Rapid Intramolecular Heterolytic Dihydrogen Activation by a Four-membered Heterocyclic Phosphane-Borane Adduct

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Supporting Informations

Experimental Section:

All reactions involving air or moisture-sensitive compounds were
10 carried out under an inert gas using Schlenk-type glassware or in a
glovebox. Solvents were dried and distilled prior to use. Unless
otherwise noted, all starting materials were commercially available
and were used without further purification. The following
instruments were used for physical characterisation of the
15 compounds: melting points: DSC 2010 TA-instruments; elemental
analyses: Foss–Heraeus CHNO-Rapid; NMR spectrometer: Bruker
AV 300 (^{1}H: 300.1 MHz; ^{13}C: 75.5 MHz; ^{31}P: 121.5 MHz; ^{19}F:
282.4 MHz), Varian INOVA (^{1}H: 499.8 MHz; ^{13}C: 125.7 MHz;
^{31}P: 202.3 MHz; ^{19}F: 470.3 MHz; ^{2}H: 76.7 MHz), Varian UNITY
20 plus (^{1}H: 599.9 MHz; ^{13}C: 150.8 MHz; ^{19}F: 564.2 MHz).
Data sets were collected with a Nonius KappaCCD diffractometer.
Programs used: data collection COLLECT (Nonius B.V., 1998),
data reduction Denzo-SMN (Z. Otwinowski, W. Minor, *Methods in
Enzymology*, **1997**, *276*, 307-326), absorption correction Denzo (Z.
25 Otwinowski, D. Borek, W. Majewski, W. Minor, *Acta Cryst.* **2003**,
A59, 228-234), structure solution SHELXS-97 (G.M. Sheldrick,
Acta Cryst. **1990**, *A46*, 467-473), structure refinement SHELXL-97
(G.M. Sheldrick, Universität Göttingen, 1997), graphics
SCHAKAL (E. Keller, Universität Freiburg, 1997).
30 Crystallographic data for this paper can be obtained free of charge
at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the
Cambridge Crystallographic Data Centre, 12 Union Road,
Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-
mail: deposit@ccdc.cam.ac.uk].

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Preparation of 2.

5.13 g (16.8 mmol) chlorodimesitylphosphine was dissolved in 60
ml thf (60 cm^3). 0.7 M vinylmagnesiumbromide in thf (24 cm^3)
was added. The solution was stirred for 1h at room temperature, the
40 solvent was removed on the rotary evaporator and the residue was
extracted with pentane (100 cm^3). The pentane was removed in the
oil pump vacuum and a brown oil could be obtained (3.93 g, 79%).
The crude product was cleaned *via* column-chromatography (silica
gel; CH$_2$Cl$_2$ Cyclohexane 2 : 8). A colorless oil (2.37 g, 48 %)
45 could be obtained. [Compound **2** contained two minor impurities
(≥ 5%) as judged from the ^{31}P spectrum (δ -36.4, δ -93.2)].
(Found: C, 80.6; H, 8.6. C$_{20}$H$_{25}$P requires C, 81.1; H, 8.5%);
δ$_H$(500 MHz; d$_6$-benzene; Me$_4$Si) 6.98 (1H, J_{PH} 26.4, $J_{HH, cis}$ 11.7,

$J_{HH, trans}$ 18, ddd, CH=), 6.69 (2H, m, J_{PH} 2.6, *m*-Mes), 5.35 (1H,
50 $J_{PH, trans}$ 26.6, $J_{HH, cis}$ 11.7, $^2J_{HH}$ 2.3, ddd, =CH$_2$), 5.29 (1H, $J_{HH, trans}$
18.0, $J_{PH, cis}$ 11.9, $^2J_{HH}$ 2.3, ddd, =CH$_2$), 2.34 (12H, s, *o*-CH$_3$^{Mes}),
2.07 (6H, s, *p*-CH$_3$^{Mes}); δ$_{C\{H\}}$(126 MHz; d$_6$-benzene; Me$_4$Si) 142.4
(d, J_{PC} 14.9, *i*-Mes), 137.9 (*p*-Mes), 131.4 (d, J_{PC} 17.2, *i*-Mes),
130.2 (d, J_{PC} 3.6, m-Mes), 129.4 (d, J_{PC} 12.9, P-C=), 121.8 (d, J_{PC}
55 17.3, =CH$_2$), 23.2 (d, J_{PC} 14.4 Hz, *o*-CH$_3$^{Mes}), 20.9 (*p*-CH$_3$^{Mes});
δ$_{P\{H\}}$(202 MHz; d$_6$-benzene; H$_3$PO$_4$) -22.0 (ν$_{1/2}$ = 2 Hz).

Preparation of 4.

Dimesitylvinylphosphane (**2**) (200 mg, 0.67 mmol) and HB(C$_6$F$_5$)$_2$
60 (**3**) (233 mg, 0.67 mmol) were suspended in pentane (20 cm^3) and
stirred for 1 h at ambient temperature. The resulting clowdy
solution was filtered and the clear filtrate evaporated to dryness in
vacuo to yield **4** (322 mg, 75%) as a yellow solid (Found: C, 58.8;
H, 3.9. C$_{32}$H$_{26}$BF$_{10}$P requires C, 59.8; H, 4.1%); δ$_H$(600 MHz;
65 C$_6$D$_6$; Me$_4$Si) 1.91 (6H, s, *p*-CH$_3$^{Mes}), 2.03 (12H, s, *o*-CH$_3$^{Mes}), 2.29
(2H, dt, J_{PH} 42 and J_{HH} 8, CH$_2$-B), 2.87 (2H, q, J_{HH} = J_{PH} 8, P-
CH$_2$), 6.44 (4H, d, J_{PH} 2.0, *m*-Mes); δ$_{C\{H\}}$(151 MHz; C$_6$D$_6$ MHz;
Me$_4$Si) 18.2 (br., CH$_2$-B), 20.5 (*p*-CH$_3$^{Mes}), 22.5 (d, J_{PC} 6.5, *o*-
CH$_3$^{Mes}), 29.4 (d, J_{PC} 37, P-CH$_2$), 119.4 (*i*-C$_6$F$_5$), 126.8 (d, J_{PC} 23, *i*-
70 Mes), 130.9 (d, J_{PC} 7.5, *m*-Mes), 137.5 (dm, J_{FC} 245, C$_6$F$_5$), 140.3
(dm, J_{FC} 252, *p*-C$_6$F$_5$), 141.0 (d, J_{PC} 2.6, *p*-Mes), 142.1 (d, J_{PC} 8.0,
o-Mes), 148.3 (dm, J_{FC} 243, C$_6$F$_5$); δ$_{P\{H\}}$(121 MHz; C$_6$D$_6$; H$_3$PO$_4$)
20.6 (ν$_{1/2}$ = 30 Hz); δ$_F$(282 MHz, C$_6$D$_6$, CFCl$_3$) -128.8 (4F), -157.0
(2F, *p*-C$_6$F$_5$), -163.6 (4F); δ$_{B\{H\}}$(96 MHz, C$_6$D$_6$, BF$_3$OEt$_2$) 8.5 (ν$_{1/2}$
75 = 460 Hz). ESI MS: m/z 643.17 ((M + H)$^+$, 100 %).

Reaction of 4 with dihydrogen, preparation of 5.

Compound **4** (1.00 g, 1.6 mmol) was dissolved in pentane (15 cm^3).
Dihydrogen gas was introduced to the solution with vigorous
80 stirring through a capillary (1.5 bar) for 15 min at room
temperature. The product precipitated during this time as a white
solid. It was collected by filtration, washed with pentane (10 cm^3)
and dried in vacuo to yield **5** as a white solid (616 mg, 60%)
(Found: C, 59.3; H, 4.3. C$_{32}$H$_{28}$BF$_{10}$P requires C, 59.7; H, 4.4%);
85 mp 81°C; δ$_H$(500 MHz; d$_8$-thf; Me$_4$Si) 1.25 (2H, br. m, CH$_2$-B),
2.32 (6H, s, *p*-CH$_3$^{Mes}), 2.45 (12H, s, *o*-CH$_3$^{Mes}), 2.80 (2H, m, P-
CH$_2$), 2.91 (1H, br., B-H), 7.11 (4H, J_{PH} 4.2, *m*-Mes), 7.87 (1H, dt,
J_{PH} 486 and J_{HH} 7.3, P-H); δ$_{C\{H\}}$(126 MHz; d$_8$-thf; Me$_4$Si) 17.8 (br.
m, CH$_2$-B), 21.0 (d, J_{PC} 1.3, *p*-CH$_3$^{Mes}), 21.9 (d, J_{PC} 6.8, *o*-CH$_3$^{Mes}),

26.9 (d, J_{PC} 34.4, P-CH$_2$), 114.8 (d, J_{PC} 76.2, i-Mes), 128.1 (br., i-C$_6$F$_5$), 132.2 (d, J_{PC} 10.8, m-Mes), 137.1 (dm, J_{FC} 247, C$_6$F$_5$), 138.3 (dm, J_{FC} 243, C$_6$F$_5$), 144.2 (d, J_{PC} 9.5, o-Mes), 145.8 (d, J_{PC} 2.7, p-Mes), 149.0 (dm, J_{FC} 237, C$_6$F$_5$); $\delta_{P\{H\}}$(121 MHz; d$_8$-thf; H$_3$PO$_4$) -6.5 ($\nu_{1/2}$ = 55 Hz); δ_P(121 MHz; d$_8$-thf; H$_3$PO$_4$) -6.5 (dm, J_{PH} 486); δ_F(282 MHz; d$_8$-thf; CFCl$_3$) -133.4 (4F), -165.8 (2F, p-C$_6$F$_5$), 168.0 (4F); $\delta_{B\{H\}}$(96 MHz; d$_8$-thf; BF$_3$OEt$_2$) -20.1 ($\nu_{1/2}$ = 67 Hz); δ_B(96 MHz; d$_8$-thf; BF$_3$OEt$_2$) -20.1 (d, J_{BH} 88). Crystal data for C$_{32}$H$_{28}$BF$_{10}$P, M = 644.32, monoclinic, space group $P2_1$/c (No. 14), 12.3680(3), b = 18.5413(5), c = 13.1716(1) Å, β = 96.361(2)°, V = 3001.90(13) Å^3, D_c = 1.426 g cm^{-3}, μ = 1.572 mm^{-1}, Z = 4, λ = 1.54178 Å, T = 223(2) K, 21035 reflections collected ($\pm h$, $\pm k$, $\pm l$), [($sin\theta$)/λ] = 0.60 Å^{-1}, 5312 independent (R_{int} = 0.060) and 4566 observed reflections [$I \geq 2\sigma(I)$], 411 refined parameters, R = 0.050, wR^2 = 0.144, CCDC 650365.

Reaction of 4 with deuterium, formation of 5-D$_2$.

Compound **4** (535 mg, 0.8 mmol) was dissolved in pentane (10 cm^3). Under vigorous stirring, deuterium (1.5 bar) was pressed on the flask for 30 min. The product precipitated during this time as a white solid. It was collected by filtration, washed with pentane (5 cm^3) and dried in vacuo to yield **5-D$_2$** as a white solid (296 mg, 55 %). δ_D(76.7 MHz; thf; Me$_4$Si) 2.94 (1D, br. B-D), 7.87 (1D, J_{PD} 75, d, P-D). ($J_{PD(calc)}$ = $\gamma(^2H)$ / $\gamma(^1H)$ $\times J_{PH(exp)}$ = 74.6 Hz)[1].
[**5-D$_2$** contains about 30% of **5**, judged from ^{31}P spectra (see below); origin as yet unexplained]. [1] E. Fluck and H. Binder, Z. Naturforsch., 1967, **22**, 805; A. A. Borisenko, N. M. Sergeyev, and Yu. A. Ustynyuk, Molec. Phys., 1971, **22**, 715.

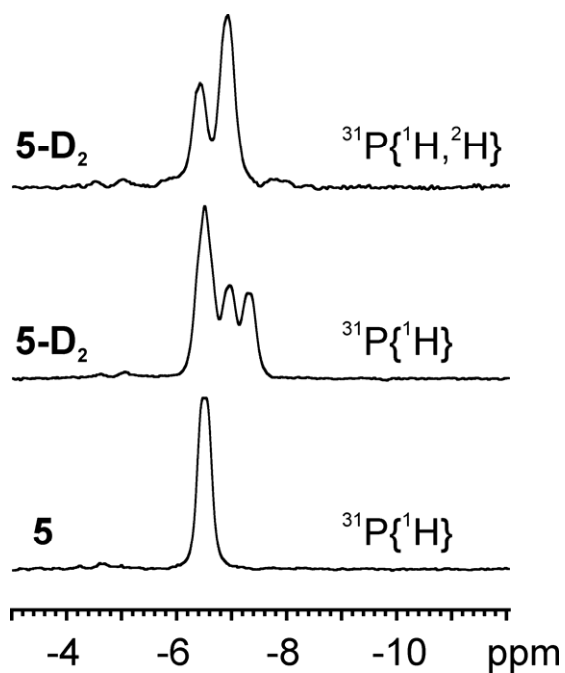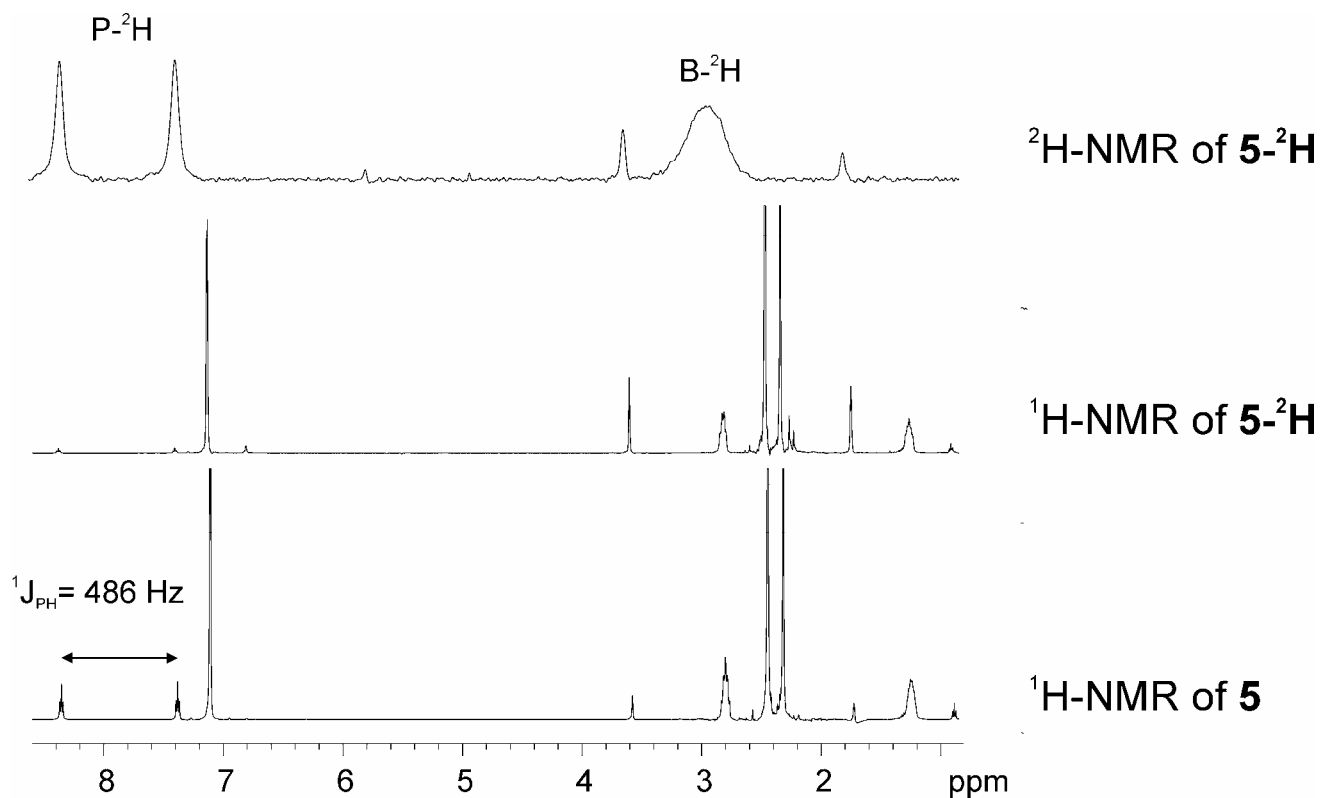### Reaction of 5 with benzaldehyde, formation of 6.

Compound **5** (542 mg, 0.8 mmol) was added to a solution of benzaldehyde (114 mg; 1.1 mmol) in thf (10 cm^3). The reaction mixture was stirred for 1 h at room temperature and then evaporated to dryness. The residue was suspended in pentane (10 cm^3) and the product collected by filtration and dried in vacuo to yield **6** as a white solid (230 mg; 36%) (Found: C, 62.1; H, 4.4. C$_{39}$H$_{34}$BF$_{10}$OP requires 62.4; H, 4.6%); δ_H(600 MHz; d$_8$-thf; Me$_4$Si) 1.37 (2H, br. m, CH$_2$-B), 2.31 (6H, s, p-CH$_3^{Mes}$), 2.32 (12H, s, o-CH$_3^{Mes}$), 2.76 (2H, m, P-CH$_2$), 4.09 (2H, s, CH$_2$Ph), 7.06 (5H, m, p-Ph + m-Mes), 7.17 (2H, m, m-Ph), 7.32 (2H, m, o-Ph), 7.86 (1H, dt, J_{PH} 492, J_{HH} 7.6, H-P); $\delta_{C\{H\}}$(151 MHz; d$_8$-thf; Me$_4$Si) 18.7 (br., CH$_2$-B), 21.0 (p-CH$_3^{Mes}$), 21.8 (d, J_{PC} 6.9, o-CH$_3^{Mes}$), 23.2 (d, J_{PC} 37.6, P-CH$_2$), 65.6 (CH$_2$Ph), 114.8 (d, J_{PC} 76.3, i-Mes), 126.1 (p-Ph), 126.8 (o-Ph), 128.1 (m-Ph), 132.1 (d, J_{PC} 10.7, m-Mes), 137.3 (dm, J_{FC} 247, C$_6$F$_5$), 138.9 (dm, J_{FC} 235, p-C$_6$F$_5$), 144.1 (d, J_{PC} 9.7, o-Mes), 145.70 (i-Ph), 145.73 (d, J_{PC} 2.7, p-Mes), 148.9 (dm, J_{FC} 238, C$_6$F$_5$); $\delta_{P\{H\}}$(121 MHz; d$_8$-thf; H$_3$PO$_4$) -4.8 ($\nu_{1/2}$ = 24 Hz); δ_P(121 MHz; d$_8$-thf; H$_3$PO$_4$) -4.8 (d, J_{PH} 492); δ_F(282 MHz, d$_8$-thf, CFCl$_3$) -133.7 (4F, o-C$_6$F$_5$), -164.3 (2F, p-C$_6$F$_5$), -167.4 (4F, m-C$_6$F$_5$); $\delta_{B\{H\}}$(96 MHz; d$_8$-thf; BF$_3$OEt$_2$) -0.3 ($\nu_{1/2}$ = 95 Hz). Crystal data for C$_{39}$H$_{34}$BF$_{10}$OP, M = 750.44, triclinic, space group P1bar (No. 2), 12.1089(8), b = 12.7662(10), c = 12.8752(8) Å, α = 104.669(3), β = 100.577(5), γ = 100.279(3)°, V = 1839.0(2) Å^3, D_c = 1.355 g cm^{-3}, μ = 1.385 mm^{-1}, Z = 2, λ = 1.54178 Å, T = 223(2) K, 20114 reflections collected ($\pm h$, $\pm k$, $\pm l$), [($sin\theta$)/λ] = 0.60 Å^{-1}, 6171 independent (R_{int} = 0.078) and 4081 observed reflections [$I \geq 2\sigma(I)$], 479 refined parameters, R = 0.077, wR^2 = 0.227, CCDC 650366.

Reaction of 4 with Oxygen.

A solution of **4** in cyclohexane was left in a schlenk flask (which was leaky) connected via a condensation bridge with a schlenk flask filled with toluene for 4 weeks. White crystals could be obtained which were isolated and dried in $vacuo$.
δ_H(300 MHz; C$_6$D$_6$; Me$_4$Si) 1.85 (6H, s, p-CH$_3^{Mes}$), 2.09 (12H, s, o-CH$_3^{Mes}$), 2.42 (2H, m, CH$_2$), only one CH$_2$ signal can be observed, 6.39 (4H, d, J_{PH} 4.4, m-Mes); $\delta_{P\{H\}}$(121 MHz; C$_6$D$_6$; H$_3$PO$_4$) 80.0 ($\nu_{1/2}$ = 3.8 Hz); δ_P(121 MHz; C$_6$D$_6$; H$_3$PO$_4$) 80.0 (t, J_{PH} 20); δ_F(282 MHz, C$_6$D$_6$, CFCl$_3$) -133.7 (4F), -159.3 (2F, p-C$_6$F$_5$), -164.4 (4F); $\delta_{B\{H\}}$(96 MHz, C$_6$D$_6$, BF$_3$OEt$_2$) 4.5 ($\nu_{1/2}$ = 600 Hz).

P-^{2}H

B-^{2}H

^{2}H-NMR of **5-^{2}H**

^{1}H-NMR of **5-^{2}H**

$^1J_{PH}$= 486 Hz

^{1}H-NMR of **5**

8   7   6   5   4   3   2   ppm

5-D$_2$ ^{31}P{^{1}H,^{2}H}

5-D$_2$ ^{31}P{^{1}H}

5 ^{31}P{^{1}H}

-4   -6   -8   -10   ppm

^{31}P NMR spectra (121 MHz; d$_8$-thf; H$_3$PO$_4$) of **5-D$_2$** (top and center) and **5** (bottom).
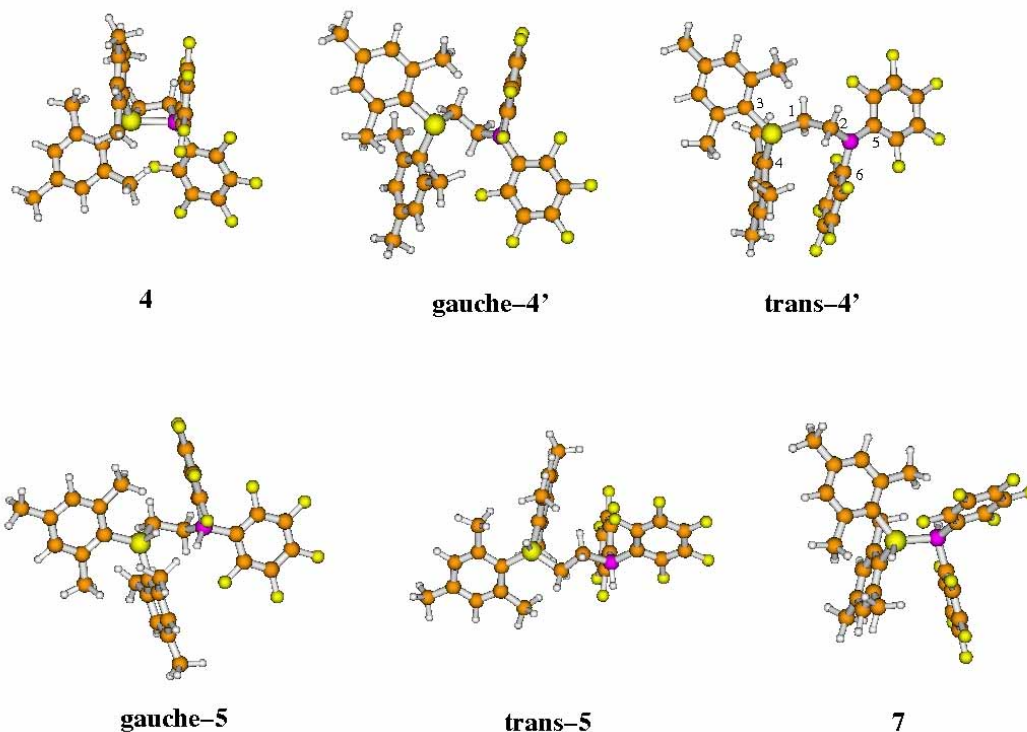
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Theoretical Methods and Technical Details of the Computations

[175] The quantum chemical calculations have been performed with slightly modified versions of the TURBOMOLE suite of programs.[1] As Gaussian AO basis, large triple-zeta (def2-TZVP) sets of Ahlrichs et al.[2] have been employed. In standard notation these are [5s3p2d1f] for B, [5s5p2d1f] for P, [5s3p2d] for C and F and [3s1p] for H. For the hydrogen atoms of the added H we employ a larger [3s2p1d] basis in order to avoid basis set superposition error (BSSE). This basis set is abbreviated in [180] the following as def2-TZVP'. In calculations on model compounds without the phenyl rings, this AO basis has been tested in comparison with a much larger QZVP set[3] and small differences on the order of ±1 kcal mol for relative energies have been observed. All geometries have been fully optimized at the DFT level using the B97-D density functional[4] that also includes an empirical correction for intramolecular dispersion (van der Waals) interactions[5, 4]. For a detailed description of this [185] dispersion correction including many illustrative examples see Ref.[6]. All energies are corrected by zero-point vibrational energies (ZPVE) employing unscaled harmonic frequencies as obtained from LDA/SV computations. The B97-D relative energies are checked by improved (spin-component scaled) Møller-Plesset perturbation theory (SCS-MP2) using the same AO basis set. In the SCS-MP2 treatments for the correlation energy (frozen-core approximation) and for the Coulomb integrals in the [190] DFT treatments, the RI-approximation has been used[7].

References

[1]   Ahlrichs, R.; Bär, M.; Häser, M.; Horn, H.; Kölmel, C. *Chem. Phys. Lett.* **1989,** *162,* 165–169.TURBOMOLE, version 5.7: R. Ahlrichs et al., Universität Karlsruhe 2003. See [195] http://www.turbomole.com.

[2]   Schäfer, A.; Huber, C.; Ahlrichs, R. *J. Chem. Phys.* **1994,** *100,* 5829–5835. The basis sets are available from the TURBOMOLE homepage via the FTP Server Button (in the subdirectories basen, jbasen, and cbasen). See http://www.turbomole.com.

[3]   Weigend, F.; Furche, F.; Ahlrichs, R. *J. Chem. Phys.* **2003,** *119,* 12753–12762.

[200] [4]   Grimme, S. *J. Comput. Chem.* **2006,** *27,* 1787-1799.

[5]   Grimme, S. *J. Comput. Chem.* **2004,** *25,* 1463-1473.

[6]   Grimme, S.; Antony, J.; Schwabe, T.; Mück-Lichtenfeld, C. *Org. Biomol. Chem.* **2007,** *5,* 741-758.

[7]   Weigend, F.; Häser, M. *Theor. Chem. Acc.* **1997,** *97,* 331-340. Weigend, F.; Köhn, A.; [205] Hättig, C. *J. Chem. Phys.* **2002,** *116,* 3175-3183. Eichkorn, K.; Treutler, O.; Öhm, H.; Häser, M.; Ahlrichs, R. *Chem. Phys. Lett.* **1995,** *240,* 283–289. Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. *Theor. Chem. Acc.* **1997,** *97,* 119–124.

Figure S1: Optimized Structures

4   **gauche–4'**   **trans–4'**

gauche–5   **trans–5**   **7**

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Table S1. Reaction Energies (in kcal/mol)

reaction	ΔE		ΔH(0 K)
	B97-D	SCS-MP2	SCS-MP2
4→gauche-4'	6.8	11.3	10.9
4→trans-4'	7.0	10.4	9.7
gauche-4'+H gauche-5	−12.1	−10.3	-4.9
gauche-5→trans-5	0.3	−2.2	-2.3
gauche-5→ethene+PH(mes)+BH(CF)	32.1	33.1	27.8
7→ PH(mes)+BH(CF)	31.6	30.9	28.7

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225 **Table S2. Important Structural Parameters (Angstroem or degree)**

	4	gauche-**4'**	trans-**4'**	gauche-**5**	trans-**5**	**7**
P–B	2.214	3.261	3.996	3.171	4.119	1.990
P–C3	1.845	1.863	1.859	1.821	1.808	1.833
P–C4	1.842	1.855	1.865	1.800	1.818	1.830
P–C1	1.842	1.880	1.906	1.823	1.811	
C1–C2	1.555	1.543	1.571	1.545	1.546	
B–C2	1.662	1.581	1.571	1.659	1.661	
B–C5	1.628	1.589	1.576	1.654	1.646	1.628
B–C6	1.627	1.583	1.588	1.641	1.663	1.635
P–H				1.393	1.399	1.399
B–H				1.224	1.218	1.205
H–H				2.160	5.109	3.705
< P–C1–C2	96.2	108.5	111.8	110.7	109.3	
< B–C2–C1	103.4	115.5	102.7	114.2	108.3	
< H–P–C1/B				104.0	105.1	109.1
< H–B–C2/P				107.2	108.9	104.4
< P–C1–C2–B	17.4	−60.2	131.5	−49.3	−145.4	
< C3–P–B–C5	21.6	40.5	5.3	12.0	70.0	56.9
< H–P–C3–C4				−114.8	−112.1	−107.3
< H–B–C5–C6				116.1	118.7	−122.9
< C3–P–C1–C2	88.3	−178.6	143.1	174.7	55.6	
< C5–B–C2–C1	−111.8	−31.7	97.4	−49.3	−171.8	

Table S3. Dipole Moments

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molecule	dipole moment [Debye]
4	7.0
gauche-4'	3.5
trans-4'	1.9
gauche-5	14.7
trans-5	17.6

B97-D/def2-TZVP'.

Discussion

In general we find good agreement between the reaction energies from DFT and wave function theory (SCS-MP2). The P-B bond is intrinsically strong (about 29 kcal/mol) but weakened in **4** by the 4-membered ring (as also indicated by the increase of R(P-B) by 22 pm). In the gas phase (and this very likely holds also for the condensed phase due to the higher dipole moment), **4** is more stable than the open forms **4'** by 7-10 kcal mol depending on the method used. This value is the minimum effective reaction barrier for the hydrogen addition process. The gauche and trans conformers of **4'** have almost the same energy and the reaction can therefore proceed from gauche-**4'** (where the P and B atoms are spatially more close) and molecular hydrogen to the adduct gauche-**5** which then yields the slightly more stable form trans-**5** that is observed in the crystal. The actual hydrogen addition reaction is exothermic by about 5 kcal/mol. The products **5** have the expected electronic structure with strong charge separation (zwitter-ionic, i.e. –0.78 charge on the CHBHCF fragment for gauche-**5**) leading to large dipole moments between 14.7 and 17.6 Debye. The also considered fragmentation reaction releasing ethene is very unfavourable (entry 5 in Table S1) and even close to thermoneutral when **7** is formed. Note, that some structures are significantly stabilized by intramolecular stacking interactions between the mesityl and the CF fragments (the B97-D computed benzene-CF complex dissociation energy is about 6 kcal/mol).

Cartesian Coordinates (in Bohr)

4

0.18526918552200	2.56723976843407	-1.40122965554050	p
-0.95577516692137	-1.40990878960997	-2.02291068172259	b
-0.76472558457380	2.50413790053560	-4.74911264731790	c
-0.84826710958847	-0.42266268643172	-5.00254771884773	c
-1.04230453588900	5.43321386949555	0.14448872407257	c
-0.20448959991383	7.83524944220173	-0.72551865636576	c
-1.18645457557537	10.01654797026878	0.38237360595240	c
-2.97901115751714	9.92144370723601	2.32701434897594	c
-3.76162462993068	7.55330954790742	3.16256973870451	c
-2.82889778854202	5.29905566726231	2.12338514204136	c
3.62773494325652	2.48617222245631	-0.85692062775398	c
5.51157010904883	2.35140659667658	-2.76657934757984	c
8.00559854312767	1.80262902315294	-2.07034940513775	c
8.73701739802163	1.40120727513243	0.42783626532372	c
6.89243034219743	1.66674984933095	2.28948794000946	c
4.37229214823062	2.20021940262082	1.71187131783367	c
-3.78188754578985	-2.32054037335943	-1.22798103715215	c
-5.90217903340929	-0.74131615067361	-1.29160165315623	c
-8.35302715578364	-1.51911795992372	-0.71046083078521	c
-8.79031096881549	-4.04585888836010	-0.10151718753503	c
-6.76122089504954	-5.72923518183082	-0.08812003150887	c
-4.33597268401611	-4.85115573576755	-0.65518746675026	c
1.36883692223097	-2.91634495341896	-0.68635155332006	c
3.65163736013849	-3.56969098835903	-1.85681478717854	c
5.76483963014747	-4.46799535658695	-0.55323818158342	c
5.64629928578029	-4.79143100095101	2.05401261445759	c
3.39391259402456	-4.24781608651728	3.30862665454415	c
1.33954019736845	-3.35491764036508	1.92870076439883	c
1.72207842106024	8.13285030231082	-2.81367364905711	c
-4.02654279050869	12.32066882067486	3.45803063782512	c
-3.79585603813922	2.87614366442377	3.28671482832177	c
5.05172767536388	2.79033949845259	-5.55259468861499	c
11.40144286729836	0.63442088947093	1.08163282560237	c
2.56770278396510	2.46692216635605	3.90835469430470	c
-5.64114385913511	1.73969436234021	-1.90389701322250	f
-10.28945753536197	0.13193113395654	-0.73888131942747	f
-11.13221065245662	-4.84788851498977	0.44753422174970	f
-7.16774811904720	-8.17846573479400	0.45399155781305	f
-2.49001889541884	-6.61961684418027	-0.65554363147823	f
3.95946001098137	-3.33423589412386	-4.38895100612200	f
7.93183322494735	-4.98342187504305	-1.78341153269893	f
7.68086907446042	-5.58537772019205	3.34698694922923	f
3.25796809959270	-4.52593501406871	5.83442410454145	f
-0.76569024493717	-2.81220239024401	3.29489352763426	f
0.37007902833822	3.52138022145949	-6.13137594967014	h
-2.66648014434119	3.31132612859974	-4.76244946833130	h

0.79721504829121	-1.10739958559152	-6.03509092091300	h
-2.52449309993484	-1.01759550807303	-6.06712451769434	h
-0.53263574062813	11.84636612175272	-0.29840108828716	h
-5.14419545230260	7.43260477820707	4.68348338419861	h
9.42279765784377	1.66694916586532	-3.55579999377053	h
7.41208464996103	1.41423434333530	4.26458296877406	h
2.11554646859205	10.13617855836649	-3.15245076202434	h
1.04116416403542	7.30710980579962	-4.58852967862641	h
3.50060603030499	7.18426981000550	-2.33526808774418	h
-5.22977331726727	11.91463509505879	5.09379458206097	h
-2.49692454949575	13.58540580277240	4.06386847453767	h
-5.16293607112919	13.35613230713191	2.06161455623187	h
-3.19729883443871	2.76341460023676	5.27064910563992	h
-3.12318203024966	1.18288508352200	2.33215108130571	h
-5.86768753415642	2.85526883324941	3.25801607525307	h
6.85064890072607	2.73587954473856	-6.57334082741327	h
3.82771934901159	1.34465726422677	-6.37906058944927	h
4.18939660470495	4.64067264450330	-5.89232063993210	h
11.89442811831440	1.20166925933487	3.01237466823150	h
12.76824721176975	1.47245814586784	-0.23185897900641	h
11.60105498553063	-1.42996966525588	0.95987463370186	h
3.45587974354349	1.78442913121351	5.64840681998697	h
2.02009694014207	4.44777859772001	4.18035887854978	h
0.82619560712946	1.39479726616376	3.63842617772958	h

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1.05972360194062	-3.17057221381749	0.17812644271387	p
-0.79963011748842	2.38005619608564	-1.74980427605512	b
0.15354202815622	-2.31618826562555	-3.14933745454284	c
0.68974590991820	0.52229453964818	-3.55470472343783	c
4.52741277454341	-2.68130213586834	0.01288325751700	c
6.11706155340948	-3.70076533807533	-1.88221821257508	c
8.67592863049514	-3.02511985923705	-1.93095323377262	c
9.73357097469823	-1.39305232072451	-0.14999619018194	c
8.16207736902401	-0.46697439360956	1.75780424528129	c
5.59260391662534	-1.07090423878483	1.87305653627488	c
0.42400310650179	-6.62167040348531	0.45176903570552	c
-2.05318032486051	-7.48818235407738	-0.14114765732341	c
-2.60294336238809	-10.07411318388151	-0.04064770555357	c
-0.82428547344861	-11.86381896862700	0.71585787714009	c
1.51833125057319	-10.96416801067680	1.52912367699789	c
2.17208690088476	-8.40114282243542	1.46189633418869	c
0.22619358310091	5.08635304684272	-0.99305371400190	c
2.80634642577505	5.62424541311271	-0.61867268589210	c
4.56482221861561	3.80705237726887	-0.87239439922523	f
3.69905213954180	7.99492731519822	0.11507339940433	c
6.17357969525152	8.39226100920938	0.50671073185291	f
1.99004469366510	9.97953692023166	0.43988808988509	c
2.81613343444203	12.26839320386863	1.11550667788878	f
-0.58744215981225	9.56447943597597	0.04326701950667	c
-2.22336402178662	11.48136245115310	0.32180380791934	f
-1.41354346218676	7.15784507092303	-0.64201871620520	c
-3.91959137460507	6.90574198488114	-1.02917746052814	f
-3.53871870079836	1.58807707298426	-0.80891400785194	c
-5.39266112019403	0.66245366547154	-2.44656956547534	c
-4.93234523852635	0.56204532753645	-4.96335207194525	f
-7.76011346180129	-0.15310379460170	-1.62403893118094	c
-9.48019526388144	-1.04537484731985	-3.26356887003296	f
-8.32049734874548	-0.07326954288371	0.95340395358072	c
-10.56621049959586	-0.88794397895414	1.78966432550259	f
-6.52733011415040	0.85242880624140	2.66032933306300	c
-7.06808934941733	0.92256486769254	5.13758568832323	f
-4.20251141672934	1.68991933580851	1.74912406314316	c
-2.52255526995638	2.57220656914181	3.45716309318707	f
5.25202304574475	-5.60214534369389	-3.83891823419724	c
12.47961077935002	-0.63466541325645	-0.28973700656175	c
4.06184918657931	0.02300418784397	4.03246381728770	c
-4.25088097425743	-5.75101301568237	-0.75547902396511	c
-1.42604951181273	-14.65147752515763	0.72017928518503	c
4.70187680662596	-7.70835420012872	2.61474752088998	c
1.11009651948153	-3.47223989600730	-4.56609885824168	h
-1.86344365931955	-2.65980645978770	-3.34818109993919	h
2.72418110917942	0.87582839752315	-3.56268237677932	h

0.02523887937312	1.03184597399878	-5.47317273788470	h
9.88364766782164	-3.83600759591351	-3.38978088914669	h
8.95365263665220	0.77556353888481	3.19541227076105	h
-4.51030472624738	-10.68993322021224	-0.51629509500531	h
2.88835157889306	-12.29859907770556	2.29349439576171	h
4.82048346526854	-4.67291875130339	-5.64601106493760	h
6.76903988783251	-6.96596904730430	-4.20663443653398	h
3.57510276028273	-6.64316140666324	-3.23497789695089	h
13.26685485658639	-0.31871022325489	1.60168615262815	h
12.69397066902870	1.13624782708467	-1.35674241052155	h
13.61074879900631	-2.08362445599368	-1.24723304887100	h
5.28098617230663	1.15046393209260	5.27107875549281	h
2.51915080090995	1.22497277331109	3.35277278029066	h
3.17494169774040	-1.46807245216215	5.17003139587055	h
-6.00642847761858	-6.57469005494631	-0.02494846197169	h
-4.50270021856317	-5.49371729454056	-2.79951335601803	h
-4.02572626821526	-3.87900401739483	0.09625675364621	h
-0.39733383323302	-15.63823882794269	2.22550447131861	h
-3.45624644716061	-14.97966895803120	0.98076444038411	h
-0.87862209832531	-15.52548816639663	-1.08515995529094	h
5.32700569161865	-9.24040144968662	3.86167065213015	h
4.59227553179790	-5.97126545929643	3.73113373573460	h
6.17126792733765	-7.40909704579280	1.18765978030424	h

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1.15535891368616	-2.29199637826034	4.43781774599708	p
0.65181098870925	-1.85200582632049	-3.08411429710246	b
2.32883345407294	-1.24315044850561	1.19807834110814	c
1.92241808136567	-3.34803942685541	-0.85578458861199	c
-1.67824251522108	-0.19810246462279	4.53466947048857	c
-1.55844132323887	2.47710846565782	4.40233317032376	c
-3.80555957820888	3.87103717080153	4.37031686734003	c
-6.17983047435340	2.72156981392237	4.48918225521869	c
-6.26537953456801	0.08967703142842	4.61764166340440	c
-4.07003674364930	-1.39048542565695	4.62595281289402	c
3.44902255503217	-0.93819148663380	6.72812062860187	c
6.08117402219310	-1.28128772324792	6.32161294628231	c
7.81512665157449	-0.24356462725355	8.03029413008356	c
7.05751994600647	1.04855674087618	10.19910476327297	c
4.46970073984055	1.13778510962197	10.70779148061757	c
2.65788098274492	0.13982020435573	9.05952714620075	c
2.12717615731253	-0.79175794675332	-5.44278884987007	c
4.75246999071366	-0.35637177145182	-5.41770692382991	c
6.11134803040462	-0.75992687975590	-3.29960963808149	f
6.08366700062004	0.57314895378608	-7.49348963876046	c
8.57998331887854	0.99783617346043	-7.36497403190509	f
4.78686041959468	1.06999197372998	-9.74030566235542	c
6.03525912344108	1.94064543891379	-11.75450753397163	f
2.18248370598108	0.65099899717230	-9.87546499793108	c

0.94961508698008	1.11320193078581	-12.04105451985343	f
0.91029882074195	-0.24411019248211	-7.74756677963453	c
-1.59164165928193	-0.63352578245619	-8.01024678442631	f
-2.23701095022361	-1.15410166897290	-2.67040389289700	c
-4.07858589736216	-2.97587850829950	-2.15162619783688	c
-3.47321169055436	-5.45929031490445	-2.25260531803188	f
-6.57088988272491	-2.36059845865426	-1.56406325307356	c
-8.28314768970163	-4.16332111374847	-1.05459313465285	f
-7.27592736970096	0.17944333708947	-1.45490179362644	c
-9.65045999322132	0.80762247180480	-0.84493520890811	f
-5.49626030666789	2.06255697588065	-1.94987069158022	c
-6.16874021960534	4.50529806675785	-1.80667783584807	f
-3.03330206082607	1.36238550733673	-2.55971377231729	c
-1.34639153289878	3.24011884323349	-2.98231639965867	f
0.88355351435082	3.96679644350774	4.44477461223265	c
-8.56446772317843	4.28441628447041	4.42914106135800	c
-4.38011110136328	-4.23621684860266	4.73977585147704	c
7.18653953016698	-2.87379930688437	4.20149906950506	c
8.95886343200170	2.23823570490651	11.96131514429895	c
-0.06163532450419	0.16879953817904	9.96403751970431	c
1.25635456764206	0.47063215157566	0.74636391848696	h
4.30419228789925	-0.67850166189373	1.23785767861886	h
3.72341996559888	-4.26347055424385	-1.29094618503129	h
0.63528018682588	-4.79358448053810	-0.11891686024801	h
-3.68962885382879	5.92447112699519	4.26130733174210	h
-8.09478047725092	-0.85055669453751	4.68947315399900	h
9.82602059915030	-0.51612251781253	7.67408895024446	h
3.82664584596619	1.97071627288513	12.47868091316045	h
0.62169946185921	5.78961833574024	3.49513210798184	h
1.45389557868636	4.34220430710812	6.40507108615205	h
2.46723787639286	2.98086570203683	3.56775200784026	h
-10.23112206670052	3.11874534036542	4.81795349961771	h
-8.81758004916542	5.16328110530974	2.56678876899271	h
-8.48547276838472	5.81233954120285	5.83079919747549	h
-6.38879086449505	-4.73529291787049	4.81312571438181	h
-3.54204313307812	-5.16498987531117	3.08756013990456	h
-3.43788273417528	-5.03886833792290	6.40356073252036	h
8.84828329834355	-3.88839074261138	4.91204968335772	h
7.82168503927507	-1.72552958808946	2.59236325551598	h
5.84685985584321	-4.27985136400723	3.48367413853369	h
8.24144372865418	2.30219206637311	13.90519756365618	h
10.74870182765696	1.19160217111596	11.95149815396303	h
9.37685647494476	4.19164712618648	11.38501955278588	h
-0.09544398885545	0.32207569492791	12.03019616056667	h
-1.06799885279779	-1.55987427831686	9.42980500832125	h
-1.14404534459064	1.75485422977393	9.18768093432821	h

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-0.68247472674720	3.97495011294625	-2.68516857818186	c
-1.20690417571496	3.29999706598373	-0.18226712204312	c
-0.67443669487748	5.19387808430038	1.57985426946069	c
0.36757119707929	7.53879642350441	0.96349974900670	c
0.90253934671738	8.08998501122249	-1.55855312744470	c
0.35954154723409	6.29248029417545	-3.40903898773530	c
-2.17149286611159	0.41037792841197	0.51871364445617	b
-5.24255996050447	-0.01260950442144	0.49695314033157	c
-6.20078218372635	-2.45137040802584	0.13612829635260	c
-8.77306290244564	-3.03120436580326	0.10333930447691	c
-10.53171931886509	-1.09683009198565	0.46008307336289	c
-9.67645948870306	1.36713128194294	0.84417530845694	c
-7.07703065612410	1.84902331450974	0.86785801081728	c
-4.58555438142715	-4.42603976672154	-0.20994477801421	f
-9.58632719725116	-5.42390198741956	-0.26118972212129	f
-13.02444714864365	-1.60772294318320	0.44136800203772	f
-11.36670948008411	3.24121401905873	1.20434873770515	f
-6.38562803459823	4.28473225719479	1.28643546120752	f
-1.14328394662493	4.80254224925220	4.07539519061779	f
0.89890591261748	9.26310694057984	2.76461111022023	f
1.93629018756535	10.32428492814469	-2.19615021100428	f
0.85629529351992	6.81457676842776	-5.85375908524978	f
-1.17073074429451	2.32618955469259	-4.59570155128038	f
-1.00734186799757	-0.66900699730052	3.22232670516982	c
1.88240778670816	-0.35686139959069	3.48831619502594	c
3.49706500642661	-1.52958599782704	0.68134024798410	p
6.89012040207683	-0.95651832394958	0.73620259639819	c
7.66116248349158	1.62384235792785	0.73275314454702	c
10.24570337331408	2.17513291294021	0.73266689910856	c
12.09110095246425	0.29181060075160	0.74391105361812	c
11.28969293138987	-2.22216753070710	0.70813689773109	c
8.73579962346445	-2.90759469715213	0.69237894100062	c
5.86640438256959	3.85689239216440	0.74854270887372	c
14.86280253357165	0.95002427940854	0.81629732862051	c
8.14274546562240	-5.70426791984554	0.56906197935908	c
2.46050559274029	-4.64856832984518	-0.19371400037362	c
1.94791134247929	-6.52418053884078	1.63979448983801	c
0.92215392252997	-8.81739685261625	0.83307714100726	c
0.39465319282616	-9.30811158455271	-1.70720182489380	c
1.00069570042450	-7.45424129110306	-3.48751046780927	c
2.02742464463508	-5.12591690257310	-2.79412893526723	c
2.46645703214817	-6.20972822466084	4.43386612558974	c
-0.83942642783473	-11.74840340974448	-2.50120550124753	c
2.58553070365344	-3.21406391691397	-4.83826899661567	c
2.70522792663944	-1.26991064812187	5.15448880602178	h
2.37851186937436	1.64792348904185	3.57892134439309	h
-1.48884789048962	-2.68119619013872	3.34272271830535	h
-1.84846424937169	0.25666894165248	4.87659829805016	h

0.52154050902202	-10.26475701697055	2.23946884660486	h
0.65017221812289	-7.81943859574773	-5.48129324466652	h
10.82293252001727	4.15005195020350	0.71012193816299	h
12.70130003610976	-3.71838332992422	0.66680232378325	h
0.91421649167647	-5.20074079649729	5.36597749551512	h
2.64876562814199	-8.06618832865319	5.33020302100402	h
4.20807458658923	-5.15270770716301	4.80722823994020	h
-0.25057617995135	-12.30361008409802	-4.40847354525976	h
-2.90456965261446	-11.51991953877352	-2.52293379492439	h
-0.39065366003705	-13.28369145712985	-1.18450447596944	h
2.41070310977430	-4.08930564572962	-6.70416679923904	h
1.23656880190230	-1.63987941544253	-4.74026393996979	h
4.50096759313717	-2.43048753549179	-4.67713893588160	h
6.82814402126013	5.53134539115758	0.00635845529902	h
5.25881209036363	4.30697283464391	2.67973427505893	h
4.15304763145946	3.57461591379934	-0.37536969492085	h
16.00516217358665	-0.51359709546798	-0.10286392378955	h
15.22533331877590	2.76517005064591	-0.11405997030625	h
15.51541400355691	1.11296488619970	2.78249503817416	h
9.90549899823970	-6.78810458396671	0.55477949686602	h
7.06886970772772	-6.18817722701905	-1.13203998345682	h
7.02275220858615	-6.34001106668833	2.18597355440725	h
-1.34726448876235	-0.93900238529922	-1.16881807517367	h
2.61763752673340	0.02477124867488	-1.25311313543715	h

trans-**5**

-4.33079838594122	-2.78334377096158	-0.47581756752530	p
2.95952704465916	-1.00100939549339	-2.53677959815801	b
-4.11109932556386	-5.32321241555506	0.22657038226956	h
2.84510281240894	-0.94222799292003	-4.83473496535818	h
-2.15118611188513	-3.36258444321408	-4.41634824951341	h
-1.85053611224491	-0.25793959706066	-3.24272049279642	h
1.16427011449089	-4.95208296352360	-1.86948890161573	h
0.65562524796642	-2.77237686609326	0.59795617917244	h
-7.50757274893925	0.69770833811720	-7.24746199019344	h
-5.21319563508730	-1.61306499879006	-6.49425179347358	h
-5.27723051246619	1.27330374477291	-4.82943224235666	h
-11.43933724993924	-0.26702588751292	-6.15874213122484	h
-16.45709025057225	-3.77621167362206	-3.34881939124207	h
-15.77177662822672	-1.20398872872012	-5.40824330728700	h
-16.49372929276850	-0.64751481764817	-2.17590963770186	h
-10.55741302175703	-5.42045785632448	3.54383226609792	h
-7.80073784887165	-3.53066950639566	3.87574213377232	h
-7.63781360348528	-6.46623858310587	2.28903473796538	h
-13.42978271354512	-4.08566587357913	0.69836934008055	h
0.00845590747018	3.73792936562515	9.08840864366544	h
-2.35246304409405	2.14990559746822	10.86068766912095	h
-3.08448583732697	5.01069350736745	9.22750705984941	h
-1.42002167728539	-1.79933832540963	8.34714316522130	h
-1.30871194556310	-5.58702093416399	6.45949659956467	h
-0.70360231379955	-5.58439589750413	3.16951155376961	h
-3.78643738059065	-6.25241175579295	4.30890085333114	h
-5.36016011859774	5.04840357041970	0.65498023660438	h
-7.02387127882681	2.34207404614299	-0.43349435651615	h
-3.84976076149384	2.89437188222343	-1.38318609068041	h
-4.01439441430302	4.95128895707123	4.70611288567538	h
-1.78985113845894	-2.25216987300104	-2.70734494904862	c
-7.59274513035887	-2.48650485067539	-1.51350181865134	c
0.75662049339330	-2.96033833417285	-1.46100734113828	c
-8.30774236363338	-1.31066784311657	-3.81309627508156	c
-6.47102321775013	-0.18054453960129	-5.68837125637532	c
-10.88580852728325	-1.17179799726969	-4.39635832606150	c
-12.75909933624656	-2.14126933793862	-2.81340782573232	c
-15.52006768934598	-1.93071653365239	-3.48645896797889	c
-12.00440227968214	-3.30445747155058	-0.56349433807522	c
-8.83013915224867	-4.79387170733901	2.59475443980254	c
-9.46704592104072	-3.50055418209856	0.12689528400496	c
-3.73101647521198	-1.04069501644974	2.40104257819327	c
-4.20917003435579	1.59257901599237	2.45801912098958	c
-5.17901949025356	3.04027371453501	0.19960822700797	c
-3.68333972912453	2.92239343588585	4.67502114938922	c
-2.67844688107613	1.74498749997407	6.81213118774669	c
-2.00694709205363	3.24485570326891	9.13534522937181	c

-2.22422451476814	-0.85561029602654	6.70611548746291	c
-2.71904656598717	-2.29216452069758	4.54862531106370	c
-2.09967125360342	-5.08262131778335	4.61678620453401	c
2.20029273451871	1.83313787778619	-1.41232238882440	c
1.08004960512040	3.71969818969307	-2.87891152261185	c
0.28175935808468	6.04834786754418	-1.91569668434161	c
0.60923506553627	6.56106672656489	0.64704354566011	c
1.73230161574791	4.74479203355456	2.19241681686918	c
2.46787961928426	2.44068610608738	1.14475306404090	c
5.87426706034566	-1.71578643726979	-1.72250450912586	c
7.86799546859828	-0.40831187977659	-2.87032948799589	c
10.41617562234542	-0.85904818582599	-2.35337005176196	c
11.06242979728729	-2.70908750817241	-0.58668389850171	c
9.14795650938644	-4.05608911610165	0.62357984655243	c
6.62603190376925	-3.52973888474749	0.03885796130537	c
4.87363978774561	-4.90646606302492	1.33782477148190	f
0.62708014501960	3.32834726997251	-5.37865234698913	f
9.75751764352817	-5.83800893759233	2.34823467633962	f
13.50647026213006	-3.18501264571180	-0.05503047327036	f
12.25922160744084	0.45707934438591	-3.52603490795002	f
7.35822324973552	1.42696812676689	-4.58525969229958	f
3.44234947665775	0.71472031991189	2.77420431088061	f
-0.21113296760915	8.76187818041831	1.63832099284950	f
2.02152014539436	5.22769025786560	4.68401755059664	f
-0.87133830044164	7.77428672716091	-3.40285367631218	f

7

-1.19418479152572	5.16426792197425	1.36943882024542	c
0.73094590863275	3.48620393688993	2.02399029464418	c
2.39060073131046	4.36258315807072	3.88927329140735	c
2.18263956868285	6.73643099623660	5.02468174980006	c
0.22886416973192	8.35114356044474	4.28837288180183	c
-1.47925070387807	7.55841160845323	2.44106974789526	c
1.23053639728612	0.67372321195089	0.88057730391121	b
0.36627061288886	-1.61035354124949	2.77363928015770	c
1.85502006341001	-3.77421661348296	3.08582573050796	c
1.15977199928722	-5.79296963850472	4.63548431164043	c
-1.11460878608710	-5.67713688130882	5.96892048057780	c
-2.65887380660912	-3.55180338286942	5.72651851783658	c
-1.89574958010605	-1.58903301333128	4.13733289204428	c
4.07012088936607	-4.00614109401927	1.83761892361132	f
2.63817608891377	-7.85067689904150	4.85374873060154	f
-1.82167727051477	-7.60511147292348	7.45890145486918	f
-4.87476153468573	-3.45157178198077	6.97151023304961	f
-3.52292401816881	0.37600616494809	3.87127988915910	f
4.31381004276225	2.87189278553732	4.67538694377025	f
3.83236309452227	7.48872605749917	6.80673572379824	f
-0.00629817975737	10.64463033195964	5.34846401145133	f
-3.37013701853979	9.10086263862521	1.72254008945447	f

-2.92096080244514	4.50803000226936	-0.42193202003525	f
-0.59006491709007	-0.22660530532381	-2.28348104738623	p
-0.37152226832348	1.57224985298675	-5.23411777643560	c
1.49079264108260	3.45687281202563	-5.64220647254306	c
1.53900440905592	4.70387172391424	-7.97216480926071	c
-0.18784141952271	4.18037665657093	-9.89984010456157	c
-2.02001962127465	2.33917915736776	-9.44848994421818	c
-2.15419160927302	1.02124134610869	-7.16026457109891	c
3.42661153778892	4.22430400850269	-3.69164531168741	c
-0.07272352274970	5.58406156098137	-12.37904116585924	c
-4.22757922001819	-0.91884334488777	-6.85502390502911	c
-0.01410408029166	-3.57335492079010	-2.93638681223812	c
2.34535143882923	-4.33294774501228	-3.94584756455094	c
2.81329209888845	-6.90520515548147	-4.30448935326023	c
1.04203750647752	-8.75764552803374	-3.66875085940922	c
-1.26970716137363	-7.96833111419964	-2.67530138476724	c
-1.84859598246721	-5.41527998962746	-2.28997425835141	c
4.40843559430422	-2.47247547914541	-4.59402488902228	c
1.64128887326724	-11.52441944747338	-4.00613528902129	c
-4.41633898155544	-4.78993976797075	-1.19712872954982	c
3.43221467647922	0.42360987253175	0.35868301893329	h
-3.19312897875048	-0.20232462143638	-1.81872052549992	h
2.98102077705156	6.13998267263415	-8.27922888089270	h
-3.39437993374262	1.90563964601098	-10.91738980966815	h
4.80409983265240	5.52106821031914	-4.53031234339532	h
4.44034786628695	2.60099888813762	-2.91607892042253	h
2.53130308700347	5.18381921945754	-2.09163741143948	h
-1.48946098159649	4.87266427072248	-13.71114110991788	h
-0.41208916383321	7.61196735869892	-12.09090876923862	h
1.80125627972696	5.39319037652192	-13.25006789165668	h
-5.34929041358542	-1.05289472569279	-8.58805126676595	h
-5.51023479029042	-0.40311734042413	-5.30634484846616	h
-3.46148314736042	-2.79477307868290	-6.42279268292085	h
4.63626904304302	-7.47273040774335	-5.07286002592906	h
-2.67513897492460	-9.38196362828136	-2.16525741786521	h
6.06763774228112	-3.46324796589259	-5.33329364153081	h
3.78220060440575	-1.09580099080274	-6.00920767342862	h
4.98739130667458	-1.42454337579676	-2.90294436822896	h
-0.03248700356151	-12.70004211149278	-3.68259684935284	h
3.11351078829694	-12.11805981055225	-2.66708665365054	h
2.35609843361838	-11.90346576444918	-5.91661332597343	h
-5.46519227303927	-6.52965183856389	-0.80582291190456	h
-4.26354638760031	-3.72967945950655	0.57192248351346	h
-5.54357505735865	-3.64690841010897	-2.51002843351154	h

PH(mes)$_2$

-0.00198798550507	-3.35974340776039	-0.17561484998137	p
-0.23986023793708	-4.08835799224143	2.39232058256171	h
-2.74522040196252	-1.17720592506196	-0.27058243260376	c

-2.83433747639141	0.74766377506407	-2.13188561503040	c
-4.93794057861180	2.34311498756294	-2.25191595128046	c
-6.99453166298333	2.08423774750280	-0.61457771445150	c
-6.90874759832665	0.13702209953024	1.16290807871366	c
-4.83862851766680	-1.50123612383795	1.36477805652640	c
2.75734232044400	-1.21972752921461	0.26674331700952	c
4.81338275516972	-1.43996517886099	-1.43640011775570	c
6.88821854160219	0.17866901528571	-1.18312309858107	c
7.00624008547731	2.01788349568785	0.71007313799494	c
4.98421779144321	2.18812401561379	2.39561599661290	c
2.86547415786286	0.60860849356455	2.21833176207529	c
-0.72317319248199	1.14142992062071	-4.01685398026817	c
-9.25563338089467	3.81499601486349	-0.81438495585916	c
-4.93471991350141	-3.55391696790121	3.35109315097092	c
4.85528683511991	-3.36642529640327	-3.55420531454967	c
9.25278980755936	3.76665790725648	0.90921398121782	c
0.78186383047764	0.92915626757870	4.14250853275869	c
-4.96863388667033	3.82319899046133	-3.68434389943698	h
-8.50172801887917	-0.12394135890502	2.44180942162975	h
8.45789781089027	-0.01057041649387	-2.50270959582376	h
5.05261770151230	3.58648395906488	3.90556627283247	h
-1.33524147064231	2.41166738729706	-5.53399349927032	h
0.96242727164282	1.94889993240263	-3.12112228492322	h
-0.14362545053723	-0.65907111618124	-4.87392836180371	h
-10.50408846189587	3.60518177494783	0.82611515991956	h
-10.36662034642967	3.39227499087809	-2.51892476905239	h
-8.66783689775684	5.80102712608012	-0.94064811421602	h
-6.78081034491571	-3.56924759407223	4.28884427965537	h
-4.60873333447786	-5.43191751825651	2.53023347024960	h
-3.47539083281116	-3.26788546143758	4.80215838237071	h
6.65781253840953	-3.27787163646532	-4.57115280291665	h
3.32544104033915	-3.02858085115505	-4.91419856496181	h
4.59497295321361	-5.29392858025265	-2.83812228608341	h
9.21277021171412	4.83765959947725	2.68209891706924	h
11.03395240970316	2.70571026515225	0.82233365654117	h
9.27065137630923	5.12745674280011	-0.66074726989757	h
1.37050599190651	2.23389219226129	5.63916535538398	h
0.28190305787177	-0.88666034474736	5.01141841158915	h
-0.94722279059690	1.66207975576746	3.26696732712480	h

$BH(C_6F_5)_2$

-0.00080899878435	-2.60526380109292	-0.00500853596712	b
-0.00153541177486	-4.86265000023084	-0.00588827876682	h
2.61644468596188	-1.25377098309490	-0.10167728347746	c
4.76727389967016	-2.45275021686236	0.91098952848630	c
4.53127825273588	-4.69005565603616	2.09462444621362	f
7.17798094817957	-1.39316686443472	0.81204558374917	c
9.17292908140651	-2.56380645869240	1.84611358490381	f
7.50590707770785	0.93740335521760	-0.39228179947099	c

9.80188238494306	1.97651124511653	-0.52031312227416	f
5.43512916090014	2.18008101130957	-1.47201584724641	c
5.78132700235144	4.39303670999603	-2.65683824963656	f
3.04792673283968	1.08160704558523	-1.30111752357898	c
1.12857015669578	2.31491566610463	-2.42557828028764	f
-2.61669986507925	-1.25148647583642	0.09434619422590	c
-4.77001254980157	-2.45052845859286	-0.91360245048387	c
-4.53766322412159	-4.68924884354331	-2.09520779468496	f
-7.18032478737413	-1.39066068695295	-0.80882019572563	c
-9.17836327455937	-2.56160465116245	-1.83660091825089	f
-7.50545803814346	0.93985261061326	0.39666751720411	c
-9.80134759034066	1.97798219802665	0.53165258341280	f
-5.43213301314942	2.18215138415255	1.47184830057288	c
-5.77525285729153	4.39485690515006	2.65778295223071	f
-3.04509966665722	1.08457016370860	1.29316023622665	c
-1.12340897312877	2.31750780569591	2.41413888296486	f

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1.25887246888114	0.00000000000000	0.00000000000000	c
-1.25887246888114	0.00000000000000	0.00000000000000	c
2.33618465716233	1.75434910236273	0.00000000000000	h
2.33618465716233	-1.75434910236273	0.00000000000000	h
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