 (br m), 7.24 (t, $^3J_{HH}$ = 7.8 Hz), 7.07 (br m), 7.05 (br m), 6.72 (br m)(each 1H, *m*,*p*-Ar), 6.73 (br d, , $^3J_{HH}$ ~ 10 Hz, 1H, OCH), 3.35, 2.97 (br, each 1H, $PCH_2$), 3.05, 2.23, 2.21, 1.99 (each s, each 3H, *o*-$CH_3^{Ar}$), 1.16 (br m, 2H, $BCH_2$).
**$^{13}$C{$^1$H} NMR** (126 MHz, [$D_2$]-dichloromethane, 193 K)[selected resonances]: δ = 143.7 (d, $^2J_{PC}$ = 7.9 Hz), 142.2 (d, $^2J_{PC}$ = 8.7 Hz), 141.7 (d, $^2J_{PC}$ = 10.0 Hz), 141.0 (d, $^2J_{PC}$ = 14.4 Hz)(*o*-Ar), 133.0 (br), 132.9 (br), 131.7 (d, $^3J_{PC}$ = 10.0 Hz, 2×C), 131.3 (d, $^3J_{PC}$ = 10.0 Hz), 130.3 (d, $^3J_{PC}$ = 11.2 Hz)(*p*,*m*-Ar), 120.2 (d, $^1J_{PC}$ = 72.1 Hz), 118.6 (d, $^1J_{PC}$ = 67.4 Hz)(*i*-Ar), 70.3 (m, OCH), 25.0 (br), 23.0 (d, $^3J_{PC}$ = 2.0 Hz), 22.2 (dd, *J* = 5.0 Hz, *J* = 2.7 Hz), 21.8 (d, $^3J_{PC}$ = 6.1 Hz)(*o*-$CH_3^{Ar}$), 21.5 (br d, $^1J_{PC}$ ~ 40 Hz, $PCH_2$), 15.4 (br, $BCH_2$), [$C_6F_5$ not listed].
**$^{11}$B{$^1$H} NMR** (160 MHz, [$D_2$]-dichloromethane, 193 K): δ = no resonance observed
**$^{19}$F NMR** (470 MHz, [$D_2$]-dichloromethane, 193 K): δ = -128.3 (1F), -132.4 (1F), -135.3 (1F), -135.6 (4F), -139.3 (1F)(each br m, *o*-$C_6F_5$), -155.3, -156.3, -157.5, -158.0 (each t, $^3J_{FF}$ = 20.8 Hz, each 1F, *p*-$C_6F_5$), -162.4 (2F), -162.7 (1F), -163.4 (1F), -163.7 (2F), -164.1 (2F)(each br m, *m*-$C_6F_5$).
**$^{31}$P{$^1$H}** NMR (202 MHz, [$D_2$]-dichloromethane, 193 K): δ = 31.2 ($\nu_{1/2}$ ~ 10 Hz).

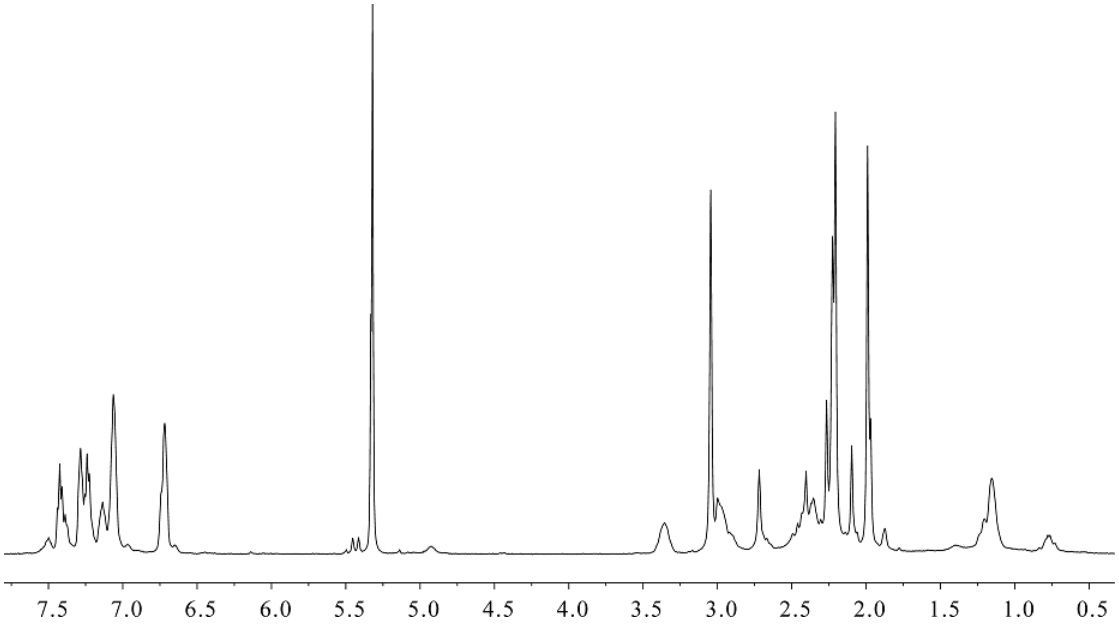



**Figure S13**: **$^1$H NMR** (500 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the isolated solid

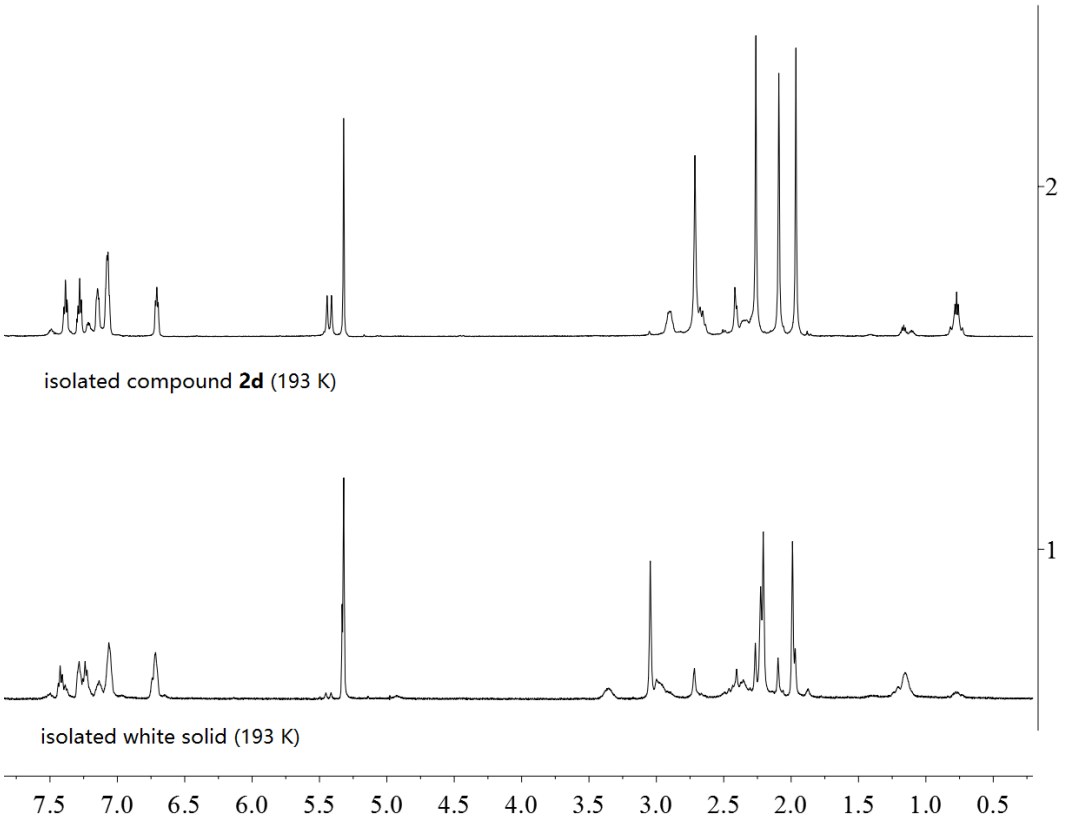



**Figure S14**: (1) **$^1$H NMR** (500 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid and (2) **$^1$H NMR** (600 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of isolated compound **2d**

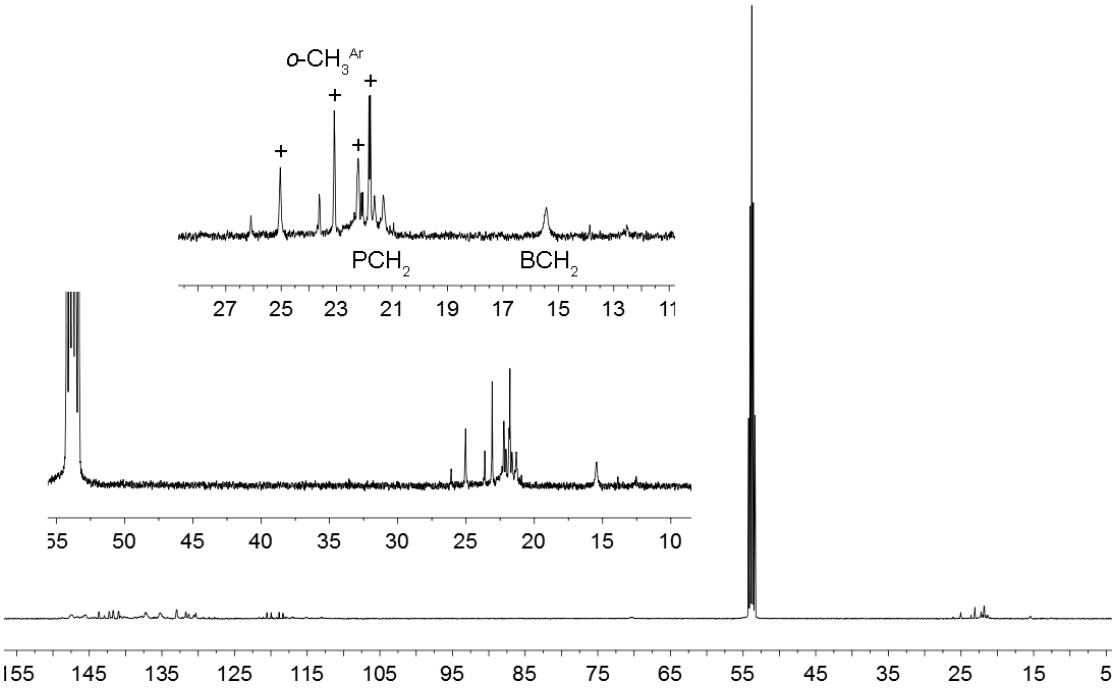



**Figure S15**: **$^{13}C\{^{1}H\}$ NMR** (126 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtaiened white solid (* pentane)

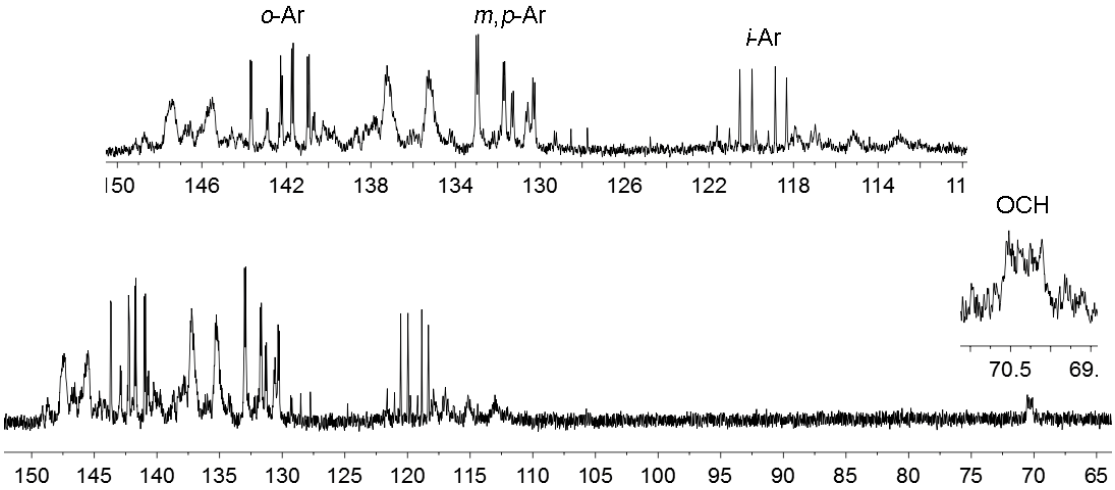



**Figure S16**: **$^{13}C\{^{1}H\}$ NMR** (126 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtained white solid

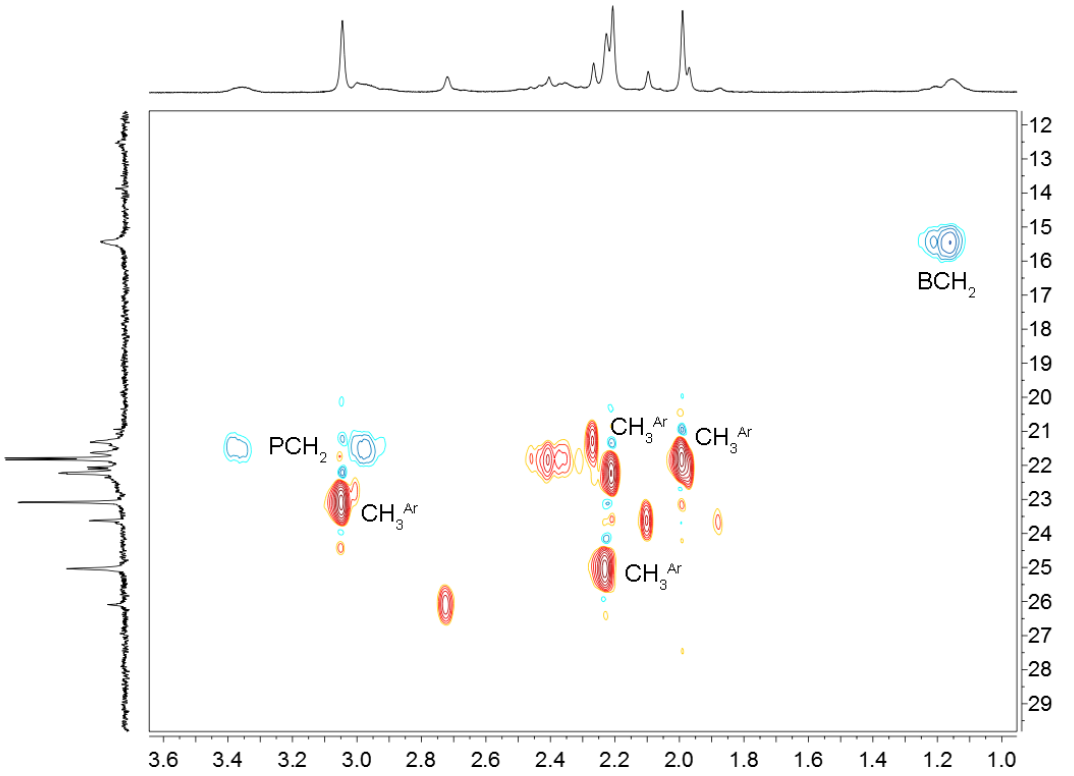



**Figure S17**: $^{1}H,^{13}C$ ghsqc (500/126 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtained white solid

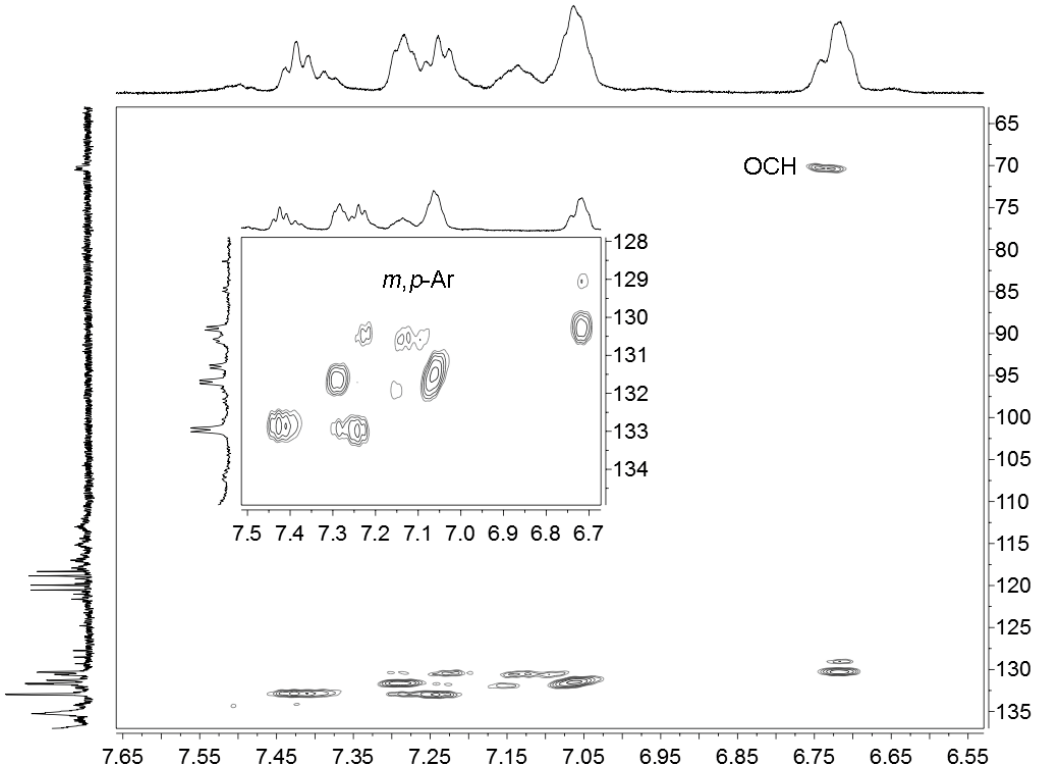



**Figure S18**: $^{1}H,^{13}C$ ghsqc (500/126 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtained white solid

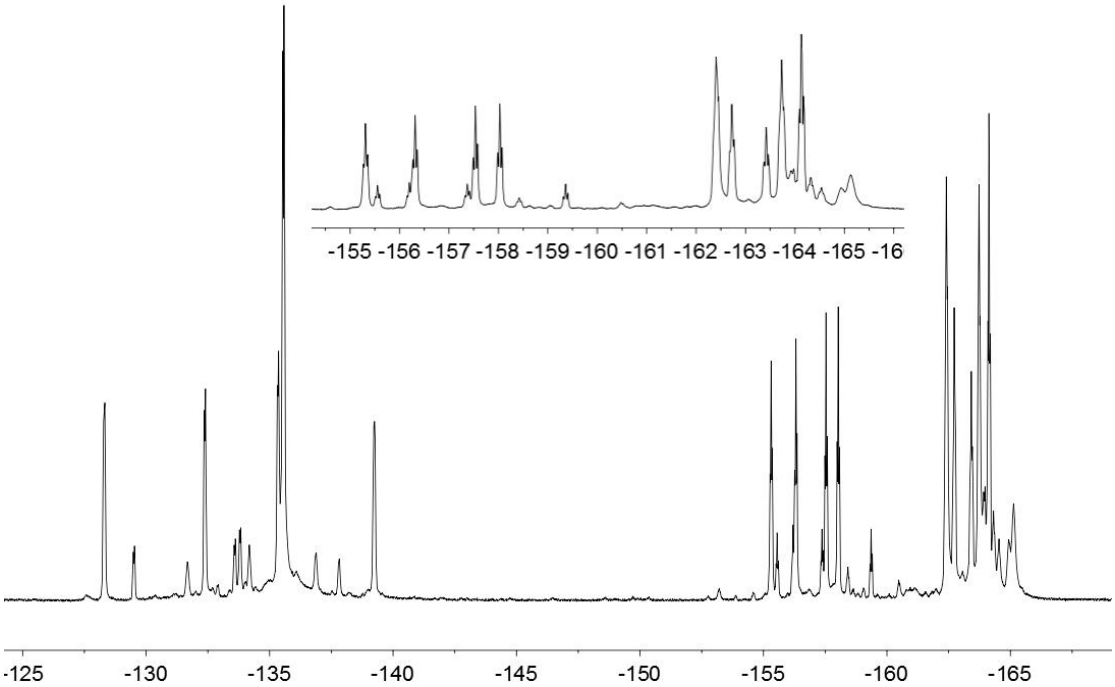



**Figure S19**: **$^{19}$F NMR** (470 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid

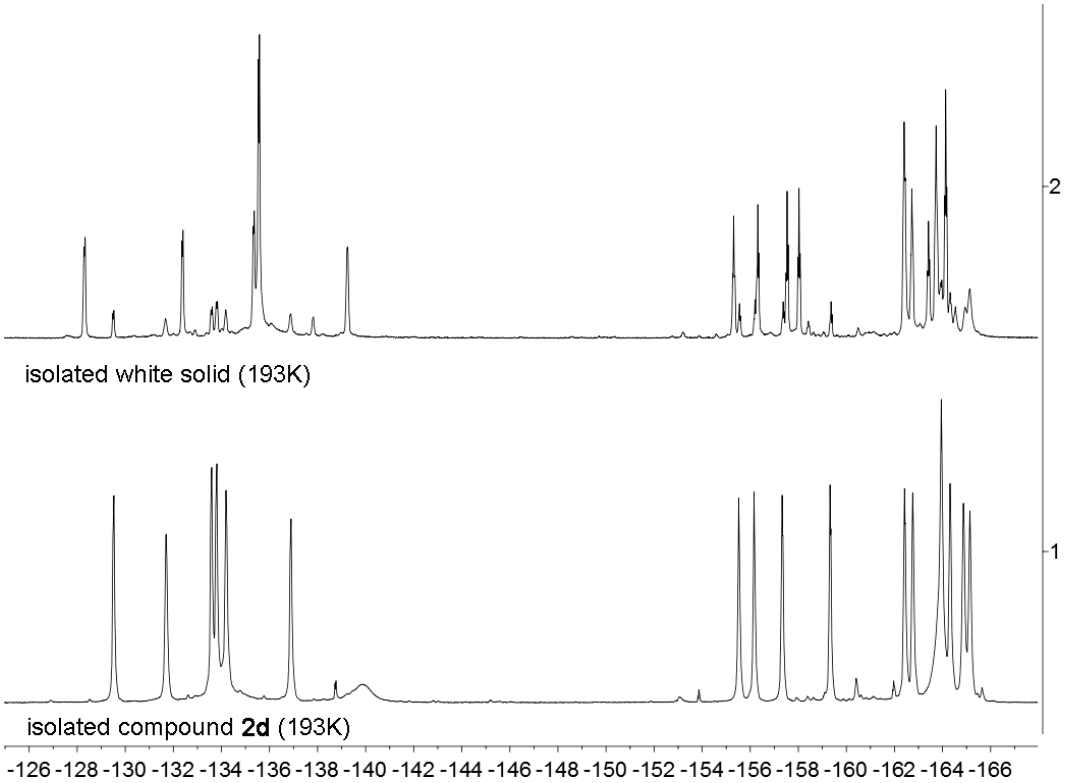



**Figure S20**: (2) **$^{19}$F NMR** (470 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid and (1) **$^{1}$H NMR** (564 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of isolated compound **2d**

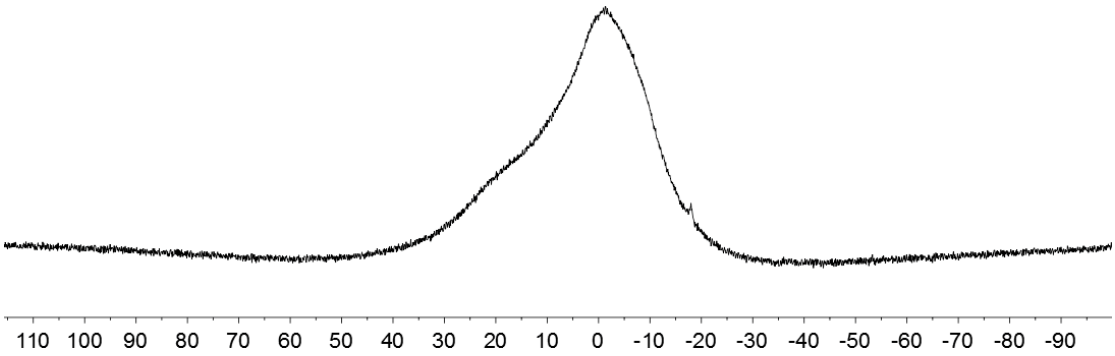



**Figure S21**: **$^{11}B\{^{1}H\}$ NMR** (160 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid

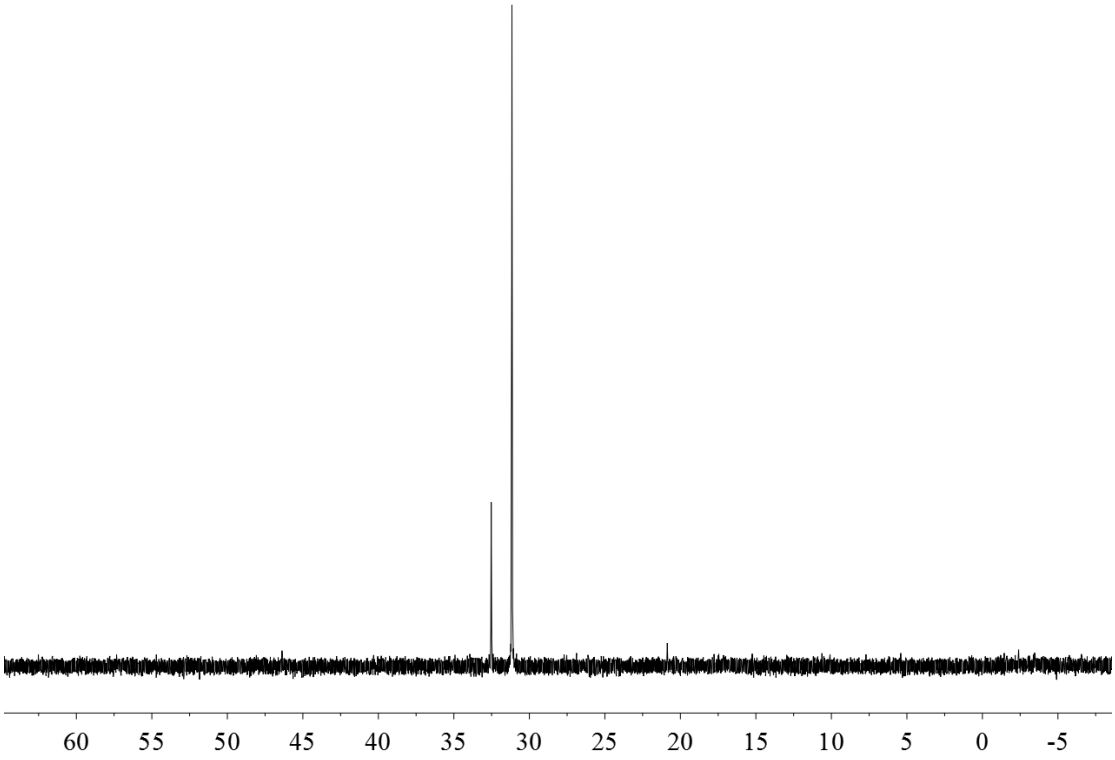



**Figure S22**: **$^{31}P\{^{1}H\}$ NMR** (202 MHz, [$D_2$]-dichloromethane, 193 K) spectrum of the obtained white solid

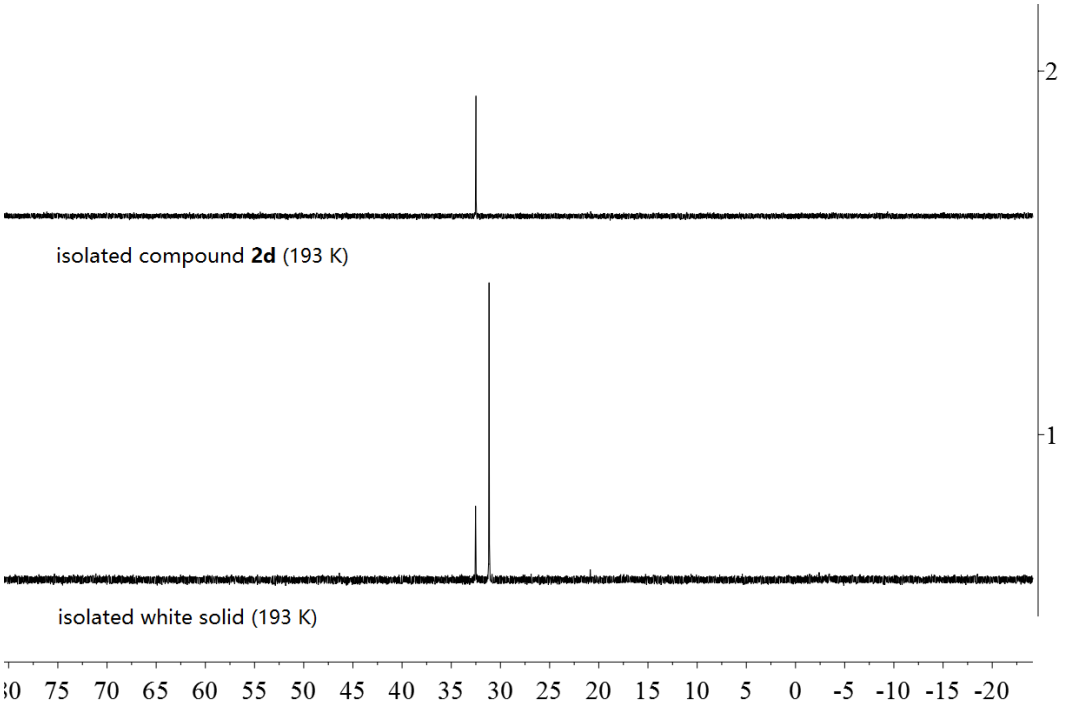
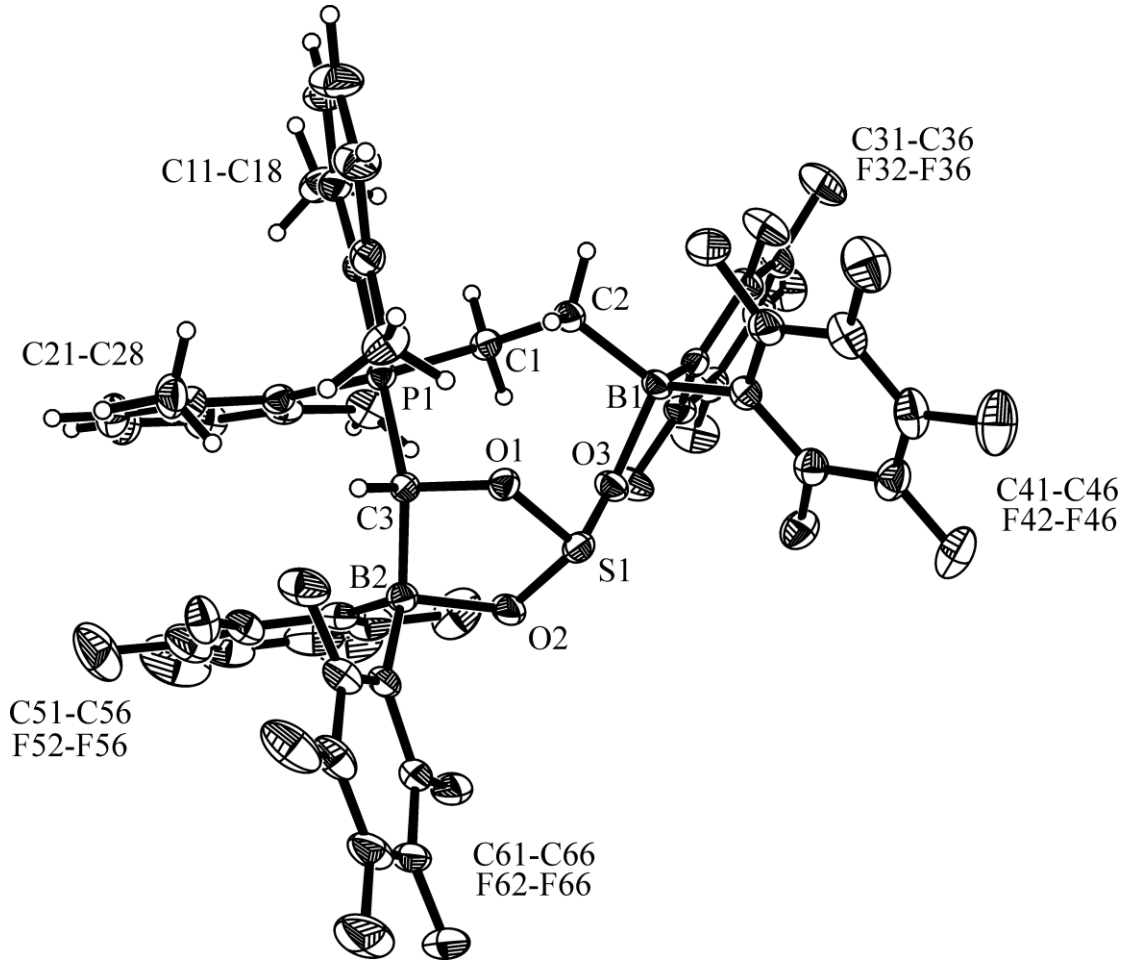



**Figure S23**: (1) **$^{31}$P NMR** (202 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of the obtained white solid and (2) **$^{31}$P NMR** (243 MHz, $[D_2]$-dichloromethane, 193 K) spectrum of isolated compound **2d**

Crystals suitable for the X-ray crystal structure analysis were obtained from a solution of the obtained white solid in $CH_2Cl_2$ (1 mL) and *n*-pentane (1 mL) at -30 °C.

**Figure S24**: **X-ray crystal structure analysis of compound 9d:** formula $C_{43}H_{23}B_2F_{20}O_3PS$, $M$ = 1052.26, colourless crystal, 0.06 x 0.04 x 0.04 mm, $a$ = 19.657(3), $b$ = 18.1222(3), $c$ = 23.6282(4) Å, $\beta$ = 99.171(1)°, $V$ = 8307.6(2) Å$^3$, $\rho_{calc}$ = 1.683 gcm$^{-3}$, $\mu$ = 0.250 mm$^{-1}$, empirical absorption correction (0.985 ≤ T ≤ 0.990), $Z$ = 8, monoclinic, space group $C2/c$ (No. 15), $\lambda$ = 0.71073 Å, $T$ = 223(2) K, $\omega$ and $\varphi$ scans, 38620 reflections collected ($\pm h$, $\pm k$, $\pm l$), 7281 independent ($R_{int}$ = 0.057) and 5697 observed reflections [$I>2\sigma(I)$], 635 refined parameters, $R$ = 0.049, $wR^2$ = 0.109, max. (min.) residual electron density 0.26 (-0.27) e.Å$^{-3}$, the hydrogen atoms were calculated and refined as riding atoms.


C11-C18
C31-C36
F32-F36
C2
C21-C28
C1
P1
B1
O1
O3
C3
C41-C46
F42-F46
S1
B2
O2
C51-C56
F52-F56
C61-C66
F62-F66

## Computational Details

All quantum chemical calculations were performed with the TURBOMOLE 7.0.2 program package.[S1] Geometry optimizations were conducted applying dispersion corrected DFT using the PBEh-3c method.[S2] The resolution-of-identity (RI) approximation for Coulomb integrals[S3] with matching default auxiliary basis sets[S4] was generally applied. The numerical quadrature grid m4 was employed as implemented in TURBOMOLE for the integration of the exchange-correlation contributions.[S5] TURBOMOLE default convergence criteria for energies and gradients were used. The optimized structures were verified as minima on the potential energy hyper surface by the absence of imaginary frequencies in the harmonic frequency calculation.

Ro-vibrational corrections to the free energies were obtained from a modified rigid rotor harmonic oscillator statistical treatment[S6] at a temperature of 298.15 K and 1 atm pressure based on analytical harmonic frequencies calculated at PBEh-3c level (geometry optimization level of theory). All frequencies were scaled by a factor of 0.95.[S2] Frequencies with wave numbers below 100 $cm^{-1}$ were treated partially as rigid rotors to avoid errors in the harmonic approximation (see Ref. [S6] for details). If present, small artificial imaginary modes below wave numbers of 30 $cm^{-1}$ were inverted and included in the entropy and enthalpy calculations.

Solvation effects were considered by the means of the COSMO-RS model[S7] as implemented in COSMOtherm version C3.0, release 16.01[S8] with the 2014 parametrization for dichloromethane (parameter file: BP_TZVP_C30_1401.ctd; Gsolv=reference option). Single point calculations were conducted at the default BP86[S9]/def-TZVP[S10] level of theory on optimized geometries. All solvation corrections were calculated for dichloromethane at a temperature of 298.15 K.

Gas phase single point energies were calculated at the PW6B95[S11] level of theory using the large def2-QZVP[S12] quadruple-$\zeta$ basis set and the m5 numerical grid.[S5] The D3 dispersion correction scheme[S13] applying Becke-Johnson (BJ) damping[S14] and including three-body-contributions (ATM) was used for single point calculations. Details about the D3 dispersion correction and its application can be found in Ref. [S15]. For a review on this topic see Ref. [S16].

Reaction path optimizations were performed with the Woelfling program[S17] as implemented in TURBOMOLE 7.0.2 in combination with a development version of the recently developed semi-empirical xTB method.[S18] Transition state structures were further refined at the PBEh-3c level of theory and verified by the existence of one large imaginary frequency with $i\omega > 30$ $cm^{-1}$.

Final free energies $G_{tot}$ were obtained from the sum of the single point energy $E$, the dispersion correction $E_{D3,\,atm}$, the ro-vibrational correction $G_{RRHO}$ and the solvation correction $\delta G_{solv}$ (Eq. 1).

$$G_{tot} = E + E_{D3,\,atm} + G_{RRHO} + \delta G_{solv} \qquad \text{(Equation 1)}$$


[S1] a) R. Ahlrichs, K. M. Armbruster, M. Bär, H.-P. Baron, R. Bauernschmitt, N. Crawford, P. Deglmann, M. Ehrig, K. Eichkorn, S. Elliott, F. Furche, F. Haase, M. Häser, C. Hättig, A. Hellweg, H. Horn, C. Huber, U. Huniar, M. Kattannek, C. Kölmel, M. Kollwitz, K. May, P. Nava, C. Ochsenfeld, H. Öhm, H. Patzelt, D. Rappoport, O. Rubner, A. Schäfer, U. Schneider, M. Sierka, O. Treutler, B. Unterreiner, M. von Arnim, F. Weigend, P. Weis, H. Weiss, *TURBOMOLE 7.0*, Universität Karlsruhe: Karlsruhe, Germany, **2015**. See also http://www.turbomole.com; b) F. Furche, R. Ahlrichs, C. Hättig, W. Klopper, M. Sierka, F. Weigend, *WIREs Comput. Mol. Sci.* **2014**, *4*, 91-100.

[S2] S. Grimme, J. G. Brandenburg, C. Bannwarth, A. Hansen, *J. Chem. Phys.* **2015**, *143*, 054107.

[S3] K. Eichkorn, O. Treutler, H. Öhm, M. Häser, R. Ahlrichs, *Chem. Phys. Lett.* **1995**, *242*, 652-660.

[S4] F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057-1065.

[S5] K. Eichkorn, F. Weigend, O. Treutler, R. Ahlrichs, *Theor. Chem. Acc.* **1997**, *97*, 119-124.

[S6] S. Grimme, *Chem. Eur. J.* **2012**, *18*, 9955-9964.

[S7] a) A. J. Klamt, *Chem. Phys.* **1995**, *99*, 2224-2235; b) F. Eckert, A. J. Klamt, *AIChE J.* **2002**, *48*, 369-385.

[S8] F. Eckert, A. J. Klamt, L. Pohler, COSMOtherm, Version C3.0, Release 16.01; COSMOlogic GmbH & Co. KG, Leverkusen, Germany, **2015**.

[S9] a) A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098-3100; b) J. P. Perdew, *Phys. Rev. B* **1986**, *33*, 8822-8824.

[S10] A. Schäfer, C. Huber, R. J. Ahlrichs, *Chem. Phys.* **1994**, *100*, 5829-5835.

[S11] Y. Zhao, D. G. Truhlar, *J. Phys. Chem. A* **2005**, *109*, 5656-5667.

[S12] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

[S13] S. Grimme, J. Antony, S. Ehrlich, H. J. Krieg, *Chem. Phys.* **2010**, *132*, 154104.

[S14] a) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456-1465; b) A. D. Becke, E. R. J. Johnson, *Chem. Phys.* **2005**, *123*, 154101.

[S15] a) S. Grimme, J. Antony, T. Schwabe, C. Mück-Lichtenfeld, *Org. Biomol. Chem.* **2007**, *5*, 741-758; b) S. Grimme, *WIREs Comput. Mol. Sci.* **2011**, *1*, 211-228; c) A. Gansäuer, C. Kube, K. Daasbjerg, R. Sure, S. Grimme, G. D. Fianu, D. V. Sadasivam, R. A. Flowers, II, *J. Am. Chem. Soc.* **2014**, *136*, 1663-1671; d) S. Grimme, H. Kruse, L. Goerigk, G. Erker, *Angew. Chem. Int. Ed.* **2010**, *49*, 1402-1405; *Angew. Chem.* **2010**, *122*, 1444-1447; e) T. Schwabe, S. Grimme, J.-P. Djukic, *J. Am. Chem. Soc.* **2009**, *131*, 14156-14157; f) H. Kruse, S. Grimme, *J. Phys. Chem. C* **2009**, *11*, 17006-

17010, g) C. M. Mömming, S. Frömel, G. Kehr, R. Fröhlich, S. Grimme, G. Erker, *J. Am. Chem. Soc.* **2009**, *131*, 12280-12289.

[S16] S. Grimme, A. Hansen, J. G. Brandenburg, C. Bannwarth, *Chem. Rev.* **2016**, *116*, 5105-5154.

[S17] P. Plessow, *J. Chem. Theory Comput.* **2013**, *9*, 1305.

[S18] S. Grimme, C. Bannwarth, *J. Chem. Phys.* **2016**, *145*, 054103.

## Absolute energy contributions

***Table 1.*** Absolute energy contributions to $G_{tot}$ and the largest imaginary frequency (ImF in $cm^{-1}$). All energy values in kcal $mol^{-1}$.

| Structure | ImF | PBEh-3c | PW6B95/ def2-QZVP | $E_{D3,\ atm}$[(a)] | $G_{RRHO}$ (298.15 K) | $G_{solv}$ ($CH_2Cl_2$) | $G_{tot}$ | ΔG |
|---|---|---|---|---|---|---|---|---|
| $2c_{calc}$ | 0 | -2626695.72 | -4200.72 | -64.89 | 339.56 | -26.64 | -2635744.13 | 0.0 |
| TS1 | *i*43.42 | -2626676.14 | -2635973.33 | -65.01 | 339.45 | -25.93 | -2635724.80 | 19.3 |
| $INT1_{calc}$ | 0 | -2626678.60 | -2635976.96 | -63.01 | 338.98 | -27.19 | -2635728.17 | 16.0 |
| $SO_2$ | 0 | -343767.69 | -344638.53 | -0.43 | -11.19 | -0.18 | -344650.33 | - |
| TS2 | *I*68.17 | -2970453.23 | -2980612.07 | -70.35 | 342.71 | -25.97 | -2980365.68 | 28.8 |
| $INT2_{calc}$ | 0 | -2970476.58 | -2980632.2 | -71.08 | 345.6 | -26.93 | -2980384.61 | 9.8 |
| TS3 | *i*68.25 | -2970463.55 | -2980622.86 | -69.2 | 344.59 | -27.18 | -2980374.66 | 19.8 |
| $9c_{calc}$ | 0 | -2970486.66 | -2980641.79 | -67.58 | 344.42 | -28.57 | -2980393.52 | 0.9 |
| TS4 | *i*46.94 | -2626676.35 | -2635975.35 | -63.86 | 339.33 | -25.30 | -2635725.18 | 19.0 |
| $2c_{open,\ calc}$ | 0 | -2626682.03 | -2635979.94 | -64.79 | 338.74 | -25.06 | -2635731.06 | 13.1 |
| $INT3_{e,\ calc}$ | 0 | -2970474.36 | -2980633.93 | -67.61 | 343.61 | -26.42 | -2980384.35 | 10.1 |
| $TS5_e$ | *i*149.79 | -2970439.11 | -2980599.28 | -67.76 | 342.34 | -31.75 | -2980356.44 | 38.0 |
| $INT3_{c,\ calc}$ | 0 | -2970474.16 | -2980632.88 | -67.24 | 343.17 | -27.86 | -2980384.81 | 9.6 |
| $TS5_c$ | *i*451.90 | -2970431.41 | -2980595.64 | -68.29 | 342.25 | -30.97 | -2980352.65 | 41.8 |

(a) Added dispersion energy correction for PW6B95.

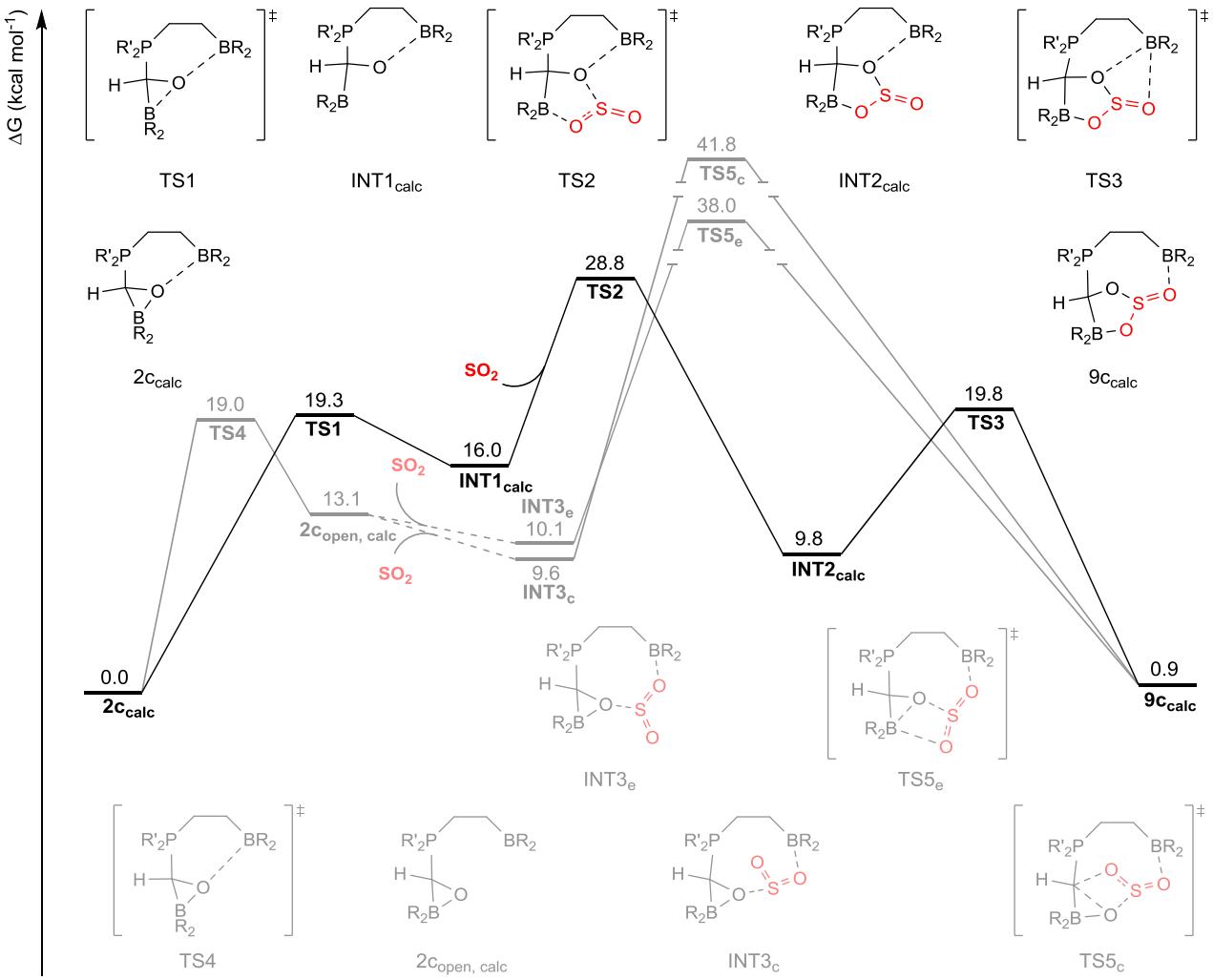



***Figure 1.*** Relative Gibbs free energy diagram of the reaction path leading to the formation of compound **9c$_{calc}$**. The paths colored in grey are much less probable possibilities. All values in kcal mol$^{-1}$ are given relative to compound **2c$_{calc}$**. R = $C_6F_5$; R' = Mes.

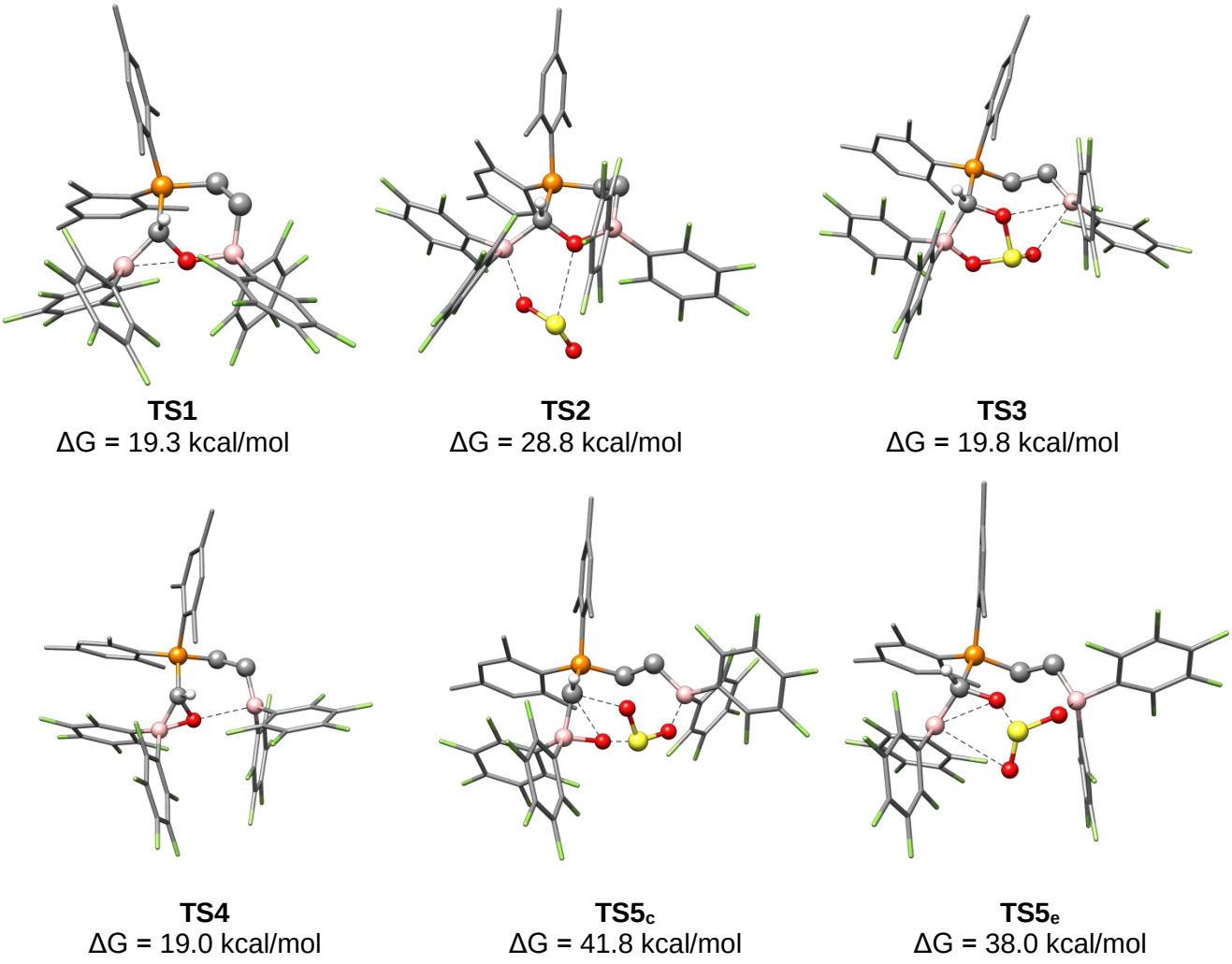



***Figure 2.*** Depiction of the calculated transition states involved in the proposed reaction paths leading to the formation of **9c**. Most hydrogen atoms are omitted for clarity. All values in kcal $mol^{-1}$. C = grey; H = white; B = pink; P = orange; F = green; S = yellow.

## Atomic cartesian coordinates in Å

**$SO_2$**

3

| | | | |
|---|---|---|---|
| S | -0.2975230 | -0.3871147 | 0.0000000 |
| O | 1.1340970 | -0.5637461 | 0.0000000 |
| O | -0.8365740 | 0.9508608 | 0.0000000 |

**$2c_{calc}$**

96

| | | | |
|---|---|---|---|
| P | 0.34930080 | -1.26904040 | -0.10692200 |
| O | 0.32940380 | 1.34302350 | 0.43597920 |
| B | 1.70298750 | 1.55002250 | 1.18227920 |
| B | -1.07927390 | 1.39968750 | -0.13121360 |
| C | 0.08808120 | 0.45558310 | -0.64730270 |
| H | 0.60353950 | 0.72598030 | -1.55338910 |
| C | 1.20291700 | -1.03222130 | 1.48575620 |
| H | 1.61952460 | -1.99114940 | 1.79635640 |
| H | 0.49034340 | -0.72144190 | 2.24361020 |
| C | 2.28998040 | 0.03012800 | 1.28339660 |
| H | 2.99905500 | -0.06546520 | 2.10300400 |
| H | 2.88188850 | -0.22227510 | 0.39583850 |
| C | 1.48305270 | -2.26156100 | -1.16031770 |
| C | 1.51487080 | -3.65372200 | -0.91266510 |
| C | 2.30697800 | -4.47073240 | -1.70716100 |
| H | 2.31526800 | -5.53530560 | -1.50321950 |
| C | 3.08543800 | -3.97565590 | -2.73912200 |
| C | 3.07501160 | -2.60746280 | -2.94012860 |
| H | 3.69726690 | -2.18993090 | -3.72255200 |
| C | 2.30615100 | -1.73312620 | -2.17800580 |
| C | 0.74575510 | -4.36011550 | 0.17035170 |
| H | 1.20397640 | -5.32685240 | 0.37202010 |
| H | 0.73854500 | -3.82532830 | 1.11663550 |
| H | -0.29036330 | -4.54304310 | -0.11211840 |
| C | 3.93912680 | -4.88364230 | -3.56958330 |
| H | 3.41148110 | -5.80134530 | -3.82822370 |
| H | 4.25456280 | -4.40544930 | -4.49539100 |
| H | 4.84045770 | -5.17077330 | -3.02512240 |
| C | 2.45330370 | -0.28164060 | -2.54562850 |
| H | 1.59160480 | 0.09937330 | -3.09542900 |
| H | 2.62977430 | 0.36113160 | -1.68702970 |
| H | 3.31172240 | -0.15698230 | -3.20251040 |
| C | -1.26035850 | -2.11341750 | -0.07777730 |
| C | -1.89290470 | -2.59234560 | 1.08543570 |
| C | -3.13548460 | -3.20143560 | 0.95488360 |
| H | -3.62378840 | -3.57038710 | 1.84914100 |
| C | -3.77243130 | -3.35697240 | -0.26662860 |
| C | -3.12765860 | -2.87667410 | -1.39548390 |
| H | -3.60609370 | -2.97759650 | -2.36260800 |
| C | -1.88694030 | -2.25939920 | -1.33075600 |
| C | -1.33587200 | -2.52478350 | 2.48106550 |
| H | -1.98315260 | -3.07128970 | 3.16380020 |
| H | -0.34499160 | -2.96660940 | 2.57088960 |
| H | -1.27197500 | -1.50914890 | 2.86448100 |
| C | -5.12334770 | -3.99552880 | -0.36397930 |
| H | -5.17598160 | -4.69304950 | -1.19964190 |
| H | -5.37938250 | -4.53869290 | 0.54417920 |
| H | -5.89248940 | -3.23895440 | -0.52299330 |
| C | -1.27999800 | -1.79052660 | -2.62365220 |
| H | -2.03164950 | -1.78847730 | -3.41056980 |
| H | -0.89636100 | -0.77267360 | -2.57596770 |
| H | -0.46911530 | -2.44322580 | -2.94889140 |
| C | 1.29019970 | 2.31988700 | 2.55069810 |
| C | 1.33865460 | 1.80147060 | 3.83358040 |
| F | 1.73628660 | 0.54139520 | 4.05430970 |
| C | 0.97747170 | 2.52118660 | 4.95899140 |
| F | 1.04328740 | 1.96940090 | 6.16685840 |
| C | 0.53926060 | 3.82369800 | 4.82199850 |
| F | 0.18606360 | 4.52515540 | 5.88984490 |
| C | 0.47076040 | 4.38815910 | 3.56248000 |
| F | 0.05438720 | 5.64022110 | 3.41909350 |
| C | 0.84908240 | 3.63348310 | 2.46814320 |
| F | 0.77290690 | 4.23121820 | 1.27652080 |
| C | 2.76583820 | 2.47592700 | 0.34900120 |
| C | 4.00049140 | 2.69377700 | 0.94623370 |
| F | 4.25267610 | 2.16370030 | 2.14780660 |
| C | 5.01263070 | 3.44447530 | 0.37746660 |
| F | 6.17203880 | 3.61243440 | 1.00319860 |
| C | 4.80724000 | 4.02231440 | -0.86142520 |
| F | 5.76370980 | 4.74129890 | -1.43329890 |
| C | 3.59542160 | 3.83955510 | -1.49675240 |
| F | 3.38359070 | 4.38798380 | -2.68870600 |
| C | 2.60932270 | 3.08394530 | -0.88348770 |
| F | 1.46440830 | 2.96488540 | -1.56665060 |
| C | -1.45631250 | 2.72064850 | -0.94018130 |
| C | -1.41740320 | 2.85058850 | -2.31648060 |
| F | -1.02920300 | 1.82706510 | -3.08561380 |
| C | -1.77692330 | 4.01528620 | -2.96911040 |
| F | -1.72227690 | 4.09820580 | -4.29393180 |
| C | -2.20131150 | 5.10304120 | -2.22841760 |
| F | -2.54849650 | 6.22626150 | -2.83899270 |
| C | -2.27237370 | 5.01181830 | -0.85016080 |
| F | -2.69297830 | 6.04899210 | -0.13812810 |
| C | -1.90527410 | 3.82768050 | -0.23937660 |
| F | -2.01229360 | 3.75856380 | 1.08790520 |
| C | -2.30470760 | 0.81002100 | 0.70539310 |
| C | -2.44728090 | 0.76566010 | 2.07715990 |
| F | -1.45729060 | 1.17771320 | 2.86987180 |
| C | -3.58495230 | 0.27493420 | 2.69801840 |
| F | -3.66234350 | 0.21846030 | 4.02285100 |

| | | | |
|---|---|---|---|
| C | -4.63805070 | -0.17589080 | 1.92682730 |
| F | -5.72682290 | -0.66687890 | 2.50287910 |
| C | -4.54762710 | -0.12328830 | 0.54713550 |
| F | -5.55867840 | -0.55485370 | -0.20032140 |
| C | -3.39353070 | 0.36389130 | -0.02875180 |
| F | -3.33135350 | 0.39702930 | -1.36159790 |

**TS1**

96

| | | | |
|---|---|---|---|
| P | 1.14034900 | -0.60481800 | -0.43730000 |
| O | -1.42937200 | -0.49730700 | 0.29780600 |
| B | -1.85864500 | -1.95253600 | 0.06901900 |
| B | -0.74579500 | 1.26920300 | 1.19355600 |
| C | -0.19575100 | -0.17206100 | 0.81247100 |
| H | 0.06614300 | -0.73633700 | 1.70128800 |
| C | 0.48633900 | -2.19784900 | -1.07504700 |
| H | 1.35428500 | -2.83148300 | -1.26592800 |
| H | -0.02089500 | -2.05242200 | -2.01895100 |
| C | -0.47700200 | -2.80984800 | -0.04615900 |
| H | -0.66480800 | -3.84041200 | -0.34323200 |
| H | 0.02174300 | -2.89999800 | 0.92612400 |
| C | 2.81880300 | -1.04628700 | 0.17296000 |
| C | 3.81325000 | -1.20917700 | -0.81617600 |
| C | 5.10843900 | -1.52830200 | -0.42882300 |
| H | 5.86282200 | -1.64202600 | -1.19889200 |
| C | 5.46436600 | -1.71155000 | 0.89630800 |
| C | 4.46394700 | -1.59501100 | 1.84588600 |
| H | 4.70834200 | -1.76168100 | 2.88823200 |
| C | 3.14961500 | -1.27984700 | 1.52077500 |
| C | 3.58478200 | -1.07344000 | -2.29715600 |
| H | 4.39618000 | -1.55620800 | -2.83926000 |
| H | 2.66562600 | -1.54871400 | -2.63657800 |
| H | 3.55201700 | -0.03314000 | -2.61854700 |
| C | 6.86533800 | -2.07607500 | 1.28104700 |
| H | 7.59636500 | -1.62326400 | 0.61239600 |
| H | 7.09996600 | -1.76081400 | 2.29671200 |
| H | 7.00809300 | -3.15728000 | 1.23450000 |
| C | 2.18453900 | -1.23295200 | 2.66962900 |
| H | 1.74932400 | -0.24755200 | 2.81407800 |
| H | 1.37589600 | -1.95487800 | 2.56239900 |
| H | 2.69628700 | -1.47893700 | 3.59771400 |
| C | 1.33660200 | 0.80448200 | -1.57731500 |
| C | 0.86604000 | 0.84743400 | -2.90497000 |
| C | 0.98686800 | 2.03687900 | -3.61055000 |
| H | 0.61472300 | 2.07018000 | -4.62747800 |
| C | 1.54745200 | 3.18338900 | -3.06525800 |
| C | 2.02922800 | 3.11017700 | -1.76989700 |
| H | 2.48329300 | 3.98559900 | -1.32027400 |
| C | 1.93844000 | 1.94665000 | -1.01517900 |
| C | 0.22839700 | -0.29719400 | -3.63994000 |
| H | -0.00196800 | -0.00081200 | -4.66101300 |
| H | 0.88091300 | -1.16739300 | -3.70796400 |
| H | -0.70976100 | -0.61379100 | -3.18843400 |
| C | 1.58886700 | 4.46105600 | -3.84519900 |
| H | 2.31628400 | 5.16180600 | -3.43811800 |
| H | 1.84019500 | 4.28485600 | -4.89073300 |
| H | 0.61412800 | 4.95313100 | -3.82894200 |
| C | 2.52236700 | 1.99383600 | 0.36724800 |
| H | 2.61314200 | 3.02492500 | 0.70431800 |
| H | 1.93033700 | 1.47747400 | 1.11855100 |
| H | 3.51742000 | 1.54759300 | 0.39481700 |
| C | -2.71754300 | -1.84474500 | -1.33485900 |
| C | -2.58602500 | -2.65556100 | -2.45127500 |
| F | -1.72617600 | -3.68623300 | -2.46186100 |
| C | -3.31240200 | -2.48570900 | -3.61910000 |
| F | -3.11989700 | -3.29044300 | -4.66205200 |
| C | -4.24615000 | -1.47291200 | -3.69656200 |
| F | -4.95025400 | -1.29096100 | -4.80706000 |
| C | -4.44424500 | -0.65744400 | -2.59929500 |
| F | -5.35635400 | 0.30853800 | -2.65187200 |
| C | -3.69358000 | -0.86330700 | -1.45557100 |
| F | -3.97763000 | -0.07260400 | -0.42188700 |
| C | -2.81231600 | -2.52535900 | 1.28670100 |
| C | -3.93821500 | -3.30864700 | 1.06563700 |
| F | -4.27702500 | -3.68750300 | -0.16852000 |
| C | -4.76500400 | -3.77308500 | 2.07619700 |
| F | -5.82961400 | -4.51564800 | 1.79174700 |
| C | -4.47820900 | -3.46556900 | 3.39093400 |
| F | -5.26093200 | -3.89665200 | 4.37085600 |
| C | -3.35326100 | -2.71636500 | 3.67021400 |
| F | -3.04229300 | -2.42169200 | 4.93022800 |
| C | -2.55472900 | -2.28690600 | 2.62719700 |
| F | -1.45029800 | -1.61666600 | 3.00074800 |
| C | -1.17086700 | 1.40595500 | 2.71468200 |
| C | -0.27093300 | 1.63177000 | 3.73761400 |
| F | 1.01835100 | 1.84468500 | 3.44236400 |
| C | -0.63423700 | 1.65274400 | 5.06896300 |
| F | 0.26689100 | 1.87598100 | 6.01758100 |
| C | -1.95876200 | 1.43611700 | 5.40567200 |
| F | -2.32800600 | 1.44791500 | 6.67598300 |
| C | -2.89460900 | 1.21736700 | 4.41205600 |
| F | -4.16464600 | 1.01910100 | 4.73172500 |
| C | -2.48997400 | 1.21859700 | 3.08870800 |
| F | -3.41480400 | 1.03215700 | 2.15641300 |
| C | -0.99740300 | 2.48418900 | 0.22552200 |
| C | -1.37306100 | 2.40820400 | -1.11438900 |
| F | -1.63740500 | 1.24889000 | -1.68938400 |
| C | -1.52936600 | 3.52236700 | -1.91749400 |
| F | -1.88477900 | 3.39308800 | -3.18858000 |
| C | -1.30346600 | 4.78020800 | -1.39600000 |
| F | -1.42260300 | 5.84987800 | -2.16550700 |
| C | -0.94407000 | 4.91316400 | -0.06924700 |
| F | -0.71804500 | 6.11701300 | 0.43942900 |
| C | -0.81236800 | 3.77951700 | 0.71046800 |

F -0.42724200 3.97929100 1.96835600

**INT1$_{calc}$**

96

B 2.62216460 -0.52783130 -0.00053570
O 1.55894930 0.52582640 -0.00064170
P -0.47962760 -0.69730450 0.97355600
C -1.01374290 -2.66541200 -1.60855350
C 1.02292210 -1.27163640 1.86389780
C -1.54177420 -3.06593000 -0.26551380
C -1.42838920 -2.27209100 0.88733580
C 0.12141520 1.28339210 3.52212030
C -2.20713650 -4.28225800 -0.18879420
C 1.97669410 -1.81949220 0.79503340
C -1.58593750 0.53031650 1.74218650
C -1.20934000 1.34370530 2.82975760
C -1.99686960 -2.72361720 2.09732620
C 4.04423180 1.22497630 1.50089590
C -2.76761120 -4.74946020 0.98880310
C -3.42254330 -0.19646850 0.07975250
C -2.87323990 0.65963900 1.18827770
C 5.19760880 1.61257250 2.16635330
C -2.65237000 -3.94965810 2.11331090
C 3.92662710 0.02344260 0.82122430
C -1.99331640 -1.96333150 3.39799750
C -3.44848280 -6.08257600 1.04669600
C -2.12547360 2.26026670 3.32185760
C 3.04846280 -0.74997090 -1.58041240
C -3.74445410 1.60499260 1.71862930
C 3.06181330 -1.93832600 -2.29069210
C 6.30101440 0.78359970 2.16363320
C 5.06397190 -0.77226340 0.85006120
C -3.39524590 2.41521310 2.78314780
C 3.41128420 0.36934870 -2.32075780
C 6.23564470 -0.42513110 1.49587180
C 3.37230380 -2.02217460 -3.63912380
C -4.34326680 3.43188080 3.34143440
C 3.72489640 0.33555400 -3.66700420
C 3.70381030 -0.87589290 -4.33296620
F 3.03006830 2.09554520 1.56158690
F 5.24965240 2.77723370 2.80830060
F 2.75490320 -3.09870210 -1.69640590
F 3.47573920 1.56774430 -1.73281510
F 7.41147640 1.14069500 2.79788840
F 5.05471580 -1.95285550 0.22189110
F 3.35114020 -3.19337820 -4.27003280
F 7.29053240 -1.23460060 1.48543190
F 4.05258750 1.44549740 -4.32098270
F 4.00113690 -0.93601020 -5.62464500
H -1.35846500 -3.35332050 -2.37806250
H 0.69794410 -2.03988740 2.56628200
H 0.95516010 1.44291810 2.84398300
H -1.36650280 -1.67684340 -1.89172030
H 1.49676860 -0.47628730 2.42750830
H -2.28748620 -4.88286760 -1.08729160
H 0.07502720 -2.67043340 -1.64997970
H 1.44206410 -2.54578980 0.17793890
H 0.27309050 0.33116110 4.03276100
H -2.70079120 -0.44541270 -0.69481040
H 0.18065370 2.05899090 4.28294310
H 2.73410820 -2.41276820 1.30876120
H -1.04600460 -1.48199300 3.63235410
H -2.71862340 -6.88048730 1.19567080
H -3.81147150 -1.13975730 0.46539730
H -4.24818660 0.31606790 -0.41222040
H -1.82848210 2.88756540 4.15430110
H -2.20701890 -2.64284970 4.22143060
H -4.16207770 -6.13608660 1.86761580
H -2.75681420 -1.18502900 3.41042510
H -3.08795830 -4.28763510 3.04657720
H -3.98213620 -6.30128110 0.12243700
H -4.72955730 1.70415030 1.27808200
H -3.91452080 4.43353070 3.29444480
H -4.56821040 3.22675790 4.38895680
H -5.28541870 3.44827180 2.79629270
C 0.36792050 0.10991640 -0.53308230
H 0.49615010 -0.70017940 -1.26938830
B -0.27361710 1.29035170 -1.38898040
C 0.43894030 2.67472180 -1.38671830
C 0.68201230 3.39581260 -0.22950680
C 0.95283200 3.19649940 -2.56463290
C 1.39927470 4.57281140 -0.22508270
C 1.69480030 4.36116910 -2.59882310
C 1.91285660 5.05063840 -1.41978030
C -1.41131670 1.08327870 -2.45488370
C -1.28178390 0.27443280 -3.57171560
C -2.56693020 1.84056170 -2.36430140
C -2.26856280 0.18268190 -4.53614880
C -3.58160990 1.76612220 -3.29778650
C -3.42578380 0.92877270 -4.39004360
F 0.77815940 2.53977900 -3.71022500
F 2.18992660 4.82118310 -3.73812190
F 2.60410700 6.17636700 -1.43349120
F 1.58659340 5.25594850 0.89501890
F 0.15243820 2.97871900 0.91314530
F -0.16279560 -0.42372990 -3.75446730
F -2.72291280 2.64929400 -1.31789810
F -4.69173350 2.47714880 -3.15930810
F -4.38369420 0.84382850 -5.29638420
F -2.11730710 -0.60188340 -5.59185350

**TS2**

99

| | | | |
|---|---|---|---|
| P | 0.90797020 | -0.01323210 | 0.18182050 |
| O | -1.64549640 | -0.19885880 | -0.10294890 |
| B | -1.66106040 | -2.99113480 | 0.59326010 |
| B | -1.06195430 | 1.43288100 | -1.80490180 |
| C | -0.67584410 | 0.81131280 | -0.29227190 |
| H | -0.83267120 | 1.58934750 | 0.44435670 |
| C | 0.69071150 | -1.78525050 | -0.26910220 |
| H | 1.68948240 | -2.20770220 | -0.34455470 |
| H | 0.26030290 | -1.84250120 | -1.26221910 |
| C | -0.11996310 | -2.58156910 | 0.78661310 |
| H | 0.41673900 | -3.52519110 | 0.91807900 |
| H | -0.01789760 | -2.09215060 | 1.75107070 |
| C | 1.29571350 | -0.13690810 | 1.97903030 |
| C | 2.51667260 | -0.77210280 | 2.30515140 |
| C | 2.85089470 | -0.94683560 | 3.64157520 |
| H | 3.79328450 | -1.42887410 | 3.87649530 |
| C | 2.02161150 | -0.55023360 | 4.67718340 |
| C | 0.82693190 | 0.05687700 | 4.33646430 |
| H | 0.15522110 | 0.37323390 | 5.12540410 |
| C | 0.44044040 | 0.27691030 | 3.01836240 |
| C | 3.50308160 | -1.35735820 | 1.32603040 |
| H | 3.24383220 | -2.39158520 | 1.09078230 |
| H | 3.60059320 | -0.81194430 | 0.39294850 |
| H | 4.49500250 | -1.38188680 | 1.77403630 |
| C | 2.39120850 | -0.81050580 | 6.10532960 |
| H | 3.45251630 | -0.63899530 | 6.28313270 |
| H | 1.82854530 | -0.17859130 | 6.79048420 |
| H | 2.18192930 | -1.84817620 | 6.37208940 |
| C | -0.87898620 | 0.97203690 | 2.84136690 |
| H | -1.53601740 | 0.49183790 | 2.12294360 |
| H | -1.41269750 | 0.99558720 | 3.78968150 |
| H | -0.74943690 | 2.01211210 | 2.53768810 |
| C | 2.29141660 | 0.89682770 | -0.57074460 |
| C | 2.85891830 | 0.50959930 | -1.79976900 |
| C | 3.92185830 | 1.24385170 | -2.30246090 |
| H | 4.35398130 | 0.94531750 | -3.25085620 |
| C | 4.43623090 | 2.35336140 | -1.64393620 |
| C | 3.83330670 | 2.73748550 | -0.45991740 |
| H | 4.19006940 | 3.62457480 | 0.04973130 |
| C | 2.76299110 | 2.04377110 | 0.09338430 |
| C | 2.38645180 | -0.66379250 | -2.60935660 |
| H | 2.77959080 | -0.60317610 | -3.62238440 |
| H | 2.73403880 | -1.61094510 | -2.19338480 |
| H | 1.30414100 | -0.71725060 | -2.70141290 |
| C | 5.56711590 | 3.13863490 | -2.23284930 |
| H | 6.43590820 | 2.50597090 | -2.41693490 |
| H | 5.27780620 | 3.57844550 | -3.18772830 |
| H | 5.87721970 | 3.94995380 | -1.57656010 |
| C | 2.18355880 | 2.62066380 | 1.35677260 |
| H | 2.39469990 | 3.68790250 | 1.39671800 |
| H | 1.10316840 | 2.52327500 | 1.42725650 |
| H | 2.61485260 | 2.16484390 | 2.24784070 |
| C | -1.96202430 | -4.41053220 | -0.05047910 |
| C | -1.18618320 | -4.93543750 | -1.08328820 |
| F | -0.13406350 | -4.27205970 | -1.54864150 |
| C | -1.44336270 | -6.15173070 | -1.68495010 |
| F | -0.68341660 | -6.59055770 | -2.67993490 |
| C | -2.49908530 | -6.92227350 | -1.23441190 |
| F | -2.75477670 | -8.09104890 | -1.79501020 |
| C | -3.27282890 | -6.46999990 | -0.18329420 |
| F | -4.26863480 | -7.21764530 | 0.27381660 |
| C | -2.99305020 | -5.24041840 | 0.38519210 |
| F | -3.75592830 | -4.89418800 | 1.41958610 |
| C | -2.83718120 | -2.31138970 | 1.40974980 |
| C | -2.68902330 | -1.92027300 | 2.73255270 |
| F | -1.54448130 | -2.14034440 | 3.38275360 |
| C | -3.70428160 | -1.33660230 | 3.46814410 |
| F | -3.49919790 | -0.97238300 | 4.72899400 |
| C | -4.93716540 | -1.13143540 | 2.88069870 |
| F | -5.91553640 | -0.56590580 | 3.56622370 |
| C | -5.14609270 | -1.54006810 | 1.57525430 |
| F | -6.33381710 | -1.37231130 | 1.01285210 |
| C | -4.11167100 | -2.13608170 | 0.88178750 |
| F | -4.38081290 | -2.55747630 | -0.35187610 |
| C | -2.31271870 | 2.51722670 | -1.69993170 |
| C | -2.86574800 | 3.13994310 | -0.59182160 |
| F | -2.40087190 | 2.91930860 | 0.64751980 |
| C | -3.92551000 | 4.03047340 | -0.65599330 |
| F | -4.40455990 | 4.58801660 | 0.45167260 |
| C | -4.48572830 | 4.33700930 | -1.87807880 |
| F | -5.50001710 | 5.18588270 | -1.95790430 |
| C | -3.97249730 | 3.74839430 | -3.01828250 |
| F | -4.49689090 | 4.03675350 | -4.20338260 |
| C | -2.91546420 | 2.86399380 | -2.90643410 |
| F | -2.46557430 | 2.34051970 | -4.04538840 |
| C | 0.12139750 | 2.11763070 | -2.66646760 |
| C | 0.53469170 | 1.75232360 | -3.93734400 |
| F | 0.02014960 | 0.69192180 | -4.55260270 |
| C | 1.51236300 | 2.44887830 | -4.63113740 |
| F | 1.89717350 | 2.05164340 | -5.84041620 |
| C | 2.10548250 | 3.55521070 | -4.05691380 |
| F | 3.06185750 | 4.21427620 | -4.70279220 |
| C | 1.71743630 | 3.95959120 | -2.79396920 |
| F | 2.29758700 | 5.01066420 | -2.22230610 |
| C | 0.73715070 | 3.24102040 | -2.14182710 |
| F | 0.38016320 | 3.66180770 | -0.92092560 |
| S | -2.39938440 | -0.77661380 | -1.50819090 |
| O | -1.87426240 | -2.10361680 | -1.80279690 |
| O | -1.59159240 | 0.19803920 | -2.45879290 |

**INT2$_{calc}$**

99

| | | | |
|---|---|---|---|
| B | 2.8868218 | -0.4612149 | 0.1119095 |
| O | 1.6046199 | -0.0749241 | 1.0169417 |
| P | -0.3877339 | -0.8630501 | -0.5934818 |
| C | 0.4337580 | 1.8296873 | -2.3977308 |
| C | 0.9455021 | -2.1101190 | -0.5690832 |
| C | -0.0876575 | 0.5963185 | -3.0737669 |
| C | -0.5243966 | -0.5632841 | -2.4066733 |
| C | -1.2044834 | -3.3042962 | 1.3862364 |
| C | -0.1605944 | 0.6462059 | -4.4598437 |
| C | 2.2147423 | -1.3887244 | -1.0463011 |
| C | -2.0575408 | -1.3567874 | -0.0688609 |
| C | -2.2852289 | -2.4626520 | 0.7725911 |
| C | -1.0574006 | -1.6344278 | -3.1591246 |
| C | 4.0889619 | -2.6167938 | 1.1666689 |
| C | -0.6514866 | -0.4011886 | -5.2207163 |
| C | -3.0545792 | 0.5817410 | -1.4685451 |
| C | -3.1510373 | -0.6274051 | -0.5788662 |
| C | 5.0578950 | -3.2682036 | 1.9067889 |
| C | -1.0997949 | -1.5221378 | -4.5448790 |
| C | 3.9633496 | -1.2313126 | 1.0869837 |
| C | -1.6722694 | -2.8994665 | -2.6109426 |
| C | -0.6762750 | -0.3310280 | -6.7165554 |
| C | -3.5941544 | -2.8217440 | 1.0609484 |
| C | 3.5149879 | 0.9158769 | -0.4934015 |
| C | -4.4375232 | -1.0395922 | -0.2569119 |
| C | 4.2334245 | 0.8851821 | -1.6803950 |
| C | 5.9716762 | -2.5329521 | 2.6346975 |
| C | 4.9053500 | -0.5454302 | 1.8509416 |
| C | -4.6865100 | -2.1349072 | 0.5532483 |
| C | 3.4111619 | 2.1707476 | 0.0878071 |
| C | 5.8904900 | -1.1569086 | 2.6089661 |
| C | 4.7506766 | 2.0134185 | -2.2923938 |
| C | -6.0826954 | -2.5445085 | 0.9063142 |
| C | 3.9013993 | 3.3275657 | -0.4910573 |
| C | 4.5704110 | 3.2478281 | -1.6976563 |
| F | 3.2439558 | -3.4299360 | 0.5280752 |
| F | 5.1117676 | -4.5948377 | 1.9279387 |
| F | 4.4772624 | -0.2821602 | -2.2828366 |
| F | 2.8418670 | 2.3109622 | 1.2860370 |
| F | 6.9040141 | -3.1397963 | 3.3508011 |
| F | 4.8974886 | 0.7843001 | 1.9150735 |
| F | 5.4184008 | 1.9208696 | -3.4370712 |
| F | 6.7505276 | -0.4286644 | 3.3101188 |
| F | 3.7586986 | 4.5012666 | 0.1105495 |
| F | 5.0530855 | 4.3413884 | -2.2693669 |
| H | -0.2710093 | 2.2401813 | -1.6755033 |
| H | 0.6743506 | -2.9227656 | -1.2401333 |
| H | -0.4718991 | -2.7240831 | 1.9406210 |
| H | 0.6095184 | 2.6139003 | -3.1311412 |
| H | 1.0583285 | -2.5316885 | 0.4234881 |
| H | 0.1812716 | 1.5448959 | -4.9593289 |
| H | 1.3856897 | 1.6587094 | -1.8957306 |
| H | 1.9763851 | -0.8081159 | -1.9413901 |
| H | -0.6757604 | -3.8999886 | 0.6409673 |
| H | -2.1887728 | 1.2090982 | -1.2773779 |
| H | -1.6388174 | -4.0065687 | 2.0944443 |
| H | 2.9060604 | -2.1455333 | -1.4108717 |
| H | -2.7169678 | -2.7395858 | -2.3405837 |
| H | 0.2622937 | -0.7014973 | -7.1329696 |
| H | -3.0248711 | 0.3022543 | -2.5223404 |
| H | -3.9309313 | 1.2130885 | -1.3280492 |
| H | -3.7631215 | -3.6675325 | 1.7167994 |
| H | -1.1866601 | -3.3152312 | -1.7337289 |
| H | -1.4793023 | -0.9360618 | -7.1353752 |
| H | -1.6493773 | -3.6748134 | -3.3750488 |
| H | -1.5076480 | -2.3499906 | -5.1134001 |
| H | -0.8059757 | 0.6913289 | -7.0690997 |
| H | -5.2738482 | -0.4716017 | -0.6483940 |
| H | -6.2670433 | -2.4045486 | 1.9718319 |
| H | -6.2546992 | -3.5979386 | 0.6838975 |
| H | -6.8242153 | -1.9617306 | 0.3626855 |
| C | 0.3704216 | 0.4632773 | 0.5263169 |
| H | 0.6059115 | 1.3244145 | -0.0827471 |
| B | -0.4515738 | 0.9353417 | 1.9378222 |
| C | -2.0749193 | 0.9324350 | 2.0018130 |
| C | -2.7872292 | 1.9530636 | 1.3925396 |
| C | -2.8430650 | 0.0602181 | 2.7644815 |
| C | -4.1556610 | 2.1116297 | 1.4926308 |
| C | -4.2152544 | 0.1901602 | 2.8965980 |
| C | -4.8787934 | 1.2162571 | 2.2555303 |
| C | 0.0374032 | 2.3945224 | 2.5166736 |
| C | -0.0479584 | 2.6113024 | 3.8888469 |
| C | 0.4259794 | 3.5063288 | 1.7851417 |
| C | 0.2616084 | 3.8142588 | 4.4977662 |
| C | 0.7429838 | 4.7275436 | 2.3509163 |
| C | 0.6657344 | 4.8819910 | 3.7207273 |
| F | -2.3014208 | -0.9703937 | 3.4050772 |
| F | -4.9055933 | -0.6862928 | 3.6203539 |
| F | -6.1969817 | 1.3255301 | 2.3510784 |
| F | -4.7780725 | 3.0919899 | 0.8449234 |
| F | -2.1383767 | 2.8394790 | 0.6278154 |
| F | -0.4773609 | 1.6399844 | 4.6966821 |
| F | 0.5118762 | 3.4591732 | 0.4497132 |
| F | 1.1098276 | 5.7505612 | 1.5896027 |
| F | 0.9641590 | 6.0436490 | 4.2817952 |
| F | 0.1633366 | 3.9524681 | 5.8145539 |
| S | 1.5647450 | -0.4505818 | 2.8550808 |
| O | 1.7280744 | -1.8777520 | 3.0059669 |
| O | 0.0462869 | -0.1596449 | 2.8448556 |

**TS3**

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| | | | |
|---|---|---|---|
| P | 0.90797020 | -0.01323210 | 0.18182050 |
| O | -1.64549640 | -0.19885880 | -0.10294890 |
| B | -1.66106040 | -2.99113480 | 0.59326010 |
| B | -1.06195430 | 1.43288100 | -1.80490180 |
| C | -0.67584410 | 0.81131280 | -0.29227190 |
| H | -0.83267120 | 1.58934750 | 0.44435670 |
| C | 0.69071150 | -1.78525050 | -0.26910220 |
| H | 1.68948240 | -2.20770220 | -0.34455470 |
| H | 0.26030290 | -1.84250120 | -1.26221910 |
| C | -0.11996310 | -2.58156910 | 0.78661310 |
| H | 0.41673900 | -3.52519110 | 0.91807900 |
| H | -0.01789760 | -2.09215060 | 1.75107070 |
| C | 1.29571350 | -0.13690810 | 1.97903030 |
| C | 2.51667260 | -0.77210280 | 2.30515140 |
| C | 2.85089470 | -0.94683560 | 3.64157520 |
| H | 3.79328450 | -1.42887410 | 3.87649530 |
| C | 2.02161150 | -0.55023360 | 4.67718340 |
| C | 0.82693190 | 0.05687700 | 4.33646430 |
| H | 0.15522110 | 0.37323390 | 5.12540410 |
| C | 0.44044040 | 0.27691030 | 3.01836240 |
| C | 3.50308160 | -1.35735820 | 1.32603040 |
| H | 3.24383220 | -2.39158520 | 1.09078230 |
| H | 3.60059320 | -0.81194430 | 0.39294850 |
| H | 4.49500250 | -1.38188680 | 1.77403630 |
| C | 2.39120850 | -0.81050580 | 6.10532960 |
| H | 3.45251630 | -0.63899530 | 6.28313270 |
| H | 1.82854530 | -0.17859130 | 6.79048420 |
| H | 2.18192930 | -1.84817620 | 6.37208940 |
| C | -0.87898620 | 0.97203690 | 2.84136690 |
| H | -1.53601740 | 0.49183790 | 2.12294360 |
| H | -1.41269750 | 0.99558720 | 3.78968150 |
| H | -0.74943690 | 2.01211210 | 2.53768810 |
| C | 2.29141660 | 0.89682770 | -0.57074460 |
| C | 2.85891830 | 0.50959930 | -1.79976900 |
| C | 3.92185830 | 1.24385170 | -2.30246090 |
| H | 4.35398130 | 0.94531750 | -3.25085620 |
| C | 4.43623090 | 2.35336140 | -1.64393620 |
| C | 3.83330670 | 2.73748550 | -0.45991740 |
| H | 4.19006940 | 3.62457480 | 0.04973130 |
| C | 2.76299110 | 2.04377110 | 0.09338430 |
| C | 2.38645180 | -0.66379250 | -2.60935660 |
| H | 2.77959080 | -0.60317610 | -3.62238440 |
| H | 2.73403880 | -1.61094510 | -2.19338480 |
| H | 1.30414100 | -0.71725060 | -2.70141290 |
| C | 5.56711590 | 3.13863490 | -2.23284930 |
| H | 6.43590820 | 2.50597090 | -2.41693490 |
| H | 5.27780620 | 3.57844550 | -3.18772830 |
| H | 5.87721970 | 3.94995380 | -1.57656010 |
| C | 2.18355880 | 2.62066380 | 1.35677260 |
| H | 2.39469990 | 3.68790250 | 1.39671800 |
| H | 1.10316840 | 2.52327500 | 1.42725650 |
| H | 2.61485260 | 2.16484390 | 2.24784070 |
| C | -1.96202430 | -4.41053220 | -0.05047910 |
| C | -1.18618320 | -4.93543750 | -1.08328820 |
| F | -0.13406350 | -4.27205970 | -1.54864150 |
| C | -1.44336270 | -6.15173070 | -1.68495010 |
| F | -0.68341660 | -6.59055770 | -2.67993490 |
| C | -2.49908530 | -6.92227350 | -1.23441190 |
| F | -2.75477670 | -8.09104890 | -1.79501020 |
| C | -3.27282890 | -6.46999990 | -0.18329420 |
| F | -4.26863480 | -7.21764530 | 0.27381660 |
| C | -2.99305020 | -5.24041840 | 0.38519210 |
| F | -3.75592830 | -4.89418800 | 1.41958610 |
| C | -2.83718120 | -2.31138970 | 1.40974980 |
| C | -2.68902330 | -1.92027300 | 2.73255270 |
| F | -1.54448130 | -2.14034440 | 3.38275360 |
| C | -3.70428160 | -1.33660230 | 3.46814410 |
| F | -3.49919790 | -0.97238300 | 4.72899400 |
| C | -4.93716540 | -1.13143540 | 2.88069870 |
| F | -5.91553640 | -0.56590580 | 3.56622370 |
| C | -5.14609270 | -1.54006810 | 1.57525430 |
| F | -6.33381710 | -1.37231130 | 1.01285210 |
| C | -4.11167100 | -2.13608170 | 0.88178750 |
| F | -4.38081290 | -2.55747630 | -0.35187610 |
| C | -2.31271870 | 2.51722670 | -1.69993170 |
| C | -2.86574800 | 3.13994310 | -0.59182160 |
| F | -2.40087190 | 2.91930860 | 0.64751980 |
| C | -3.92551000 | 4.03047340 | -0.65599330 |
| F | -4.40455990 | 4.58801660 | 0.45167260 |
| C | -4.48572830 | 4.33700930 | -1.87807880 |
| F | -5.50001710 | 5.18588270 | -1.95790430 |
| C | -3.97249730 | 3.74839430 | -3.01828250 |
| F | -4.49689090 | 4.03675350 | -4.20338260 |
| C | -2.91546420 | 2.86399380 | -2.90643410 |
| F | -2.46557430 | 2.34051970 | -4.04538840 |
| C | 0.12139750 | 2.11763070 | -2.66646760 |
| C | 0.53469170 | 1.75232360 | -3.93734400 |
| F | 0.02014960 | 0.69192180 | -4.55260270 |
| C | 1.51236300 | 2.44887830 | -4.63113740 |
| F | 1.89717350 | 2.05164340 | -5.84041620 |
| C | 2.10548250 | 3.55521070 | -4.05691380 |
| F | 3.06185750 | 4.21427620 | -4.70279220 |
| C | 1.71743630 | 3.95959120 | -2.79396920 |
| F | 2.29758700 | 5.01066420 | -2.22230610 |
| C | 0.73715070 | 3.24102040 | -2.14182710 |
| F | 0.38016320 | 3.66180770 | -0.92092560 |
| S | -2.39938440 | -0.77661380 | -1.50819090 |
| O | -1.87426240 | -2.10361680 | -1.80279690 |
| O | -1.59159240 | 0.19803920 | -2.45879290 |

**TS4**

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| | | | |
|---|---|---|---|
| P | 1.13497130 | 0.02200190 | -0.48881680 |
| O | -1.45212080 | -0.12916840 | -0.16450670 |
| B | -1.35230480 | -2.61337740 | -0.43531070 |
| B | -1.46781140 | 1.06409110 | 0.69526870 |
| C | -0.27693130 | 0.02759410 | 0.63509510 |
| H | -0.18466640 | -0.69022160 | 1.43801830 |
| C | 0.54907790 | -1.18487890 | -1.74249260 |
| H | 1.35632860 | -1.40640240 | -2.43890510 |
| H | -0.27393040 | -0.76014190 | -2.30415880 |
| C | 0.12706080 | -2.45184530 | -0.97758220 |
| H | 0.22856360 | -3.29699970 | -1.67072460 |
| H | 0.85370960 | -2.69103210 | -0.19694550 |
| C | 2.71657040 | -0.74838150 | 0.03882960 |
| C | 3.77643650 | -0.68632600 | -0.89389230 |
| C | 4.95686090 | -1.36499180 | -0.62109520 |
| H | 5.76039670 | -1.31332950 | -1.34674530 |
| C | 5.14235560 | -2.10086860 | 0.53764870 |
| C | 4.10523720 | -2.11991200 | 1.45373430 |
| H | 4.23140310 | -2.67018790 | 2.37864520 |
| C | 2.89821440 | -1.46250040 | 1.23777690 |
| C | 3.75954560 | 0.10744330 | -2.17384470 |
| H | 4.57876620 | -0.21107630 | -2.81619920 |
| H | 2.84926060 | -0.00284820 | -2.75899350 |
| H | 3.88718140 | 1.17311430 | -1.98405040 |
| C | 6.40948570 | -2.86447770 | 0.77321610 |
| H | 6.56761470 | -3.06900240 | 1.83092210 |
| H | 6.37985580 | -3.82540130 | 0.25592540 |
| H | 7.27939510 | -2.32422880 | 0.40115920 |
| C | 1.88181030 | -1.57780580 | 2.33815920 |
| H | 1.47350260 | -0.61925400 | 2.65053320 |
| H | 1.04846860 | -2.22274510 | 2.05937020 |
| H | 2.33660090 | -2.02596410 | 3.21929330 |
| C | 1.50464970 | 1.73179330 | -0.96973650 |
| C | 1.14311450 | 2.30998860 | -2.19849560 |
| C | 1.44052240 | 3.64724760 | -2.41413010 |
| H | 1.15126400 | 4.09633250 | -3.35744750 |
| C | 2.07667020 | 4.43304080 | -1.46090460 |
| C | 2.41254250 | 3.84234840 | -0.25568390 |
| H | 2.88690140 | 4.44001780 | 0.51343420 |
| C | 2.13361620 | 2.50902020 | 0.01951960 |
| C | 0.43872480 | 1.57062610 | -3.29937770 |
| H | 0.26411670 | 2.23171210 | -4.14587360 |
| H | 1.01818770 | 0.72541930 | -3.67377490 |
| H | -0.53386320 | 1.19424510 | -2.98819510 |
| C | 2.33973680 | 5.88481960 | -1.71805760 |
| H | 2.89091790 | 6.34435900 | -0.89961140 |
| H | 2.91513000 | 6.02862940 | -2.63295740 |
| H | 1.40441540 | 6.43372370 | -1.83453030 |
| C | 2.50629280 | 1.99837130 | 1.38279330 |
| H | 2.68460570 | 2.83418110 | 2.05632360 |
| H | 1.71556120 | 1.40499550 | 1.84034520 |
| H | 3.41452420 | 1.39604120 | 1.35986000 |
| C | -2.63014080 | -2.30581520 | -1.29983740 |
| C | -2.64497170 | -2.29310100 | -2.68685180 |
| F | -1.55059980 | -2.62655610 | -3.37745710 |
| C | -3.76759090 | -1.96484280 | -3.42316070 |
| F | -3.73493980 | -1.96864590 | -4.75024970 |
| C | -4.93559740 | -1.63262840 | -2.76200870 |
| F | -6.01644130 | -1.31038860 | -3.45151810 |
| C | -4.97361380 | -1.64625250 | -1.37884020 |
| F | -6.09593380 | -1.34089520 | -0.74679360 |
| C | -3.83452540 | -1.99268530 | -0.68007610 |
| F | -3.91203250 | -1.99150510 | 0.64590250 |
| C | -1.55247200 | -3.62181580 | 0.77928880 |
| C | -1.60605690 | -4.95374970 | 0.40004340 |
| F | -1.48920110 | -5.25364030 | -0.89848310 |
| C | -1.77856550 | -5.99253170 | 1.29340650 |
| F | -1.82097710 | -7.25072770 | 0.87829800 |
| C | -1.90678160 | -5.69734510 | 2.63885950 |
| F | -2.06949820 | -6.67224090 | 3.51899820 |
| C | -1.86351100 | -4.38075200 | 3.06052430 |
| F | -1.98890940 | -4.09718710 | 4.34905630 |
| C | -1.69085640 | -3.36964670 | 2.12999920 |
| F | -1.66897610 | -2.11908580 | 2.58622370 |
| C | -2.37844370 | 0.98279300 | 2.01465420 |
| C | -1.87657480 | 0.92882030 | 3.30151430 |
| F | -0.55688540 | 0.98334200 | 3.51905000 |
| C | -2.68549870 | 0.80377530 | 4.41741190 |
| F | -2.16157980 | 0.74206530 | 5.63829920 |
| C | -4.05646100 | 0.73991550 | 4.25363280 |
| F | -4.84731230 | 0.61861950 | 5.31201760 |
| C | -4.60229210 | 0.80626030 | 2.98379640 |
| F | -5.92023750 | 0.75148920 | 2.82730190 |
| C | -3.75567730 | 0.92996130 | 1.89834190 |
| F | -4.30745240 | 1.00339430 | 0.68527580 |
| C | -1.47361550 | 2.49138360 | -0.02655670 |
| C | -2.12550580 | 2.74406350 | -1.22057130 |
| F | -2.75633630 | 1.76151780 | -1.86706150 |
| C | -2.14335510 | 3.99587310 | -1.81325680 |
| F | -2.75734010 | 4.19259840 | -2.97679120 |
| C | -1.50000620 | 5.04863500 | -1.19135660 |
| F | -1.47901860 | 6.25060720 | -1.75914380 |
| C | -0.85589060 | 4.84324080 | 0.01403800 |
| F | -0.21278330 | 5.84885000 | 0.60207140 |
| C | -0.86640180 | 3.58032030 | 0.57152060 |
| F | -0.23767960 | 3.41672490 | 1.73765640 |

**2c$_{open, calc}$**

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| | | | |
|---|---|---|---|
| P | 0.12082580 | -1.02592380 | 0.18230890 |
| O | -1.03439060 | 1.06102890 | 1.14671340 |
| B | 2.73783640 | 1.08088450 | 1.66848080 |
| B | -1.75170630 | 1.37559940 | -0.07749170 |
| C | -0.30884950 | 0.71175570 | -0.01628330 |
| H | 0.57196860 | 1.31942160 | -0.22691230 |
| C | 1.07386770 | -1.05257600 | 1.75185380 |
| H | 1.12805590 | -2.08059770 | 2.10295030 |
| H | 0.48265260 | -0.51101360 | 2.47957660 |
| C | 2.48301080 | -0.46761210 | 1.64374480 |
| H | 3.01877800 | -0.77339240 | 2.55864850 |
| H | 3.05171920 | -0.95508860 | 0.84987150 |
| C | 1.28201880 | -1.75332950 | -1.02664650 |
| C | 1.72842170 | -3.07224810 | -0.80256070 |
| C | 2.65657200 | -3.62656340 | -1.67526880 |
| H | 2.98461840 | -4.64511570 | -1.50087250 |
| C | 3.16882880 | -2.92835040 | -2.75645330 |
| C | 2.70068840 | -1.64245940 | -2.96934730 |
| H | 3.06480830 | -1.08336120 | -3.82334200 |
| C | 1.76580820 | -1.03805170 | -2.13848560 |
| C | 1.28661070 | -3.95987380 | 0.33195490 |
| H | 1.93504660 | -3.83859350 | 1.20202730 |
| H | 0.25971980 | -3.79977880 | 0.64989600 |
| H | 1.36105710 | -5.00438990 | 0.03355350 |
| C | 4.19949130 | -3.53591890 | -3.65792120 |
| H | 4.15069160 | -4.62393100 | -3.65158750 |
| H | 4.08073020 | -3.19973970 | -4.68726610 |
| H | 5.20409280 | -3.25195380 | -3.33879210 |
| C | 1.32755350 | 0.34469650 | -2.52038440 |
| H | 0.25842700 | 0.50361970 | -2.41872640 |
| H | 1.82733750 | 1.10915610 | -1.92610310 |
| H | 1.58256340 | 0.54423790 | -3.55944570 |
| C | -1.38929290 | -2.04512120 | 0.26927750 |
| C | -2.03073830 | -2.38183430 | 1.47694620 |
| C | -3.17460720 | -3.17289040 | 1.42439650 |
| H | -3.67203300 | -3.41712220 | 2.35499180 |
| C | -3.71773700 | -3.62855850 | 0.23698680 |
| C | -3.09005930 | -3.25442890 | -0.94149680 |
| H | -3.51595850 | -3.56479750 | -1.88903530 |
| C | -1.94928080 | -2.46777720 | -0.95707900 |
| C | -1.61634200 | -1.92669260 | 2.84904250 |
| H | -2.40064590 | -2.16472350 | 3.56421530 |
| H | -0.71305880 | -2.42505760 | 3.19995880 |
| H | -1.46536020 | -0.85183700 | 2.89634270 |
| C | -4.97381000 | -4.44298320 | 0.20837280 |
| H | -4.82601840 | -5.37923280 | -0.33083570 |
| H | -5.32160660 | -4.68421910 | 1.21108940 |
| H | -5.77423860 | -3.90163050 | -0.29767410 |
| C | -1.41135420 | -2.10199220 | -2.31183060 |
| H | -2.19520700 | -2.21166030 | -3.05977040 |
| H | -1.07207650 | -1.07134040 | -2.37198230 |
| H | -0.58238320 | -2.74331250 | -2.61151960 |
| C | 1.70156860 | 2.12488100 | 2.19619820 |
| C | 0.99232240 | 1.97173510 | 3.37526890 |
| F | 1.26165330 | 0.93109230 | 4.16898780 |
| C | 0.03566930 | 2.87327260 | 3.79369340 |
| F | -0.61397460 | 2.69628760 | 4.93465950 |
| C | -0.23428320 | 3.97915250 | 3.00675230 |
| F | -1.14769000 | 4.85283310 | 3.38611580 |
| C | 0.46614870 | 4.18144550 | 1.83052730 |
| F | 0.22060400 | 5.25039010 | 1.08796810 |
| C | 1.42249740 | 3.26195060 | 1.45325000 |
| F | 2.06094560 | 3.46047730 | 0.29790830 |
| C | 4.16356330 | 1.60600540 | 1.26009520 |
| C | 4.86849110 | 2.43442300 | 2.12335970 |
| F | 4.33969110 | 2.75541340 | 3.30069920 |
| C | 6.13016080 | 2.91746860 | 1.83179630 |
| F | 6.78067010 | 3.68919180 | 2.68939620 |
| C | 6.71563060 | 2.58051590 | 0.62361890 |
| F | 7.91788200 | 3.03734780 | 0.32273940 |
| C | 6.04480850 | 1.76205810 | -0.26877500 |
| F | 6.60574420 | 1.44739050 | -1.42781640 |
| C | 4.79318560 | 1.28298890 | 0.06750020 |
| F | 4.17220020 | 0.51121450 | -0.82284580 |
| C | -1.84859100 | 2.94853790 | -0.41932330 |
| C | -1.23771740 | 3.60091840 | -1.47285810 |
| F | -0.43712800 | 2.93665460 | -2.31163610 |
| C | -1.41359700 | 4.95150920 | -1.72594990 |
| F | -0.80576930 | 5.53647550 | -2.75399700 |
| C | -2.23167380 | 5.69535400 | -0.89859050 |
| F | -2.41218580 | 6.98964690 | -1.12794050 |
| C | -2.85863440 | 5.08629310 | 0.17376610 |
| F | -3.64602770 | 5.79869460 | 0.97217670 |
| C | -2.65389320 | 3.73658020 | 0.38796960 |
| F | -3.28088440 | 3.17474610 | 1.42373290 |
| C | -3.08830210 | 0.57614970 | -0.46151000 |
| C | -3.96166700 | 0.02668210 | 0.46081410 |
| F | -3.71225920 | 0.11554780 | 1.76550140 |
| C | -5.11324480 | -0.64560350 | 0.08998740 |
| F | -5.90510990 | -1.19940310 | 1.00521160 |
| C | -5.43239900 | -0.76339630 | -1.24865840 |
| F | -6.52092220 | -1.43232960 | -1.61790240 |
| C | -4.60392490 | -0.20217100 | -2.20235710 |
| F | -4.89973990 | -0.32293060 | -3.49432150 |
| C | -3.46290100 | 0.45820490 | -1.78787490 |
| F | -2.67796390 | 0.98297820 | -2.73542440 |

**INT3$_e$**

99

| | | | |
|---|---|---|---|
| P | -0.9922047 | -0.0837300 | -0.2274426 |
| O | 1.4754330 | -0.7608398 | -0.5687702 |
| B | 1.5956769 | 2.8922756 | 0.1856484 |
| B | 1.3796713 | -2.0279300 | 0.2461048 |
| C | 0.5454521 | -0.7038686 | 0.5271928 |
| H | 0.8896659 | -0.0754930 | 1.3445530 |
| C | -0.4706818 | 1.5421050 | -0.8847365 |
| H | -1.3264800 | 1.9889564 | -1.3855441 |
| H | 0.2823321 | 1.3868319 | -1.6520697 |
| C | 0.0372791 | 2.4477294 | 0.2583267 |
| H | -0.5894194 | 3.3390901 | 0.2964800 |
| H | -0.1315810 | 1.9851153 | 1.2357533 |
| C | -2.3775421 | 0.3368976 | 0.8791674 |
| C | -3.5789219 | 0.7435484 | 0.2581623 |
| C | -4.6323647 | 1.1632591 | 1.0581497 |
| H | -5.5523197 | 1.4755604 | 0.5772436 |
| C | -4.5524277 | 1.1913624 | 2.4426078 |
| C | -3.3734254 | 0.7626939 | 3.0271922 |
| H | -3.2913750 | 0.7559343 | 4.1075264 |
| C | -2.2824934 | 0.3331549 | 2.2801187 |
| C | -3.8469366 | 0.7001888 | -1.2237614 |
| H | -4.7126425 | 1.3162221 | -1.4604754 |
| H | -3.0307752 | 1.0645691 | -1.8432883 |
| H | -4.0661491 | -0.3146910 | -1.5572310 |
| C | -5.7039837 | 1.6778579 | 3.2678974 |
| H | -6.6464154 | 1.2449400 | 2.9325362 |
| H | -5.5782035 | 1.4321542 | 4.3209533 |
| H | -5.8015707 | 2.7621873 | 3.1928306 |
| C | -1.0804119 | -0.1359416 | 3.0438357 |
| H | -0.7016770 | -1.0891148 | 2.6838802 |
| H | -0.2613959 | 0.5835623 | 3.0174134 |
| H | -1.3313803 | -0.2766275 | 4.0932893 |
| C | -1.5587450 | -1.3342856 | -1.4141121 |
| C | -1.3598359 | -1.2407931 | -2.8025949 |
| C | -1.8500603 | -2.2598415 | -3.6118842 |
| H | -1.6887382 | -2.1902985 | -4.6806860 |
| C | -2.5245860 | -3.3584943 | -3.1058561 |
| C | -2.6942905 | -3.4358477 | -1.7312462 |
| H | -3.2030395 | -4.2945654 | -1.3077622 |
| C | -2.2206759 | -2.4566881 | -0.8715673 |
| C | -0.6424509 | -0.1198769 | -3.4987259 |
| H | -0.6121321 | -0.3082094 | -4.5697423 |
| H | -1.1368410 | 0.8421151 | -3.3658609 |
| H | 0.3902020 | -0.0213911 | -3.1702435 |
| C | -3.0107047 | -4.4560766 | -4.0008118 |
| H | -4.0004283 | -4.8032670 | -3.7054172 |
| H | -3.0608159 | -4.1370066 | -5.0403508 |
| H | -2.3400434 | -5.3156090 | -3.9550170 |
| C | -2.4610897 | -2.6729589 | 0.5964857 |
| H | -2.6390866 | -3.7293546 | 0.7913939 |
| H | -1.6197931 | -2.3805247 | 1.2214113 |
| H | -3.3366968 | -2.1260522 | 0.9476661 |
| C | 2.1015258 | 3.6924956 | -1.1369428 |
| C | 1.2831905 | 4.2638994 | -2.0953533 |
| F | -0.0499340 | 4.1833933 | -1.9987604 |
| C | 1.7635059 | 4.9617317 | -3.1904610 |
| F | 0.9255026 | 5.4860647 | -4.0791051 |
| C | 3.1252697 | 5.1162342 | -3.3558290 |
| F | 3.6020688 | 5.7804605 | -4.3987721 |
| C | 3.9862007 | 4.5727211 | -2.4207382 |
| F | 5.2981546 | 4.7145262 | -2.5656901 |
| C | 3.4598909 | 3.8850896 | -1.3447349 |
| F | 4.3384961 | 3.3781201 | -0.4708838 |
| C | 1.9823692 | 3.6707936 | 1.5651250 |
| C | 1.9951328 | 5.0562207 | 1.6417491 |
| F | 1.6911858 | 5.7937260 | 0.5716665 |
| C | 2.2868403 | 5.7563344 | 2.8001323 |
| F | 2.2877131 | 7.0842239 | 2.8081739 |
| C | 2.5719401 | 5.0613603 | 3.9589171 |
| F | 2.8535225 | 5.7113868 | 5.0792876 |
| C | 2.5423141 | 3.6802998 | 3.9423891 |
| F | 2.7903871 | 2.9997648 | 5.0565237 |
| C | 2.2426221 | 3.0207387 | 2.7636126 |
| F | 2.1912077 | 1.6837502 | 2.8454731 |
| C | 2.6469249 | -2.2740200 | 1.1941359 |
| C | 2.6173621 | -2.3126840 | 2.5758672 |
| F | 1.4744410 | -2.1071845 | 3.2303053 |
| C | 3.7437178 | -2.5644954 | 3.3404306 |
| F | 3.6732823 | -2.5941877 | 4.6646613 |
| C | 4.9543473 | -2.7878573 | 2.7106516 |
| F | 6.0404262 | -3.0286714 | 3.4277044 |
| C | 5.0290623 | -2.7592983 | 1.3286569 |
| F | 6.1895341 | -2.9697572 | 0.7219616 |
| C | 3.8792011 | -2.5071959 | 0.6058197 |
| F | 3.9715963 | -2.4803432 | -0.7268848 |
| C | 0.8506162 | -3.3199178 | -0.5176565 |
| C | 0.9128046 | -3.5057146 | -1.8883959 |
| F | 1.4140909 | -2.5609312 | -2.6790085 |
| C | 0.4602007 | -4.6611875 | -2.5006834 |
| F | 0.5022765 | -4.7907009 | -3.8224087 |
| C | -0.0580398 | -5.6840323 | -1.7299874 |
| F | -0.5146900 | -6.7871388 | -2.3101722 |
| C | -0.1143361 | -5.5481525 | -0.3549193 |
| F | -0.6189524 | -6.5251514 | 0.3907912 |
| C | 0.3472935 | -4.3786822 | 0.2174438 |
| F | 0.2786755 | -4.2689697 | 1.5471218 |
| S | 3.0227037 | 0.5492423 | -0.7333212 |
| O | 2.8482783 | 0.9092137 | -2.1188292 |
| O | 2.4571964 | 1.5455477 | 0.2523140 |

**TS5$_e$**

99

| | | | |
|---|---|---|---|
| P | -0.6701448 | -0.4761692 | 0.6178860 |
| O | 1.6191446 | 0.1164595 | -0.0529646 |
| B | 1.7173808 | 2.8832021 | 0.5388576 |
| B | 1.0278378 | -1.5965710 | -1.6435912 |
| C | 0.9346252 | -1.0960158 | -0.1234224 |
| H | 1.3464389 | -1.8421322 | 0.5550634 |
| C | -0.5967513 | 1.3348847 | 0.3585247 |
| H | -1.6050165 | 1.6961563 | 0.5508003 |
| H | -0.4081124 | 1.4748575 | -0.7042911 |
| C | 0.4191999 | 2.1160312 | 1.2325165 |
| H | -0.1635359 | 2.8875117 | 1.7405806 |
| H | 0.7818869 | 1.4955447 | 2.0548139 |
| C | -0.8322629 | -0.7833909 | 2.4157575 |
| C | -2.1273266 | -0.6468024 | 2.9678494 |
| C | -2.3240760 | -0.9387318 | 4.3087326 |
| H | -3.3215174 | -0.8290425 | 4.7190628 |
| C | -1.2924162 | -1.3450209 | 5.1414346 |
| C | -0.0235967 | -1.4086540 | 4.5971328 |
| H | 0.8095676 | -1.6734062 | 5.2372017 |
| C | 0.2415561 | -1.1259223 | 3.2599080 |
| C | -3.3442213 | -0.1801531 | 2.2146278 |
| H | -4.0797712 | 0.2072378 | 2.9176061 |
| H | -3.1354582 | 0.6297214 | 1.5191479 |
| H | -3.8212695 | -0.9843644 | 1.6550909 |
| C | -1.5481634 | -1.6626267 | 6.5825800 |
| H | -2.2432232 | -2.4973173 | 6.6830841 |
| H | -0.6317149 | -1.9286647 | 7.1061287 |
| H | -1.9906434 | -0.8104364 | 7.0995973 |
| C | 1.6911546 | -1.2054900 | 2.8659767 |
| H | 1.9492473 | -2.1820773 | 2.4504324 |
| H | 1.9935512 | -0.4316310 | 2.1682912 |
| H | 2.3139537 | -1.0756567 | 3.7486946 |
| C | -2.0282872 | -1.3738727 | -0.2091042 |
| C | -2.9799634 | -0.7730258 | -1.0585935 |
| C | -3.9551096 | -1.5791949 | -1.6348976 |
| H | -4.6882221 | -1.1128412 | -2.2827777 |
| C | -4.0351079 | -2.9443908 | -1.4100492 |
| C | -3.0857447 | -3.5124191 | -0.5765011 |
| H | -3.1191138 | -4.5789663 | -0.3873255 |
| C | -2.0874219 | -2.7626049 | 0.0308330 |
| C | -3.0844253 | 0.6945380 | -1.3710998 |
| H | -3.7909932 | 0.8506146 | -2.1837513 |
| H | -3.4637624 | 1.2629259 | -0.5200367 |
| H | -2.1528276 | 1.1589258 | -1.6750417 |
| C | -5.0891811 | -3.7801975 | -2.0678659 |
| H | -5.4295242 | -4.5827911 | -1.4146179 |
| H | -5.9563657 | -3.1852018 | -2.3499843 |
| H | -4.6999917 | -4.2426962 | -2.9758181 |
| C | -1.1523098 | -3.5111545 | 0.9429576 |
| H | -1.2329717 | -4.5808272 | 0.7597858 |
| H | -0.1019224 | -3.2626005 | 0.8086163 |
| H | -1.3921596 | -3.3396595 | 1.9926186 |
| C | 1.4129020 | 3.6018720 | -0.9014121 |
| C | 0.1577553 | 4.0250673 | -1.3110555 |
| F | -0.8944522 | 3.9553355 | -0.4781198 |
| C | -0.1108944 | 4.5729159 | -2.5524221 |
| F | -1.3508922 | 4.9301817 | -2.8846981 |
| C | 0.9245955 | 4.7615576 | -3.4444788 |
| F | 0.6931765 | 5.2862084 | -4.6418973 |
| C | 2.2073249 | 4.4207050 | -3.0640456 |
| F | 3.2191860 | 4.6383878 | -3.8980204 |
| C | 2.4285434 | 3.8717855 | -1.8125187 |
| F | 3.7027746 | 3.6538423 | -1.4977930 |
| C | 2.2854019 | 3.9236989 | 1.6760472 |
| C | 2.1849117 | 5.3044647 | 1.6037519 |
| F | 1.5929046 | 5.8965505 | 0.5644008 |
| C | 2.6673556 | 6.1594656 | 2.5827785 |
| F | 2.5440097 | 7.4774281 | 2.4535546 |
| C | 3.2785292 | 5.6356393 | 3.7032070 |
| F | 3.7453692 | 6.4372914 | 4.6532990 |
| C | 3.3896403 | 4.2643862 | 3.8302314 |
| F | 3.9635518 | 3.7455763 | 4.9140654 |
| C | 2.8943324 | 3.4469199 | 2.8308244 |
| F | 3.0175470 | 2.1311026 | 3.0467988 |
| C | 2.3652962 | -2.2718124 | -2.0779354 |
| C | 3.0537840 | -3.2011184 | -1.3039342 |
| F | 2.5346589 | -3.6308034 | -0.1512453 |
| C | 4.2525482 | -3.7601451 | -1.6945831 |
| F | 4.8645490 | -4.6584115 | -0.9369826 |
| C | 4.8104327 | -3.3770279 | -2.9030572 |
| F | 5.9587366 | -3.8973874 | -3.2883219 |
| C | 4.1594350 | -2.4620661 | -3.7114529 |
| F | 4.6950087 | -2.1067799 | -4.8669265 |
| C | 2.9503182 | -1.9364920 | -3.2980826 |
| F | 2.3580823 | -1.0720519 | -4.1014784 |
| C | -0.1078101 | -1.4573751 | -2.7131549 |
| C | -0.4980574 | -0.2959591 | -3.3492259 |
| F | 0.0996510 | 0.8517587 | -3.0491534 |
| C | -1.5058073 | -0.2867825 | -4.2972820 |
| F | -1.8775509 | 0.8425450 | -4.8799609 |
| C | -2.1430341 | -1.4719016 | -4.6211667 |
| F | -3.1260799 | -1.4733835 | -5.5069930 |
| C | -1.7648251 | -2.6557438 | -4.0113158 |
| F | -2.3816582 | -3.7897422 | -4.3177090 |
| C | -0.7528985 | -2.6254404 | -3.0756736 |
| F | -0.3897995 | -3.7620150 | -2.4734921 |
| S | 3.2026440 | 0.6439229 | -0.4223432 |
| O | 3.1717226 | 0.7958432 | -1.8733538 |
| O | 2.9561634 | 1.9520966 | 0.3518692 |

**INT3$_c$**

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| | | | |
|---|---|---|---|
| P | -0.8770214 | -0.2753603 | -0.0445757 |
| O | 1.7669251 | -0.5488907 | 0.0463499 |
| B | 1.5079797 | 3.0123572 | 0.0995337 |
| B | 1.6325363 | -2.0250625 | 0.3615039 |
| C | 0.6113853 | -0.8982753 | 0.8198861 |
| H | 0.6983513 | -0.5742111 | 1.8511754 |
| C | -0.2817964 | 1.2951866 | -0.7554898 |
| H | -1.0644436 | 1.7476744 | -1.3607071 |
| H | 0.5430596 | 1.0714074 | -1.4253599 |
| C | 0.1208905 | 2.2265392 | 0.4064630 |
| H | -0.6919227 | 2.9328078 | 0.5726140 |
| H | 0.2021422 | 1.6813437 | 1.3477765 |
| C | -2.3055814 | 0.2265548 | 0.9795082 |
| C | -3.4692844 | 0.5858562 | 0.2612729 |
| C | -4.5698712 | 1.0606729 | 0.9603093 |
| H | -5.4559299 | 1.3369043 | 0.4002226 |
| C | -4.5756203 | 1.1940236 | 2.3396562 |
| C | -3.4300550 | 0.8255297 | 3.0215359 |
| H | -3.4102721 | 0.9166240 | 4.1006889 |
| C | -2.2924197 | 0.3447897 | 2.3811466 |
| C | -3.6488957 | 0.4573107 | -1.2295657 |
| H | -4.4945779 | 1.0631656 | -1.5501005 |
| H | -2.7959785 | 0.7886138 | -1.8173054 |
| H | -3.8556364 | -0.5726015 | -1.5209354 |
| C | -5.7809160 | 1.7221551 | 3.0550886 |
| H | -6.6650901 | 1.1230104 | 2.8346348 |
| H | -5.6407308 | 1.7244693 | 4.1345061 |
| H | -5.9993367 | 2.7456181 | 2.7475485 |
| C | -1.1457070 | -0.0241401 | 3.2795672 |
| H | -0.8134101 | -1.0516473 | 3.1422313 |
| H | -0.2882419 | 0.6387465 | 3.1582516 |
| H | -1.4496784 | 0.0615293 | 4.3205461 |
| C | -1.4227913 | -1.5966676 | -1.1628686 |
| C | -1.1931615 | -1.5853401 | -2.5519453 |
| C | -1.6425749 | -2.6603493 | -3.3037700 |
| H | -1.4584191 | -2.6559906 | -4.3720462 |
| C | -2.3052767 | -3.7432692 | -2.7400418 |
| C | -2.5062060 | -3.7364255 | -1.3709128 |
| H | -2.9983821 | -4.5808114 | -0.9035216 |
| C | -2.0735830 | -2.6903070 | -0.5639877 |
| C | -0.4842576 | -0.4865138 | -3.2921482 |
| H | -0.4128158 | -0.7336136 | -4.3493230 |
| H | -1.0093066 | 0.4669677 | -3.2295796 |
| H | 0.5332563 | -0.3266881 | -2.9409450 |
| C | -2.7430220 | -4.8937909 | -3.5927518 |
| H | -3.2439746 | -5.6626067 | -3.0077190 |
| H | -3.4298066 | -4.5659219 | -4.3738323 |
| H | -1.8897385 | -5.3580507 | -4.0887047 |
| C | -2.3247689 | -2.8191903 | 0.9124512 |
| H | -2.5135607 | -3.8602490 | 1.1666006 |
| H | -1.4770823 | -2.5078615 | 1.5210502 |
| H | -3.1932731 | -2.2412713 | 1.2284710 |
| C | 1.3741941 | 3.8113181 | -1.3151556 |
| C | 0.6627954 | 5.0030418 | -1.3185485 |
| F | 0.1250266 | 5.4524620 | -0.1801041 |
| C | 0.4540858 | 5.7720023 | -2.4484850 |
| F | -0.2338469 | 6.9068278 | -2.3851548 |
| C | 0.9648408 | 5.3408222 | -3.6582687 |
| F | 0.7751446 | 6.0565599 | -4.7587585 |
| C | 1.6625711 | 4.1504797 | -3.7114353 |
| F | 2.1408146 | 3.7187855 | -4.8741638 |
| C | 1.8507075 | 3.4108694 | -2.5542218 |
| F | 2.5111157 | 2.2594142 | -2.7038567 |
| C | 2.0887765 | 3.9784453 | 1.2709289 |
| C | 3.2844608 | 4.6486518 | 1.0494601 |
| F | 3.9290206 | 4.4839623 | -0.1077611 |
| C | 3.8719243 | 5.4932964 | 1.9734875 |
| F | 5.0188818 | 6.1076949 | 1.7062097 |
| C | 3.2496826 | 5.6937150 | 3.1913716 |
| F | 3.7924116 | 6.4973516 | 4.0953119 |
| C | 2.0593614 | 5.0469613 | 3.4596135 |
| F | 1.4563893 | 5.2323808 | 4.6299924 |
| C | 1.5064818 | 4.2093073 | 2.5058034 |
| F | 0.3540274 | 3.6230888 | 2.8441740 |
| C | 2.5924884 | -2.5876474 | 1.5074016 |
| C | 2.1327507 | -3.0914039 | 2.7105058 |
| F | 0.8251975 | -3.0910160 | 2.9828781 |
| C | 2.9780323 | -3.6118904 | 3.6742315 |
| F | 2.4982250 | -4.0849599 | 4.8173436 |
| C | 4.3404330 | -3.6363847 | 3.4362746 |
| F | 5.1629961 | -4.1302756 | 4.3479154 |
| C | 4.8426299 | -3.1446999 | 2.2438628 |
| F | 6.1486182 | -3.1657962 | 2.0156752 |
| C | 3.9614354 | -2.6366063 | 1.3081927 |
| F | 4.4640673 | -2.1667238 | 0.1647556 |
| C | 1.4810370 | -2.9470362 | -0.9261504 |
| C | 2.0571551 | -2.6630120 | -2.1528845 |
| F | 2.7624402 | -1.5459871 | -2.3264222 |
| C | 1.9210157 | -3.4969803 | -3.2499962 |
| F | 2.4644324 | -3.1776889 | -4.4186303 |
| C | 1.1974708 | -4.6676278 | -3.1254474 |
| F | 1.0298516 | -5.4636430 | -4.1740711 |
| C | 0.6288312 | -4.9991779 | -1.9096792 |
| F | -0.0865814 | -6.1128348 | -1.7932867 |
| C | 0.7914287 | -4.1422441 | -0.8400636 |
| F | 0.2370699 | -4.4855227 | 0.3244351 |
| S | 3.0926081 | 0.7767080 | 0.7577331 |
| O | 2.6449606 | 0.8773094 | 2.1308165 |
| O | 2.6404316 | 1.9229526 | -0.1182821 |

**TS5$_c$**

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| | | | |
|---|---|---|---|
| P | -0.8872567 | -0.2570336 | -0.0216125 |
| O | 2.1794474 | -0.4333089 | -0.1905901 |
| B | 1.5243283 | 2.9891522 | 0.1384506 |
| B | 1.7495540 | -1.7860640 | 0.2912525 |
| C | 0.4660997 | -1.0439405 | 0.9393855 |
| H | 0.3699179 | -0.9449150 | 2.0078090 |
| C | -0.2256129 | 1.2672150 | -0.7714016 |
| H | -0.9879982 | 1.6527975 | -1.4467742 |
| H | 0.6373855 | 1.0059168 | -1.3744602 |
| C | 0.0782749 | 2.2738215 | 0.3532428 |
| H | -0.7238531 | 3.0106657 | 0.3688888 |
| H | 0.0417826 | 1.8025550 | 1.3318466 |
| C | -2.3288309 | 0.2966752 | 0.9565911 |
| C | -3.4826212 | 0.5994209 | 0.1963763 |
| C | -4.6113926 | 1.0722863 | 0.8497966 |
| H | -5.4887148 | 1.3058949 | 0.2576178 |
| C | -4.6539751 | 1.2618363 | 2.2215564 |
| C | -3.5112158 | 0.9657007 | 2.9421147 |
| H | -3.5154911 | 1.1161571 | 4.0146458 |
| C | -2.3443076 | 0.4918836 | 2.3512509 |
| C | -3.6215950 | 0.4291651 | -1.2949927 |
| H | -2.7520932 | 0.7426110 | -1.8680225 |
| H | -3.8298105 | -0.6059087 | -1.5661528 |
| H | -4.4527683 | 1.0333702 | -1.6540051 |
| C | -5.8885117 | 1.7874012 | 2.8865560 |
| H | -6.7597933 | 1.1799337 | 2.6399433 |
| H | -5.7879898 | 1.8031964 | 3.9701911 |
| H | -6.1015648 | 2.8060354 | 2.5595409 |
| C | -1.2117079 | 0.2103796 | 3.2996915 |
| H | -1.0314317 | -0.8604372 | 3.4184841 |
| H | -0.2772643 | 0.6952957 | 3.0265772 |
| H | -1.4622591 | 0.5814027 | 4.2908603 |
| C | -1.4336565 | -1.6287356 | -1.0746928 |
| C | -1.2051802 | -1.6708939 | -2.4639638 |
| C | -1.6903079 | -2.7580847 | -3.1735480 |
| H | -1.5152160 | -2.7960750 | -4.2424980 |
| C | -2.3802417 | -3.8008138 | -2.5670896 |
| C | -2.5747421 | -3.7409803 | -1.1973159 |
| H | -3.0872460 | -4.5552807 | -0.6995441 |
| C | -2.1110349 | -2.6794716 | -0.4305012 |
| C | -0.4809359 | -0.6112205 | -3.2434566 |
| H | -0.3524557 | -0.9291365 | -4.2759677 |
| H | -1.0330561 | 0.3292446 | -3.2741901 |
| H | 0.5132921 | -0.3971574 | -2.8593402 |
| C | -2.8401046 | -4.9763470 | -3.3712818 |
| H | -3.5355662 | -5.6011886 | -2.8141319 |
| H | -3.3305374 | -4.6616734 | -4.2921925 |
| H | -1.9912594 | -5.6007229 | -3.6548627 |
| C | -2.3678138 | -2.7479400 | 1.0500497 |
| H | -2.5194766 | -3.7824921 | 1.3515282 |
| H | -1.5411555 | -2.3838520 | 1.6617426 |
| H | -3.2575263 | -2.1852810 | 1.3331293 |
| C | 1.5072887 | 3.7470520 | -1.3121821 |
| C | 0.8271353 | 4.9523233 | -1.4191984 |
| F | 0.2113774 | 5.4616518 | -0.3466434 |
| C | 0.7259201 | 5.6795313 | -2.5908300 |
| F | 0.0625818 | 6.8310755 | -2.6260261 |
| C | 1.3177759 | 5.1891259 | -3.7394249 |
| F | 1.2305119 | 5.8635503 | -4.8791976 |
| C | 1.9873460 | 3.9827707 | -3.6912559 |
| F | 2.5414250 | 3.4932432 | -4.7967561 |
| C | 2.0671901 | 3.2866977 | -2.4946820 |
| F | 2.7049013 | 2.1148900 | -2.5508121 |
| C | 1.9941317 | 4.0121084 | 1.3206117 |
| C | 3.2060352 | 4.6754526 | 1.1751859 |
| F | 3.9378257 | 4.4850702 | 0.0768182 |
| C | 3.7212550 | 5.5460391 | 2.1182078 |
| F | 4.8875569 | 6.1529695 | 1.9242321 |
| C | 3.0072687 | 5.7833973 | 3.2778491 |
| F | 3.4813503 | 6.6125061 | 4.1988349 |
| C | 1.7970791 | 5.1477742 | 3.4687642 |
| F | 1.1023288 | 5.3682630 | 4.5823219 |
| C | 1.3178412 | 4.2846288 | 2.4971466 |
| F | 0.1345793 | 3.7168949 | 2.7627205 |
| C | 2.7323889 | -2.4596090 | 1.3874867 |
| C | 2.3466906 | -2.9625037 | 2.6172946 |
| F | 1.0691903 | -2.8840650 | 3.0161590 |
| C | 3.2270315 | -3.5696964 | 3.4941557 |
| F | 2.8067958 | -4.0344225 | 4.6642930 |
| C | 4.5582990 | -3.6908097 | 3.1417998 |
| F | 5.4146603 | -4.2683402 | 3.9694553 |
| C | 4.9887922 | -3.2112243 | 1.9181251 |
| F | 6.2625732 | -3.3310044 | 1.5709648 |
| C | 4.0737061 | -2.6129039 | 1.0714793 |
| F | 4.5194379 | -2.1742190 | -0.1048259 |
| C | 1.5288269 | -2.7948522 | -0.9467814 |
| C | 2.0697974 | -2.6557563 | -2.2151262 |
| F | 2.7875555 | -1.5884510 | -2.5474112 |
| C | 1.8760424 | -3.6020027 | -3.2109044 |
| F | 2.3853144 | -3.4196732 | -4.4231848 |
| C | 1.1361247 | -4.7368723 | -2.9440349 |
| F | 0.9199892 | -5.6356523 | -3.8961280 |
| C | 0.6016405 | -4.9245094 | -1.6829144 |
| F | -0.1265978 | -6.0054260 | -1.4222363 |
| C | 0.8177451 | -3.9607016 | -0.7209159 |
| F | 0.2908134 | -4.1670471 | 0.4909034 |
| S | 2.9053607 | 0.6252378 | 0.8369104 |
| O | 2.6581372 | 1.9331703 | 0.0759348 |
| O | 2.0044696 | 0.4732591 | 2.0172857 |

**9c$_{calc}$**

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| | | | |
|---|---|---|---|
| P | -0.3071964 | -0.8378887 | -0.1032089 |
| S | 1.7893401 | 2.2667944 | -0.2348705 |
| B | 1.4027419 | 1.6392562 | 2.5952217 |
| B | 0.1946306 | 1.4793132 | -2.0333836 |
| O | 1.8874457 | 0.6443981 | -0.5074855 |
| O | 0.3846065 | 2.4670791 | -0.8896959 |
| O | 1.5569293 | 2.4659934 | 1.2389332 |
| C | -0.4865871 | 0.2199307 | 1.3688496 |
| H | -0.7301858 | 1.2232969 | 1.0218030 |
| H | -1.3523428 | -0.1169889 | 1.9252788 |
| C | 0.7805303 | 0.1880435 | 2.2458252 |
| H | 1.5736716 | -0.4075028 | 1.7888055 |
| H | 0.5556426 | -0.3513811 | 3.1668567 |
| C | 0.7840126 | 0.1202502 | -1.2600068 |
| H | 1.1920057 | -0.5794393 | -1.9770513 |
| C | 0.3709976 | -2.4248371 | 0.5305338 |
| C | 1.6493579 | -2.9377402 | 0.2315659 |
| C | 2.0168675 | -4.1712056 | 0.7627726 |
| H | 3.0003663 | -4.5571922 | 0.5236758 |
| C | 1.1871512 | -4.9189269 | 1.5771835 |
| C | -0.0565041 | -4.3877265 | 1.8764374 |
| H | -0.7240177 | -4.9417926 | 2.5263846 |
| C | -0.4822875 | -3.1615270 | 1.3859986 |
| C | 2.6909546 | -2.2789775 | -0.6291630 |
| H | 3.6102224 | -2.8599112 | -0.5982176 |
| H | 2.9452895 | -1.2759861 | -0.3005249 |
| H | 2.4027161 | -2.2297710 | -1.6795304 |
| C | 1.6088002 | -6.2477106 | 2.1248049 |
| H | 0.9540927 | -7.0442924 | 1.7687110 |
| H | 1.5633134 | -6.2559542 | 3.2143449 |
| H | 2.6267781 | -6.4998666 | 1.8332402 |
| C | -1.8325195 | -2.7072693 | 1.8736696 |
| H | -2.3844093 | -3.5547752 | 2.2753919 |
| H | -2.4603341 | -2.2702756 | 1.1024272 |
| H | -1.7338324 | -1.9886273 | 2.6888365 |
| C | -1.8354826 | -1.2480063 | -1.0159346 |
| C | -1.7444713 | -2.2395779 | -2.0107622 |
| C | -2.8815572 | -2.5726574 | -2.7389644 |
| H | -2.7945853 | -3.3222440 | -3.5161846 |
| C | -4.1061976 | -1.9722437 | -2.5162966 |
| C | -4.1763735 | -1.0054650 | -1.5229152 |
| H | -5.1259777 | -0.5186735 | -1.3320247 |
| C | -3.0781617 | -0.6221191 | -0.7681005 |
| C | -0.4949170 | -2.9979519 | -2.3611752 |
| H | -0.5814997 | -3.4078457 | -3.3656151 |
| H | -0.3296173 | -3.8306542 | -1.6773360 |
| H | 0.4064383 | -2.3919124 | -2.3612996 |
| C | -5.3116848 | -2.3116095 | -3.3362474 |
| H | -5.6347749 | -1.4499829 | -3.9218946 |
| H | -6.1501685 | -2.6051113 | -2.7040658 |
| H | -5.1125650 | -3.1266753 | -4.0294673 |
| C | -3.3400457 | 0.4180011 | 0.2853311 |
| H | -4.3081461 | 0.8836417 | 0.1120430 |
| H | -2.6114986 | 1.2208574 | 0.3081355 |
| H | -3.3803994 | -0.0201664 | 1.2843738 |
| C | 2.8813259 | 1.4342746 | 3.2448437 |
| C | 2.9941511 | 1.1738445 | 4.6024373 |
| F | 1.8930530 | 1.1010373 | 5.3559087 |
| C | 4.2001787 | 0.9587834 | 5.2448169 |
| F | 4.2437708 | 0.7163528 | 6.5497873 |
| C | 5.3702600 | 0.9902202 | 4.5101779 |
| F | 6.5390480 | 0.7849993 | 5.1020156 |
| C | 5.3089714 | 1.2221605 | 3.1498899 |
| F | 6.4259641 | 1.2356657 | 2.4302054 |
| C | 4.0788126 | 1.4280000 | 2.5493653 |
| F | 4.1066701 | 1.6094961 | 1.2192730 |
| C | 0.5143321 | 2.6853131 | 3.4681446 |
| C | 0.9960762 | 3.9745137 | 3.6597914 |
| F | 2.1738922 | 4.3257120 | 3.1433198 |
| C | 0.3237815 | 4.9427001 | 4.3825739 |
| F | 0.8324452 | 6.1602592 | 4.5309555 |
| C | -0.8936794 | 4.6313112 | 4.9590958 |
| F | -1.5577777 | 5.5435462 | 5.6545919 |
| C | -1.4085861 | 3.3596836 | 4.8071669 |
| F | -2.5749597 | 3.0455486 | 5.3633995 |
| C | -0.7001334 | 2.4209242 | 4.0760883 |
| F | -1.2608609 | 1.2063074 | 3.9976169 |
| C | 1.1895657 | 1.9530889 | -3.2599592 |
| C | 2.1859998 | 1.2382322 | -3.9067321 |
| F | 2.4846405 | -0.0196211 | -3.5561060 |
| C | 2.9400243 | 1.7510016 | -4.9496346 |
| F | 3.8816533 | 1.0134351 | -5.5262599 |
| C | 2.7090779 | 3.0384292 | -5.3898312 |
| F | 3.4211387 | 3.5428238 | -6.3849818 |
| C | 1.7241105 | 3.7945378 | -4.7820869 |
| F | 1.4878358 | 5.0313981 | -5.1988021 |
| C | 0.9964403 | 3.2443125 | -3.7436749 |
| F | 0.0550321 | 4.0166009 | -3.2045120 |
| C | -1.3192021 | 1.4772936 | -2.5775080 |
| C | -1.6295986 | 0.6019702 | -3.6059675 |
| F | -0.6935332 | -0.2565059 | -4.0266453 |
| C | -2.8627379 | 0.5503882 | -4.2206915 |
| F | -3.1173779 | -0.3304732 | -5.1824134 |
| C | -3.8524471 | 1.4196209 | -3.8003727 |
| F | -5.0588232 | 1.3675398 | -4.3516218 |
| C | -3.5878313 | 2.3192212 | -2.7871539 |
| F | -4.5435429 | 3.1432567 | -2.3719526 |
| C | -2.3327302 | 2.3409523 | -2.1989899 |
| F | -2.1509920 | 3.2254500 | -1.2215818 |