Electronic supplementary information (ESI) for:

Gas Phase Chemical Vapor Deposition Chemistry of Triethylboron Probed by Boron-Carbon Thin Film Deposition and Quantum Chemical Calculations

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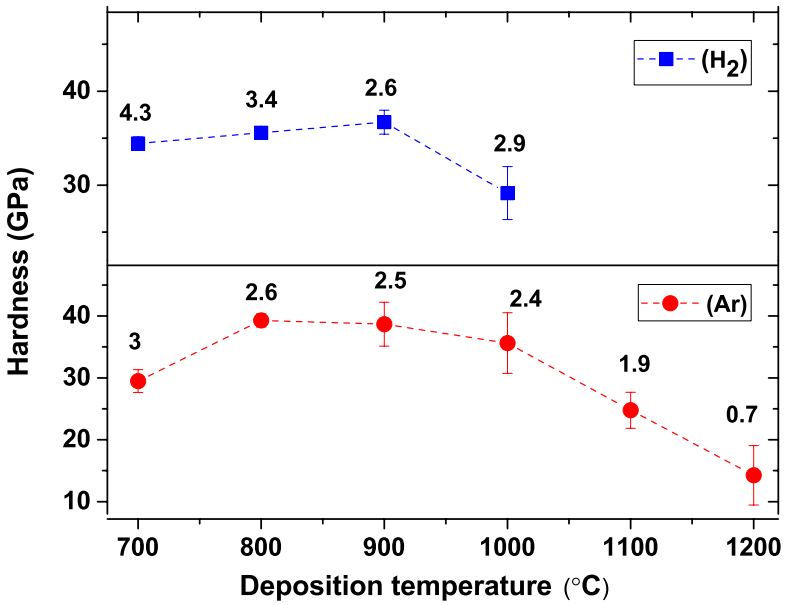
Supporting Table 1: Relative amounts of B, C and H in B_xC films deposited in H_2 and Ar atmosphere, respectively. Results for 400 – 600 °C are taken from a previous publication[1]

	ERDA atomic %					
	In H_2			In Ar		
Deposition temperature °C	B	C	H	B	C	H
400	71	3	25	56	20	24
500	79	6	15	66	19	15
600	79	17	4	75	21	4
700	82	18	< 0.1	75	25	< 0.3
800	77	23	< 0.1	72	28	< 0.1
900	72	28	< 0.1	71	29	< 0.1
1000	74	26	< 0.1	71	29	< 0.1
1100	8	92	< 0.1	65	35	< 0.1
1200	8	92	< 0.1	42	58	< 0.1

Supporting Table 2: Film densities for B_xC films deposited in H_2 and Ar atmosphere, as obtained from XRR.

Atmosphere	H_2	Ar	H_2	Ar	Ar
Deposition temperature (˚C)	700	700	900	900	1000
B/C ratio	4.5	3	2.6	2.5	2.4
Film density (g/cm^3)	2.42	2.40	2.43	2.59	2.65



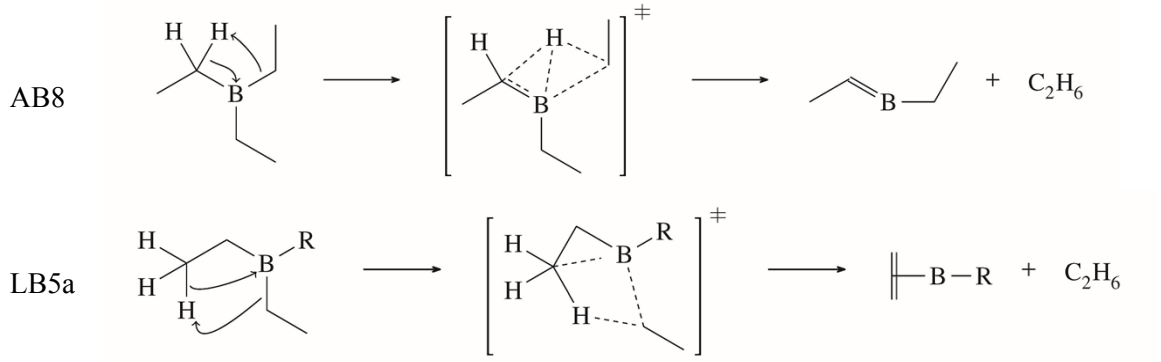
Supporting Figure 1. Hardness from nanoindentation of B_xC films deposited in H_2 and Ar atmosphere as a function of deposition temperature. The B/C ratios of the films are given as inserts by the data points.

Supporting Table 3: Computationally investigated reaction catalogue of TEB.

Index	Reaction scheme
	Radical cleavages
RB1	$B(C_2H_5)_3 \rightarrow B(C_2H_5)_2\bullet + C_2H_5\bullet$
RB2	$B(C_2H_5)_2\bullet \rightarrow B(C_2H_5) + C_2H_5\bullet$
RB3	$B(C_2H_5) \rightarrow B + C_2H_5\bullet$
RB4	$B(C_2H_5)H_2 \rightarrow B(C_2H_5)H\bullet + C_2H_5\bullet$
RB5	$B(C_2H_5)H\bullet \rightarrow BH + C_2H_5\bullet$
RB6	$B(C_2H_5)H_2 \rightarrow BH_2\bullet + C_2H_5\bullet$
RB7	$B(C_2H_5)(C_2H_4) \rightarrow B(C_2H_4) + C_2H_5\bullet$
RB8	$B(C_2H_4)H \rightarrow B(C_2H_4) + H\bullet$
RB9	$B(C_2H_5)H_2 \rightarrow B(C_2H_5)_2\bullet + H\bullet$
RB10	$B(C_2H_5)H_2 \rightarrow B(C_2H_5)H\bullet + H\bullet$
RB11	$B(C_2H_5)H\bullet \rightarrow B(C_2H_5) + H\bullet$
RB12	$BH_3 \rightarrow BH_2\bullet + H\bullet$
RB13	$BH_2\bullet \rightarrow BH + H\bullet$
RB14	$BH \rightarrow B + H\bullet$
RB15	$B(C_2H_5)_2\bullet \rightarrow B(C_2H_5)(C_2H_4) + H\bullet$
RB16	$B(C_2H_5) \rightarrow B(C_2H_4) + H\bullet$
RB17	$B(C_2H_3)H_2 \rightarrow B(C_2H_3)H\bullet + H\bullet$
RB18	$B(C_2H_5)(C_2H_3)H \rightarrow B(C_2H_5)(C_2H_3)\bullet + H\bullet$
RB19	$B(C_2H_3)H\bullet \rightarrow B(C_2H_3) + H\bullet$
RB20	$B(C_2H_5)(C_2H_3)H \rightarrow B(C_2H_3)H\bullet + C_2H_5\bullet$
RB21	$B(C_2H_5)(C_2H_3)\bullet \rightarrow B(C_2H_3) + C_2H_5\bullet$
RB22	$B(C_2H_3)H_2 \rightarrow BH_2\bullet + C_2H_3$
RB23	$B(C_2H_5)(C_2H_3)H \rightarrow B(C_2H_5)H\bullet + C_2H_3$
RB24	$B(C_2H_5)(C_2H_3)\bullet \rightarrow B(C_2H_5) + C_2H_3$
RB25	$B(C_2H_3)H\bullet \rightarrow BH + C_2H_3$
RB26	$B(C_2H_3) \rightarrow B + C_2H_3$
	β-H eliminations
BB1	$B(C_2H_5)_3 \rightarrow B(C_2H_5)_2H + C_2H_4$
BB2	$B(C_2H_5)_2H \rightarrow B(C_2H_5)H_2 + C_2H_4$
BB3	$B(C_2H_5)H_2 \rightarrow BH_3 + C_2H_4$
BB4	$B(C_2H_5)H\bullet \rightarrow BH_2\bullet + C_2H_4$
BB5	$B(C_2H_5)_2\bullet \rightarrow B(C_2H_5)H\bullet + C_2H_4$
BB6	$B(C_2H_5) \rightarrow BH + C_2H_4$
BB7	$B(C_2H_5)(C_2H_4) \rightarrow B(C_2H_4)H + C_2H_4$
BB8	$B(C_2H_5)(C_2H_3)H \rightarrow B(C_2H_3)H_2 + C_2H_4$
BB9	$B(C_2H_5)(C_2H_3)\bullet \rightarrow B(C_2H_3)H\bullet + C_2H_4$
	alkane-/alkene-eliminations
AB1	$B(C_2H_5)_3 \rightarrow B(C_2H_5) + C_4H_{10}$
AB2	$B(C_2H_5)_2\bullet \rightarrow B + C_4H_{10}$
AB3	$B(C_2H_5)_2\bullet \rightarrow B(C_2H_4) + C_2H_6$
AB4	$B(C_2H_5)H_2 \rightarrow BH + C_4H_{10}$
AB5	$B(C_2H_5)H_2 \rightarrow B(C_2H_5) + C_2H_6$
AB6	$B(C_2H_5)H_2 \rightarrow BH + C_2H_6$
AB7	$B(C_2H_5)H\bullet \rightarrow B + C_2H_6$
AB8	$B(C_2H_5)_3 \rightarrow B(C_2H_5)(C_2H_4) + C_2H_6$
AB9	$B(C_2H_5)(C_2H_3)H \rightarrow B(C_2H_3) + C_2H_6$
AB10	$B(C_2H_5)(C_2H_3)H \rightarrow BH + C_4H_8$
AB11	$B(C_2H_5)(C_2H_3)H \rightarrow B(C_2H_5) + C_2H_4$
AB12	$B(C_2H_3)H\bullet \rightarrow B + C_2H_4$
AB13	$B(C_2H_5)(C_2H_3)\bullet \rightarrow B + C_4H_8$
AB14	$B(C_2H_3)H_2 \rightarrow BH + C_2H_4$
	H_2-eliminations
HB1	$B(C_2H_5)H_2 \rightarrow B(C_2H_5)(C_2H_4) + H_2$
HB2	$B(C_2H_5)H_2 \rightarrow B(C_2H_5) + H_2$
HB3	$B(C_2H_5)H_2 \rightarrow B(C_2H_4)H + H_2$
HB4	$B(C_2H_5)H\bullet \rightarrow B(C_2H_4) + H_2$

HB5	$BH_3 \rightarrow BH + H_2$
HB6	$BH_2\bullet \rightarrow B + H_2$
HB7	$B(C_2H_3)H_2 \rightarrow B(C_2H_3) + H_2$
	α-H reactions
LB1	$B(C_2H_5)_3 \rightarrow B(C_2H_5)(C_4H_9)H$
LB2	$B(C_2H_5)_2 \rightarrow B(C_4H_9)H$
LB3	$B(C_2H_5)H_2 \rightarrow B(C_4H_9)H_2$
LB4	$B(C_2H_5)(C_4H_9)H \rightarrow B(C_6H_{13})H_2$
LB5	$B(C_2H_5)_3 \rightarrow B(C_2H_5)(C_2H_3)H + C_2H_6$
LB6	$B(C_2H_5)_2\bullet \rightarrow B(C_2H_3)H\bullet + C_2H_6$
LB7	$B(C_2H_5)H_2 \rightarrow B(C_2H_3)H_2 + C_2H_6$
LB8	$B(C_2H_5)(C_2H_3)H \rightarrow B(C_2H_3)H_2 + C_2H_4$
LB5a	$B(C_2H_5)_3 \rightarrow B(C_2H_5)(\eta^2\text{-}C_2H_4) + C_2H_6$
LB5b	$B(C_2H_5)(\eta^2\text{-}C_2H_4) \rightarrow B(C_2H_5)(C_2H_3)H$
	H_2-assisted alkane eliminations
H2BB1	$B(C_2H_5)_3 + H_2 \rightarrow B(C_2H_5)_2H + C_2H_6$
H2BB2	$B(C_2H_5)_2H + H_2 \rightarrow B(C_2H_5)H_2 + C_2H_6$
H2BB3	$B(C_2H_5)H_2 + H_2 \rightarrow BH_3 + C_2H_6$

Supporting Figure 2. Schemes of selected reactions from Supporting Table 3.



Supporting Table 4: Reaction and Gibbs energies at different temperatures for all decomposition reactions of TEB and its derivatives investigated at CVD conditions[a].

	PBE-D3(BJ)/def2-TZVPP					MP2/def2-TZVPP					CCSD(T)
Index	ΔE	ΔG (I)	ΔG (II)	ΔG (III)	ΔG (IV)	ΔE	ΔG (I)	ΔG (II)	ΔG (III)	ΔG (IV)	ΔE[b]
					Radical cleavages						
RB1	418.5	251.7	229.5	191.0	77.8	445.8	279.2	257.3	219.1	106.7	430.2
RB2	340.2	202.8	184.9	153.8	62.8	337.4	185.0	165.0	130.3	28.3	303.9
RB3	379.6	275.7	261.1	235.6	157.9	374.1	265.6	250.6	224.2	143.6	360.7
RB4	428.5	269.7	248.9	212.8	106.4	447.2	284.7	263.6	226.8	118.0	436.7
RB5	383.6	261.9	246.1	218.5	137.3	371.9	239.7	222.5	192.5	103.8	330.2
RB6	442.1	294.3	275.2	241.9	144.1	449.8	298.9	279.6	245.9	146.5	438.2
RB7	468.0	323.6	304.8	272.3	176.7	496.7	338.7	319.1	285.2	177.8	469.4
RB8	469.1	360.3	346.5	322.2	248.7	487.0	372.2	358.7	357.1	255.9	483.9
RB9	432.9	314.5	299.3	272.5	191.5	443.2	328.6	314.1	288.6	211.3	451.4
RB10	438.4	316.6	301.1	273.7	190.8	445.0	329.3	314.8	289.3	211.9	457.1
RB11	344.6	247.6	235.3	213.5	147.9	333.3	228.8	215.6	192.2	121.5	318.6
RB12	447.5	336.9	323.1	298.8	225.0	449.2	336.5	322.6	298.1	223.6	459.4
RB13	380.0	284.2	272.0	250.3	184.0	367.2	270.1	257.8	236.0	169.2	349.2
RB14	340.5	261.3	250.3	230.6	168.5	335.5	254.8	243.6	223.9	161.3	349.1
RB15	204.8	100.3	87.2	64.2	-5.5	198.8	85.4	71.4	46.6	-28.7	209.3
RB16	332.6	221.1	207.2	182.7	108.5	358.1	239.1	225.4	201.4	120.8	374.9

RB17	430.1	305.7	290.0	262.3	178.3	455.3	340.3	325.9	300.5	223.5	467.1[d]
RB18	413.1	286.0	269.9	241.3	154.7	460.7	339.6	325.6	301.1	228.0	452.5
RB19	368.3	272.1	259.7	237.9	172.5	337.9	229.7	216.0	191.9	119.0	332.5[d]
RB20	413.2	248.9	227.5	190.2	80.3	450.5	290.4	269.6	233.3	126.4	439.8[d]
RB21	368.4	234.9	217.3	186.9	98.0	327.8	180.5	160.0	124.1	17.4	310.8
RB22	507.8	361.7	343.1	310.9	216.1	538.8	388.3	369.3	336.2	238.6	509.0
RB23	487.3	327.2	306.5	270.6	164.8	529.3	368.8	400.3	312.5	206.9	500.7
RB24	418.7	288.8	271.9	242.8	157.9	402.0	258.1	238.2	203.5	100.5	366.8
RB25	457.7	340.2	325.1	298.9	221.8	450.7	318.1	301.2	271.7	184.2	391.0[d]
RB26	429.9	329.5	315.7	291.6	217.8	448.3	343.2	328.8	303.6	226.6	416.7
	β-H eliminations										
BB1	156.5	13.5	-5.4	-38.0	-133.5	158.4	6.0	-14.0	-48.7	-150.6	146.4
BB2	160.9	29.4	12.3	-17.4	-104.1	158.0	10.9	-8.4	-41.8	-139.9	147.1
BB3	165.5	33.7	16.5	-13.4	-100.6	156.5	17.9	-0.2	-31.5	-123.1	146.3
BB4	174.5	54.0	38.5	11.7	-66.4	160.6	25.1	7.6	-22.7	-111.4	148.6
BB5	166.5	31.5	14.1	-16.2	-104.8	159.9	11.6	-7.7	-41.1	-139.2	152.9
BB6	209.9	90.6	75.2	48.5	-30.3	194.4	66.3	49.8	21.1	-63.8	179.2
BB7	169.7	39.7	22.8	-6.4	-91.7	165.6	22.0	3.3	-29.1	-124.1	153.1
BB8	154.0	19.5	1.9	-28.6	-117.7	151.0	5.5	-13.5	-46.4	-143.1	140.3
BB9	170.9	39.1	22.0	-7.6	-94.2	145.7	6.3	-13.2	-47.0	-147.5	155.0[d]
	Alkane/alkene eliminations										
AB1	376.0	247.8	230.5	200.6	113.9	372.4	231.0	211.8	178.6	81.8	344.4
AB2	337.1	271.8	262.0	245.2	194.0	300.7	217.5	205.1	183.6	118.7	274.9
AB3	232.3	114.5	98.6	71.3	-7.7	245.9	105.4	87.3	56.4	-41.6	227.6
AB4	429.5	325.0	311.1	287.1	217.0	408.5	291.3	275.6	248.4	168.6	377.2
AB5	332.6	207.9	190.7	161.1	75.3	331.0	194.9	176.0	143.5	48.8	304.1
AB6	381.6	269.1	253.7	227.0	149.1	367.4	250.3	234.2	206.4	124.9	336.2
AB7	283.7	213.8	202.9	183.9	126.8	257.8	175.8	163.0	141.0	74.4	228.1
AB8	182.9	42.5	23.3	-9.9	-106.7	195.0	45.9	25.5	-9.7	-112.8	188.4
AB9	341.1	211.5	193.7	163.0	73.8	338.9	201.4	182.5	149.8	54.6	312.1
AB10	449.5	333.2	317.9	291.4	213.4	420.2	297.8	281.7	253.7	171.4	389.2
AB11	354.4	219.7	201.4	169.7	77.5	354.4	213.1	193.9	160.7	63.7	325.6
AB12	320.9	246.5	235.0	215.1	155.1	278.0	188.4	175.0	151.6	80.9	246.5[d]
AB13	376.8	308.5	298.3	280.7	227.2	295.0	213.0	199.8	176.5	104.8	285.8
AB14	410.4	290.8	274.7	246.9	164.9	397.8	273.9	257.2	228.3	143.1	364.5
	H_2-eliminations										
HB1	198.9	71.6	55.0	26.1	-59.9	208.7	77.9	61.1	31.7	-55.9	207.3
HB2	344.1	221.0	204.8	176.6	92.8	345.1	222.0	206.0	178.1	95.0	322.3
HB3	207.6	81.8	65.6	37.1	-47.5	216.2	89.0	72.8	44.5	-40.1	213.3
HB4	238.4	125.5	110.9	85.6	10.5	258.2	131.9	116.6	90.2	3.9	240.0
HB5	388.6	277.9	263.6	238.5	163.1	383.0	270.4	256.0	230.6	154.3	355.2
HB6	281.7	202.3	190.7	170.3	106.6	269.4	188.7	177.0	156.4	92.0	244.9
HB7	359.6	234.5	218.2	189.6	104.9	360.0	233.9	217.6	189.0	104.0	337.2
	α-H reactions										
LB1	46.7	50.7	51.6	53.1	57.5	40.0	37.9	37.8	37.8	37.6	40.9
LB2	59.6	76.8	79.6	84.5	99.2	45.7	51.2	52.4	54.3	60.2	48.0
LB3	52.4	63.2	65.0	68.1	77.5	41.7	46.6	47.5	49.2	54.0	43.6
LB4	45.0	59.3	61.7	66.1	78.8	39.9	46.1	47.3	49.3	55.4	41.7
LB5	134.6	1.7	-16.1	-46.6	-135.7	135.0	-12.2	-31.9	-65.9	-165.5	124.9
LB6	129.3	-1.1	-18.1	-47.4	-133.2	139.7	-1.0	-19.6	-51.7	-145.8	134.5[d]
LB7	132.1	7.7	-8.8	-37.3	-120.0	127.6	-12.7	-31.4	-63.7	-158.0	118.8
LB8	154.0	19.5	1.9	-28.6	-117.7	151.0	5.5	-13.5	-46.4	-143.1	140.3
LB5a	158.8	21.4	2.9	-29.1	-37.8	169.8	25.8	6.5	-27	-125.0	169.7
LB5b	-24.1	-19.8	-18.9	-17.5	-97.8	-34.8	-38.0	-38.34	-38.9	-40.5	-44.8
	H_2-assisted alkane eliminations										
H2BB1	-15.9	-29.0	-31.7	-35.9	-46.7	-13.9	-32.1	-35.7	-41.6	-87.0	-18.9
H2BB2	-11.6	-13.2	-14.2	-15.5	-17.5	-14.2	-27.2	-30.1	-34.7	-76.3	-18.2
H2BB3	-7.1	-8.9	-10.0	-11.5	-14.0	-15.8	-20.3	-21.9	-24.3	-59.5	-19.0

[a] Electronic energy changes ΔE and the Gibbs reaction-energy ΔG at 673.15 K (I), 773.15 K (II), 948.15 K (III) and 1473.15 K (IV) for p = 0.05 atm in kJ/mol.
[b] CCSD(T)/def2-TZVPP single-point calculation on MP2/def2-TZVPP optimized structure.
[c] The CCSD(T) energy of $B(C_2H_3)H\bullet$ was calculated on the structure on PBE-D3(BJ) level due to inconsistencies with the MP2 structure.

Supporting Table 5: Reaction barriers at CVD conditions[a] and imaginary modes $\tilde{\nu}_{imag}^{\ddagger}$ of transition states of selected gas phase decomposition reactions for TEB and derivatives.

	PBE-D3(BJ)/def2-TZVPP						MP2/def2-TZVPP					
Index	$\Delta E^{\ddagger}$	$\Delta G^{\ddagger}$ (I)	$\Delta G^{\ddagger}$ (II)	$\Delta G^{\ddagger}$ (III)	$\Delta G^{\ddagger}$ (IV)	$\tilde{\nu}_{imag}^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta G^{\ddagger}$ (I)	$\Delta G^{\ddagger}$ (II)	$\Delta G^{\ddagger}$ (III)	$\Delta G^{\ddagger}$ (IV)	$\tilde{\nu}_{imag}^{\ddagger}$
AB6	372.1	364.5	365.3	366.7	372.0	734.2	405.9	397.2	398.2	399.9	406.1	1044.7
AB8	220.2	234.2	238.7	246.7	271.6	778.1	246.0	246.9	249.4	254.0	268.7	1379.9
AB9	408.5	405.9	407.6	410.9	421.5	451.2	456.3	452.1	453.9	457.4	468.6	519.8
AB11	381.3	371.7	372.7	374.6	380.7	705.3	413.2	400.7	401.8	403.7	410.1	999.6
HB2	351.0	334.6	334.8	335.1	336.6	407.1	389.7	368.4	358.0	367.7	366.9	557.8
LB5a[b]	196.4	221.9	227.8	238.4	271.0	705.4	215.0	225.3	229.9	238.0	361.9	119.2
H2BB1	71.5	217.5	239.1	277.2	391.4	946.0	88.7	223.9	244.6	281.0	263.2	1585.9
H2BB2	47.3	189.6	210.4	247.0	357.0	945.4	73.6	207.6	227.6	262.8	390.7	1582.2
H2BB3	18.3	145.5	163.9	196.2	293.3	943.9	53.4	180.4	198.9	231.6	368.9	1572.8

[a] Electronic barriers $\Delta E^{\ddagger}$ and Gibbs activation enthalpies ΔG at 673.15 K (I), 773.15 K (II), 948.15 K (III) and 1473.15 K (IV) for p = 0.05 atm in kJ/mol.
[b] LB5a is the first step for reaction LB5 in Supporting Table 5. No TS was found leading from LB5a→LB5.

Supporting Table 6: Statistical error measures of reaction energies ΔE.[a]

	RMS in kJ·mol^{-1}			MAE in kJ·mol^{-1}			RAD in %			RMD in %		
	nr[b]	r[b]	all	nr[b]	r[b]	all	nr[b]	r[b]	all	nr[b]	r[b]	all
PBE:MP2	10.4	25.9	21.0	29.3	81.8	81.8	4.5	6.4	5.6	20.5	23.4	23.4
PBE:CC	27.0	36.0	32.6	60.3	91.0	91.0	9.1	8.4	8.7	16.8	24.2	24.2
MP2:CC	19.7	21.9	21.1	33.3	59.7	59.7	6.3	5.5	5.8	8.5	13.2	13.2

[a] Root mean square (RMS), maximum absolute error (MAE), relative average deviation (RAD) and relative maximum deviation (RMD). Deviations of method 1 relative to method 2 (method 1: method 2), with the methods used PBE-D3(BJ)/def2-TZVPP (PBE), MP2/def2-TZVPP (MP2) and CCSD(T)/def2-TZVPP//MP2/def2-TZVPP.
[b] Deviations for reactions containing radicals (r) and reactions containing no radicals (nr).

Supporting Table 7: Cartesian coordinates and SCF energies E of all compounds and transition states (TS) computed.

	PBE-D3(BJ)/def2-TZVPP				MP2/def2-TZVPP			
Element or	Coordinates[b]			E[a]	Coordinates[b]			E[a]
Compound	x	y	z		x	y	z	
B				-24.6101				-24.5758
$B(C_2H_3)$				-102.5967				-102.4538
C	0.0163	0.0000	-0.0991		0.0150	0.0000	-0.0966	
C	0.0470	0.0000	1.2507		0.0462	0.0000	1.2516	
B	1.4593	0.0000	-0.6266		1.4570	0.0000	-0.6253	
H	-0.9269	0.0000	-0.6513		-0.9204	0.0000	-0.6391	
H	1.0066	0.0000	1.7821		0.9983	0.0000	1.7736	
H	-0.8491	0.0000	1.8769		-0.8431	0.0000	1.8685	
$B(C_2H_3)H$				-103.2366				-103.0823
C	0.1486	-0.1590	-0.0437		-0.0953	0.0000	0.0324	
C	0.0598	0.0003	1.3279		-0.0185	0.0000	1.3501	
B	1.1760	-0.4150	-1.0093		1.1999	0.0000	-0.7958	
H	-0.7955	-0.0275	-0.6116		-1.0809	0.0000	-0.4248	
H	0.9341	-0.1008	1.9684		0.9448	0.0000	1.8440	
H	-0.8886	0.2329	1.8069		-0.8950	0.0000	1.9878	
H	1.8841	-0.8473	-1.8492		1.3545	0.0000	-1.9721	
$B(C_2H_3)H_2$				-103.9000				-103.7555
C	-0.0281	0.2086	0.2055		-0.0360	0.2095	0.2005	
B	0.0325	0.0538	1.7344		0.0366	0.0569	1.7312	
C	1.0295	-0.1235	-0.5657		1.0258	-0.1252	-0.5597	
H	-0.9229	0.5899	-0.2991		-0.9189	0.5816	-0.3067	
H	1.9468	-0.5088	-0.1128		1.9298	-0.5012	-0.0976	
H	1.0268	-0.0280	-1.6554		1.0268	-0.0367	-1.6393	
H	-0.8961	0.3441	2.4402		-0.8775	0.3404	2.4392	
H	1.0432	-0.3712	2.2321		1.0451	-0.3603	2.2115	
$B(C_2H_4)$				-103.1974				-103.0418
B	-0.2542	0.5618	0.4383		-0.3239	0.2973	-0.0714	
C	0.0652	-0.0290	1.6595		0.0633	-0.1111	1.1676	
C	1.2908	0.0203	2.5320		1.3079	0.0255	1.9985	
H	1.7147	-0.9854	2.6749		1.7211	-0.9513	2.2454	
H	1.0499	0.4200	3.5289		1.0975	0.5418	2.9340	
H	2.0740	0.6539	2.0991		2.0733	0.5883	1.4714	
H	-0.7817	-0.6426	2.0095		-0.7801	-0.6612	1.5962	
$B(C_2H_4)H$				-103.8757				-103.7271
C	0.0610	-0.2551	0.0503		0.0494	-0.2634	0.0515	
C	0.0796	0.0405	1.5274		0.0796	0.0400	1.5261	
B	0.8413	0.1455	-1.0194		0.8330	0.1553	-1.0101	
H	0.2150	-0.8792	2.1169		0.2207	-0.8691	2.1094	

H	-0.8677	0.4964	1.8536		-0.8550	0.4964	1.8505	
H	0.8902	0.7293	1.7949		0.8871	0.7237	1.7766	
H	-0.7337	-0.9449	-0.2844		-0.7323	-0.9465	-0.2891	
H	1.4532	0.4742	-1.9743		1.4564	0.4705	-1.9498	
$B(C_2H_5)$				-103.8237				-103.6781
B	-0.0331	-0.0001	0.3844		-0.0004	-0.0001	0.3892	
C	0.0129	0.0000	1.9210		0.0051	0.0000	1.9313	
C	1.4343	0.0001	2.5256		1.4270	0.0001	2.5214	
H	-0.5699	-0.8854	2.2464		-0.5630	-0.8801	2.2540	
H	-0.5700	0.8855	2.2462		-0.5630	0.8802	2.2539	
H	1.9988	-0.8859	2.2087		1.9829	-0.8788	2.2027	
H	1.3913	0.0002	3.6218		1.3916	0.0002	3.6075	
H	1.9988	0.8860	2.2086		1.9829	0.8790	2.2026	
	$B(C_2H_5)(C_2H_3)$			-181.8060				-181.5383
C	-0.1850	-0.1573	-0.1227		-0.2662	-0.1659	-0.1385	
C	0.2751	0.0483	1.3329		0.3379	0.0578	1.2544	
B	0.8680	-0.4585	-1.1867		0.7155	-0.4549	-1.2762	
C	1.6278	-0.8154	-2.3557		1.5759	-0.8184	-2.3390	
C	2.3746	-0.0876	-3.2741		2.4122	-0.0830	-3.1752	
H	-0.7759	0.7124	-0.4697		-0.8992	0.6771	-0.4291	
H	-0.9076	-0.9960	-0.1827		-0.9479	-1.0249	-0.1254	
H	0.9596	0.9029	1.4106		0.9990	0.9214	1.2548	
H	0.8090	-0.8358	1.7044		0.9215	-0.8056	1.5649	
H	-0.5797	0.2372	1.9978		-0.4421	0.2288	1.9941	
H	1.6203	-1.9110	-2.4950		1.5513	-1.8989	-2.4970	
H	2.4569	0.9965	-3.2122		2.4974	0.9877	-3.0849	
H	2.9101	-0.5827	-4.0814		2.9977	-0.5680	-3.9375	
	$B(C_2H_5)(C_2H_3)H$			-182.4630				-182.2136
C	0.0792	-0.2616	-0.1755		0.0551	-0.2651	-0.1888	
C	0.1728	0.1829	1.2913		0.1987	0.1921	1.2670	
B	1.4177	-0.6901	-0.8607		1.3957	-0.7224	-0.8595	
C	1.7234	-0.4845	-2.3673		1.7744	-0.4377	-2.3374	
C	1.1382	0.4731	-3.1129		1.1160	0.4572	-3.0981	
H	2.2473	-1.2509	-0.1819		2.1563	-1.3601	-0.1888	
H	-0.5028	0.4605	-0.7717		-0.4964	0.4737	-0.7708	
H	-0.5214	-1.1968	-0.2252		-0.5659	-1.1723	-0.2092	
H	0.7224	1.1305	1.3820		0.7952	1.1012	1.3337	
H	0.7089	-0.5619	1.8959		0.6970	-0.5699	1.8641	
H	-0.8187	0.3339	1.7414		-0.7680	0.3999	1.7230	
H	2.5119	-1.0750	-2.8487		2.6296	-0.9284	-2.7903	
H	0.3655	1.1247	-2.6967		0.2633	1.0000	-2.7117	
H	1.4185	0.6663	-4.1518		1.4119	0.6828	-4.1151	
	$B(C_2H_5)(C_2H_4)$			-182.4446				-182.1908
B	-0.4860	0.5104	0.7735		-0.4816	0.5126	0.7701	
C	0.7354	0.1083	1.6044		0.7467	0.1065	1.5980	

C	0.5091	-0.2088	3.0934		0.4971	-0.2061	3.0776	
C	-1.5703	0.9308	0.0097		-1.5710	0.9373	0.0166	
C	-2.6038	0.1393	-0.7545		-2.5989	0.1363	-0.7434	
H	-2.4329	-0.9423	-0.6755		-2.4176	-0.9333	-0.6586	
H	-2.5974	0.3958	-1.8258		-2.5897	0.3875	-1.8040	
H	-3.6217	0.3387	-0.3834		-3.6051	0.3286	-0.3709	
H	0.0731	0.6520	3.6165		0.0612	0.6515	3.5853	
H	1.4514	-0.4710	3.5948		1.4232	-0.4681	3.5865	
H	-0.1841	-1.0513	3.2151		-0.1947	-1.0386	3.1859	
H	1.4690	0.9291	1.4892		1.4722	0.9201	1.4926	
H	1.2227	-0.7423	1.0928		1.2201	-0.7424	1.0958	
H	-1.6839	2.0243	-0.0332		-1.6813	2.0210	-0.0146	
	$B(C_2H_5)(C_4H_9)H$			-262.2328				-261.8806
C	0.4660	-0.6455	-0.1076		0.4672	-0.6639	-0.1112	
C	0.1128	0.1875	1.1298		0.1256	0.1883	1.1108	
B	1.6115	-0.1367	-1.0374		1.6162	-0.1525	-1.0391	
C	1.6935	-0.4913	-2.5632		1.6918	-0.5001	-2.5654	
C	0.9607	0.6948	-3.2434		0.9629	0.6875	-3.2325	
C	3.1151	-0.6457	-3.1167		3.1082	-0.6360	-3.1149	
C	3.8673	-1.8217	-2.4953		3.8549	-1.8059	-2.4862	
H	2.4680	0.5892	-0.5782		2.4646	0.5675	-0.5855	
H	1.1166	-1.4068	-2.7900		1.1255	-1.4076	-2.7973	
H	-0.4363	-0.9145	-0.6834		-0.4276	-0.9164	-0.6852	
H	0.8700	-1.6323	0.2163		0.8600	-1.6386	0.2222	
H	0.9612	0.5616	-4.3360		0.9573	0.5610	-4.3157	
H	1.4622	1.6511	-3.0297		1.4691	1.6295	-3.0145	
H	-0.0856	0.7815	-2.9176		-0.0720	0.7752	-2.9009	
H	-0.3295	1.1515	0.8407		-0.2910	1.1486	0.8095	
H	1.0094	0.4094	1.7253		1.0181	0.3926	1.7002	
H	-0.6093	-0.3221	1.7836		-0.6026	-0.2968	1.7592	
H	3.6720	0.2879	-2.9300		3.6517	0.2924	-2.9218	
H	3.0763	-0.7678	-4.2131		3.0756	-0.7606	-4.2008	
H	4.8793	-1.9247	-2.9104		4.8598	-1.9113	-2.8923	
H	3.3357	-2.7691	-2.6701		3.3225	-2.7412	-2.6606	
H	3.9672	-1.6949	-1.4062		3.9460	-1.6711	-1.4073	
	$B(C_2H_5)(\eta^2\text{-}C_2H_4)$			-182.4538				-182.2004
C	-2.3142	2.4061	0.3937		-2.3116	2.4338	0.4162	
C	-3.1423	1.3843	-0.3955		-3.1402	1.3775	-0.3151	
H	-2.9347	1.4561	-1.4719		-2.9112	1.3761	-1.3791	
H	-4.2225	1.5293	-0.2511		-4.2091	1.5503	-0.1991	
H	-2.8983	0.3581	-0.0884		-2.9202	0.3815	0.0653	
B	-0.7742	2.3309	0.2678		-0.7739	2.3323	0.2642	
C	0.4842	1.6951	-0.3370		0.4529	1.7234	-0.4267	
C	0.6026	2.8743	0.6724		0.6239	2.8203	0.6642	
H	-2.5593	2.3678	1.4721		-2.5647	2.4735	1.4790	
H	-2.5996	3.4405	0.1193		-2.5641	3.4382	0.0516	

H	0.9567	3.8334	0.2848		0.9776	3.7877	0.3310	
H	1.0185	2.6513	1.6588		1.0599	2.5094	1.6050	
H	0.8213	0.7096	-0.0038		0.7778	0.7234	-0.1686	
H	0.7592	1.8919	-1.3768		0.7004	2.0009	-1.4434	
$B(C_2H_5)_2$				-183.0222				-182.7663
B	-0.3279	-0.3578	0.3351		-0.2960	-0.3364	0.2997	
C	-0.0524	0.2067	1.7500		-0.0878	0.1660	1.7563	
C	1.3029	-0.0711	2.4122		1.2802	-0.0435	2.4041	
C	-1.6064	-0.2834	-0.5422		-1.6000	-0.2947	-0.5517	
C	-2.8032	0.5222	-0.0005		-2.7481	0.5642	-0.0064	
H	-1.9046	-1.3312	-0.7415		-1.9155	-1.3441	-0.6232	
H	-1.3139	0.0794	-1.5446		-1.3657	-0.0228	-1.5830	
H	-3.1432	0.1281	0.9674		-3.0269	0.2548	0.9997	
H	-3.6594	0.4946	-0.6898		-3.6351	0.4933	-0.6342	
H	-2.5350	1.5769	0.1525		-2.4611	1.6137	0.0420	
H	1.4635	-1.1506	2.5362		1.5263	-1.1025	2.4503	
H	1.3790	0.3983	3.4035		1.3128	0.3549	3.4171	
H	2.1262	0.3089	1.7925		2.0599	0.4457	1.8236	
H	-0.8834	-0.1344	2.4022		-0.8784	-0.2936	2.3642	
H	-0.2287	1.3008	1.6713		-0.3511	1.2325	1.7457	
$B(C_2H_5)_2H$				-183.6867				-183.4349
B	0.5875	-0.0025	0.3121		0.5871	0.0006	0.3090	
C	-0.0713	-0.1353	1.7231		-0.0444	-0.1466	1.7337	
H	0.7605	-0.4950	2.3682		0.8047	-0.4531	2.3639	
H	-0.7705	-0.9910	1.7392		-0.7126	-1.0110	1.7687	
C	-0.7092	1.1136	2.3394		-0.7102	1.0932	2.3277	
H	0.7759	1.0999	-0.1539		0.7577	1.0971	-0.1462	
C	1.0675	-1.2254	-0.5394		1.0697	-1.2211	-0.5469	
C	0.8961	-2.6398	0.0224		0.8694	-2.6224	0.0250	
H	2.1243	-1.0377	-0.8121		2.1277	-1.0458	-0.7763	
H	0.5571	-1.1318	-1.5194		0.5869	-1.1316	-1.5274	
H	1.4374	-2.7620	0.9718		1.3682	-2.7301	0.9876	
H	1.2695	-3.4081	-0.6692		1.2631	-3.3919	-0.6373	
H	-0.1607	-2.8665	0.2243		-0.1870	-2.8355	0.1836	
H	0.0057	1.9478	2.3698		-0.0198	1.9351	2.3382	
H	-1.0656	0.9394	3.3648		-1.0528	0.9274	3.3481	
H	-1.5701	1.4503	1.7445		-1.5736	1.3914	1.7345	
$B(C_2H_5)_3$				-262.2506				-261.8958
B	0.5050	0.0994	0.1821		0.5050	0.0994	0.1821	
C	-0.0044	-0.0214	1.6697		-0.0026	-0.0321	1.6684	
H	0.8130	-0.4895	2.2527		0.8100	-0.4897	2.2456	
H	-0.7812	-0.8109	1.6812		-0.7778	-0.8080	1.6748	
C	-0.5145	1.2303	2.3890		-0.5081	1.2239	2.3743	
C	0.4854	1.4977	-0.5470		0.4817	1.5015	-0.5374	
C	0.9855	1.5948	-1.9908		0.9827	1.5843	-1.9774	

H	1.0428	2.2052	0.0978		1.0413	2.1978	0.0988	
H	-0.5506	1.8833	-0.4758		-0.5463	1.8783	-0.4719	
C	1.0344	-1.1780	-0.5763		1.0359	-1.1711	-0.5847	
C	1.0439	-2.5267	0.1482		1.0412	-2.5098	0.1497	
H	2.0509	-0.9357	-0.9438		2.0447	-0.9315	-0.9422	
H	0.4575	-1.2555	-1.5187		0.4570	-1.2506	-1.5128	
H	1.6654	-2.4929	1.0548		1.6587	-2.4666	1.0462	
H	1.4357	-3.3342	-0.4867		1.4271	-3.3139	-0.4754	
H	0.0329	-2.8212	0.4649		0.0370	-2.7923	0.4640	
H	0.2629	2.0058	2.4488		0.2679	1.9866	2.4281	
H	-0.8392	1.0132	3.4166		-0.8324	1.0142	3.3927	
H	-1.3709	1.6764	1.8630		-1.3536	1.6618	1.8449	
H	2.0354	1.2787	-2.0757		2.0221	1.2671	-2.0533	
H	0.9200	2.6197	-2.3831		0.9200	2.5980	-2.3711	
H	0.4023	0.9495	-2.6636		0.4009	0.9405	-2.6361	
$B(C_2H_5)H$				-104.4545				-104.3048
C	0.1196	-0.0319	-0.0507		0.1072	-0.0294	-0.0526	
C	0.0545	-0.0010	1.4821		0.0552	-0.0014	1.4743	
B	1.4864	-0.0352	-0.7546		1.4917	-0.0358	-0.7436	
H	1.7122	-0.0899	-1.9345		1.7063	-0.0954	-1.9122	
H	-0.4532	-0.8924	-0.4559		-0.4531	-0.8849	-0.4495	
H	-0.4150	0.8415	-0.4851		-0.4148	0.8408	-0.4748	
H	0.5359	-0.8896	1.9116		0.5397	-0.8813	1.8927	
H	-0.9823	0.0303	1.8455		-0.9694	0.0247	1.8412	
H	0.5801	0.8776	1.8791		0.5753	0.8721	1.8621	
$B(C_2H_5)H_2$				-105.1211				-104.9741
B	0.2507	0.1980	0.2845		0.2514	0.2056	0.2896	
C	0.1258	0.1695	1.8292		0.1169	0.1473	1.8400	
H	1.1046	0.0256	2.3174		1.0919	0.0231	2.3157	
H	-0.3548	-0.8307	1.9623		-0.3652	-0.8337	1.9873	
C	-0.7097	1.2452	2.5295		-0.7079	1.2380	2.5196	
H	-0.5047	0.8481	-0.3938		-0.4788	0.8836	-0.3677	
H	-0.2213	2.2271	2.4589		-0.2278	2.2095	2.4132	
H	-0.8587	1.0287	3.5967		-0.8381	1.0503	3.5841	
H	-1.7000	1.3422	2.0633		-1.6959	1.3135	2.0683	
H	1.0678	-0.4935	-0.2673		1.0534	-0.4771	-0.2692	
$B(C_4H_9)H$				-182.9995				-182.7489
C	-0.0524	0.0576	-0.0321		-0.0431	0.0516	-0.0243	
C	-0.0244	0.0383	1.5253		-0.0265	0.0297	1.5231	
C	1.4215	0.0068	2.0541		1.4137	0.0071	2.0424	
C	1.4925	-0.0144	3.5801		1.4783	-0.0028	3.5646	
B	-0.8156	1.3205	1.8676		-0.8053	1.3166	1.9080	
H	-0.4000	2.4505	1.9181		-0.3578	2.4217	1.9438	
H	-0.5466	-0.8771	1.8525		-0.5378	-0.8787	1.8480	
H	0.4999	-0.8150	-0.4115		0.5063	-0.8108	-0.4014	

H	0.4364	0.9573	-0.4340		0.4435	0.9480	-0.4102	
H	-1.0741	0.0126	-0.4321		-1.0537	0.0104	-0.4278	
H	1.9624	0.8858	1.6670		1.9438	0.8801	1.6549	
H	1.9347	-0.8809	1.6441		1.9243	-0.8744	1.6451	
H	2.5303	-0.0623	3.9370		2.5053	-0.0473	3.9232	
H	0.9567	-0.8835	3.9894		0.9436	-0.8626	3.9678	
H	1.0349	0.8894	4.0109		1.0216	0.8970	3.9790	
$B(C_4H_9)H_2$				-183.6668				-183.4190
C	-0.1091	0.0480	-0.0178		-0.0952	0.0396	-0.0162	
C	-0.0675	0.0233	1.5414		-0.0676	0.0164	1.5339	
C	1.3751	0.0378	2.0555		1.3689	0.0389	2.0429	
C	1.4552	-0.0044	3.5809		1.4385	0.0076	3.5644	
B	-0.9210	1.2888	1.8390		-0.9139	1.2835	1.8647	
H	-0.3843	2.3625	1.9581		-0.3702	2.3406	1.9859	
H	-0.5676	-0.9061	1.8620		-0.5577	-0.9060	1.8534	
H	0.4845	-0.7927	-0.4076		0.4887	-0.7969	-0.4004	
H	0.3318	0.9716	-0.4226		0.3510	0.9559	-0.4062	
H	-1.1291	-0.0484	-0.4140		-1.1056	-0.0443	-0.4149	
H	1.8762	0.9476	1.6845		1.8607	0.9416	1.6715	
H	1.9310	-0.8162	1.6311		1.9210	-0.8107	1.6321	
H	2.4954	-0.0051	3.9347		2.4669	0.0082	3.9223	
H	0.9659	-0.9062	3.9782		0.9479	-0.8842	3.9545	
H	0.9527	0.8680	4.0260		0.9376	0.8771	3.9919	
H	-2.1239	1.2415	1.8350		-2.1055	1.2426	1.8844	
$B(C_6H_{13})H_2$				-262.2157				-261.8654
C	-0.0807	0.1434	0.0564		-0.0285	0.0494	-0.0241	
C	-0.0219	-0.0940	1.5995		-0.0308	0.0114	1.5275	
C	1.3814	-0.0266	2.2025		1.3811	0.0245	2.1185	
C	2.2482	-1.2169	1.7590		2.2039	-1.1868	1.6805	
C	3.7206	-1.1189	2.1584		3.6338	-1.1928	2.2107	
B	-0.9275	1.1590	1.5581		-0.8801	1.2873	1.8147	
C	1.2802	0.0721	3.7273		1.2842	0.1108	3.6393	
H	-0.4196	2.2501	1.6100		-0.3413	2.3529	1.8650	
H	-0.5149	-1.0416	1.8510		-0.5414	-0.9047	1.8367	
H	-0.5733	-0.6706	-0.4824		0.3364	-0.8907	-0.4329	
H	0.9118	0.3627	-0.3518		0.6157	0.8503	-0.3885	
H	-0.6893	1.0626	-0.2067		-1.0280	0.2074	-0.4347	
H	1.8570	0.9007	1.8315		1.8837	0.9285	1.7538	
H	2.2659	0.1645	4.2023		2.2593	0.2102	4.1121	
H	0.7906	-0.8237	4.1403		0.8046	-0.7859	4.0374	
H	0.6812	0.9457	4.0198		0.6858	0.9724	3.9404	
H	-2.1209	1.0556	1.4553		-2.0706	1.2401	1.8650	
H	1.8093	-2.1416	2.1722		1.6853	-2.0945	2.0042	
H	2.1827	-1.3159	0.6629		2.2381	-1.2201	0.5909	
H	4.2977	-1.9652	1.7611		4.2063	-2.0113	1.7771	
H	3.8511	-1.1168	3.2491		3.6648	-1.3077	3.2921	

H	4.1736	-0.1949	1.7686		4.1412	-0.2611	1.9585	
BH				-25.2394				-25.2034
B	0.0000	0.0000	0.1792		0.0000	0.0000	0.1922	
H	0.0000	0.0000	1.4313		0.0000	0.0000	1.4183	
BH_2				-25.8838				-25.8431
B	0.2291	0.0000	0.1620		0.2263	0.0000	0.1600	
H	0.0192	0.0000	1.3403		0.0308	0.0000	1.3270	
H	1.2701	0.0000	-0.4286		1.2613	0.0000	-0.4133	
BH_3				-26.5538				-26.5140
B	-0.0001	0.0002	0.0000		0.0000	0.0002	0.0000	
H	0.0001	0.0000	1.1986		0.0000	0.0000	1.1869	
H	1.0381	0.0000	-0.5992		1.0279	0.0000	-0.5935	
H	-1.0381	0.0005	-0.5994		-1.0279	0.0005	-0.5935	
C_2H_3				-77.8228				-77.7072
C	0.1040	0.0000	0.0425		0.0970	0.0000	0.0610	
C	0.0091	0.0000	1.3473		0.0083	0.0000	1.3392	
H	0.8754	0.0000	-0.7223		0.8730	0.0000	-0.6841	
H	-0.9547	0.0000	1.8661		-0.9445	0.0000	1.8511	
H	0.8994	0.0000	1.9951		0.8994	0.0000	1.9616	
C_2H_4				-78.5043				-78.4006
C	0.0000	0.0000	-0.0010		0.0000	0.0001	-0.0007	
C	0.0000	0.0002	1.3318		0.0000	0.0002	1.3316	
H	0.9284	-0.0002	1.9053		0.9226	-0.0002	1.8937	
H	-0.9284	0.0005	1.9052		-0.9227	0.0005	1.8936	
H	0.9284	-0.0004	-0.5744		0.9227	-0.0004	-0.5628	
H	-0.9283	0.0003	-0.5744		-0.9226	0.0003	-0.5628	
C_2H_5				-79.0690				-78.9597
C	0.1230	0.2152	0.0601		0.1173	0.2052	0.0589	
C	0.0174	0.0305	1.5275		0.0176	0.0308	1.5315	
H	1.0020	-0.1234	-0.4860		0.9967	-0.1150	-0.4740	
H	-0.6150	0.8005	-0.4860		-0.6050	0.8003	-0.4740	
H	0.5191	-0.8883	1.8652		0.5123	-0.8812	1.8606	
H	-1.0288	-0.0035	1.8652		-1.0193	-0.0059	1.8606	
H	0.4929	0.8622	2.0867		0.4909	0.8590	2.0691	
C_2H_6				-79.7364				-79.6308
C	0.0000	0.0000	-0.0043		0.0000	0.0000	-0.0025	
C	0.0000	-0.0001	1.5235		0.0000	-0.0001	1.5217	
H	1.0230	0.0001	-0.4058		1.0149	0.0000	-0.3947	
H	-0.5116	0.8859	-0.4057		-0.5075	0.8789	-0.3947	
H	-0.5114	-0.8860	-0.4058		-0.5074	-0.8789	-0.3947	
H	0.5114	0.8859	1.9250		0.5073	0.8788	1.9139	
H	0.5116	-0.8860	1.9249		0.5075	-0.8790	1.9139	
H	-1.0230	-0.0002	1.9250		-1.0149	-0.0003	1.9139	
C_4H_{10}				-158.2837				-158.0759
C	-0.0040	-0.0063	0.0145		-0.0044	-0.0070	0.0073	

C	0.0071	0.0118	1.5423		0.0046	0.0075	1.5301	
H	1.0313	0.0112	-0.3650		1.0212	0.0045	-0.3682	
H	-0.4802	0.9134	-0.3646		-0.4811	0.9013	-0.3678	
H	0.5061	-0.8822	1.9447		0.4988	-0.8814	1.9216	
H	-1.0164	0.0270	1.9451		-1.0123	0.0207	1.9219	
H	0.5334	0.8929	1.9345		0.5254	0.8799	1.9211	
C	-0.7291	-1.2209	-0.5672		-0.7288	-1.2202	-0.5601	
C	-0.7404	-1.2390	-2.0951		-0.7378	-1.2346	-2.0829	
H	-1.2665	-2.1201	-2.4873		-1.2586	-2.1071	-2.4739	
H	0.2832	-1.2541	-2.4978		0.2790	-1.2478	-2.4747	
H	-1.2394	-0.3450	-2.4974		-1.2321	-0.3458	-2.4743	
H	-1.7645	-1.2384	-0.1877		-1.7544	-1.2317	-0.1845	
H	-0.2530	-2.1406	-0.1881		-0.2520	-2.1285	-0.1849	
C_4H_8				-157.0524				-156.8501
C	0.0392	0.0681	0.0751		0.0468	0.0780	0.0923	
C	-0.0385	-0.1027	1.5994		-0.0449	-0.1165	1.6056	
C	1.3136	-0.1022	2.2484		1.3071	-0.1193	2.2445	
C	1.7289	0.7694	3.1719		1.7228	0.7741	3.1451	
H	0.6485	-0.7253	-0.3818		0.6550	-0.7039	-0.3610	
H	0.4969	1.0319	-0.1879		0.5064	1.0366	-0.1420	
H	-0.9600	0.0278	-0.3802		-0.9387	0.0474	-0.3692	
H	-0.6594	0.6936	2.0388		-0.6527	0.6730	2.0492	
H	-0.5461	-1.0571	1.8239		-0.5472	-1.0638	1.8136	
H	2.0044	-0.8830	1.9081		1.9909	-0.8996	1.9252	
H	1.0751	1.5658	3.5359		1.0695	1.5669	3.4850	
H	2.7311	0.7201	3.5986		2.7186	0.7337	3.5617	
H				-0.4996				-0.4998
H_2				-1.1664				-1.1646
H	0.0000	0.0000	-0.0212		0.0000	0.0000	-0.0145	
H	0.0000	0.0000	0.7292		0.0000	0.0000	0.7225	
TS-AB11				-182.3177				-182.0562
C	0.1180	-0.1203	0.0955		0.0782	-0.1802	0.0504	
C	-0.0029	0.0616	1.6184		0.0222	0.1159	1.5525	
B	1.5747	0.0548	-0.4351		1.4988	0.0892	-0.5648	
C	1.1208	-0.5779	-2.3838		1.0763	-0.6069	-2.3534	
C	1.0523	0.4519	-3.2232		1.1158	0.4943	-3.1071	
H	2.1179	-0.3996	-1.5863		2.0751	-0.5470	-1.6162	
H	-0.4639	0.6641	-0.4311		-0.6269	0.4625	-0.4894	
H	-0.3493	-1.0690	-0.2271		-0.2521	-1.2053	-0.1528	
H	0.4289	1.0205	1.9340		0.3180	1.1441	1.7509	
H	0.5369	-0.7311	2.1528		0.7043	-0.5315	2.0998	
H	-1.0533	0.0332	1.9408		-0.9810	-0.0356	1.9491	
H	0.6269	-1.5454	-2.4938		0.4635	-1.4838	-2.5149	
H	1.6117	1.3686	-3.0012		1.8028	1.2866	-2.8177	
H	0.4460	0.4482	-4.1311		0.4698	0.6573	-3.9578	
TS-AB6				-104.9794				-104.8195

B	-0.1234	0.1096	-0.3339		-0.1222	0.1101	-0.2753	
C	0.0278	-0.0314	1.8208		0.0295	-0.0343	1.8023	
H	1.1232	-0.0117	1.8344		1.1168	-0.0121	1.8294	
H	-0.3308	-1.0657	1.8672		-0.3287	-1.0598	1.8620	
C	-0.6187	0.8925	2.8420		-0.6160	0.8882	2.8275	
H	-0.4945	0.6562	0.7723		-0.5016	0.6672	0.8005	
H	-0.2761	1.9295	2.7214		-0.2744	1.9146	2.7010	
H	-0.3667	0.5761	3.8647		-0.3650	0.5733	3.8391	
H	-1.7139	0.8877	2.7535		-1.7010	0.8808	2.7330	
H	0.5862	-0.8686	-0.3314		0.5758	-0.8538	-0.3085	
TS-AB8				-262.1668				-261.8021
B	-0.0730	-0.1734	0.0273		0.1367	0.1984	-0.0129	
C	-0.0526	-0.0027	1.8235		0.2400	0.7508	1.6743	
H	0.9157	0.2860	2.2589		1.0304	1.4801	1.8603	
H	-0.1040	-1.0962	1.9385		0.6468	-0.2130	1.9861	
C	-1.2127	0.6909	2.5233		-1.0295	1.0792	2.4465	
C	-1.1556	0.5370	-0.6389		-1.1845	0.3318	-0.6041	
C	-1.4653	0.5258	-2.1049		-1.5614	-0.0303	-2.0118	
H	0.1642	0.8727	0.7148		-0.1063	1.3513	0.4471	
H	-1.8145	1.1934	-0.0575		-1.9989	0.7530	-0.0177	
C	1.0804	-1.1164	-0.5148		1.5239	-0.3057	-0.5765	
C	2.5109	-0.5975	-0.2898		1.8556	-1.7303	-0.1102	
H	0.9242	-1.2815	-1.5935		2.3319	0.3663	-0.2749	
H	0.9905	-2.1187	-0.0563		1.5087	-0.2868	-1.6682	
H	2.6550	0.3807	-0.7714		1.9106	-1.7935	0.9775	
H	3.2693	-1.2832	-0.6957		2.8124	-2.0747	-0.5018	
H	2.7336	-0.4684	0.7801		1.0881	-2.4309	-0.4379	
H	-1.2386	1.7676	2.3004		-1.5061	1.9836	2.0678	
H	-1.1247	0.5857	3.6137		-0.8035	1.2411	3.4990	
H	-2.1743	0.2658	2.2111		-1.7483	0.2674	2.3670	
H	-0.7730	-0.1086	-2.6741		-1.9752	0.8229	-2.5518	
H	-1.4353	1.5385	-2.5396		-2.3314	-0.8056	-2.0133	
H	-2.4883	0.1512	-2.2841		-0.7082	-0.4066	-2.5733	
TS-AB9				-182.3074				-182.0398
C	0.0377	0.1925	0.2882		0.0631	0.3315	0.3768	
C	-0.1302	-0.2623	1.7402		-0.1250	-0.4494	1.6779	
B	1.8585	0.1160	0.0151		1.8081	0.3749	0.1081	
C	2.5652	1.4351	-0.3550		2.5302	1.6808	-0.3044	
C	3.2404	1.8312	-1.4623		3.2821	1.6518	-1.4339	
H	0.8521	1.0647	-0.1194		0.8629	1.2981	0.0412	
H	-0.7104	1.0120	0.1043		-0.6636	1.1719	0.4008	
H	-0.2118	-0.5898	-0.4367		-0.2026	-0.2612	-0.4968	
H	0.2661	0.4838	2.4406		0.2833	0.0994	2.5230	
H	0.4092	-1.2007	1.9088		0.3971	-1.3992	1.6099	
H	-1.1996	-0.3933	1.9680		-1.1891	-0.6069	1.8627	
H	2.6050	2.1148	0.5192		2.4215	2.6405	0.2013	

H	3.2685	1.2176	-2.3629		3.4707	0.7156	-1.9414	
H	3.7697	2.7826	-1.4959		3.6816	2.5563	-1.8732	
TS-AB11				-182.3177				-182.0562
C	0.1180	-0.1203	0.0955		0.0782	-0.1802	0.0504	
C	-0.0029	0.0616	1.6184		0.0222	0.1159	1.5525	
B	1.5747	0.0548	-0.4351		1.4988	0.0892	-0.5648	
C	1.1208	-0.5779	-2.3838		1.0763	-0.6069	-2.3534	
C	1.0523	0.4519	-3.2232		1.1158	0.4943	-3.1071	
H	2.1179	-0.3996	-1.5863		2.0751	-0.5470	-1.6162	
H	-0.4639	0.6641	-0.4311		-0.6269	0.4625	-0.4894	
H	-0.3493	-1.0690	-0.2271		-0.2521	-1.2053	-0.1528	
H	0.4289	1.0205	1.9340		0.3180	1.1441	1.7509	
H	0.5369	-0.7311	2.1528		0.7043	-0.5315	2.0998	
H	-1.0533	0.0332	1.9408		-0.9810	-0.0356	1.9491	
H	0.6269	-1.5454	-2.4938		0.4635	-1.4838	-2.5149	
H	1.6117	1.3686	-3.0012		1.8028	1.2866	-2.8177	
H	0.4460	0.4482	-4.1311		0.4698	0.6573	-3.9578	
TS-BB1-tBu				-497.8164				
B	-0.2799	0.1109	-0.0957					
C	-0.1123	-0.0681	1.5571					
C	-0.4453	1.2425	2.3007					
C	-2.2131	0.2036	-0.4960					
C	-1.4985	1.3612	-0.8265					
C	0.5718	-0.7526	-1.2439					
C	0.4066	-0.2039	-2.6811					
H	-0.6134	-0.2097	-3.0801					
H	1.0178	-0.8049	-3.3736					
H	0.7778	0.8312	-2.7446					
H	0.2694	2.0313	2.0204					
H	-0.3641	1.0932	3.3901					
H	-1.4491	1.6379	2.1070					
H	-1.6089	2.2488	-0.2028					
H	0.1631	1.2654	-0.2593					
H	-1.1688	1.5507	-1.8456					
C	-2.6816	-0.8094	-1.5193					
H	-2.7749	-1.8050	-1.0657					
H	-2.0548	-0.8949	-2.4061					
H	-3.6922	-0.5171	-1.8501					
C	-3.2394	0.2878	0.6210					
H	-4.1494	0.7395	0.1916					
H	-2.9401	0.9018	1.4724					
H	-3.5251	-0.7045	0.9891					
C	2.0995	-0.5977	-1.0133					
H	2.4643	-1.1552	-0.1472					
H	2.3878	0.4564	-0.8868					
H	2.6391	-0.9855	-1.8932					

C	0.2872	-2.2668	-1.2276				
H	0.9360	-2.7892	-1.9512				
H	-0.7500	-2.5152	-1.4802				
H	0.4972	-2.6940	-0.2365				
C	1.3603	-0.3443	1.9380				
H	1.4547	-0.3031	3.0361				
H	2.0523	0.3955	1.5155				
H	1.6867	-1.3447	1.6286				
C	-0.9008	-1.2450	2.1681				
H	-1.9835	-1.0960	2.1644				
H	-0.6003	-1.3943	3.2190				
H	-0.6904	-2.1815	1.6326				
TS-BB3-tBu				-183.6493			
B	-0.0806	-0.1085	0.2947				
C	0.0160	-0.0246	2.0382				
C	-0.5839	-1.2296	1.6086				
H	-0.8509	0.7475	-0.0465				
H	-1.6665	-1.3499	1.6487				
H	-0.6046	-1.1560	-0.1230				
H	-0.0093	-2.1557	1.5951				
H	1.0488	-0.1776	-0.1077				
C	1.4433	-0.0432	2.5490				
H	1.4499	-0.1621	3.6448				
H	1.9583	0.8978	2.3133				
H	2.0213	-0.8638	2.1068				
C	-0.8512	1.0728	2.6229				
H	-1.8751	1.0314	2.2321				
H	-0.4412	2.0648	2.3906				
H	-0.8917	0.9769	3.7202				
TS-H2BB1				-263.3910			-263.0266
C	0.0085	-0.0231	0.1211	0.0124	-0.0143	0.1128	
C	-0.0378	0.0407	1.6466	-0.0108	0.0692	1.6347	
B	1.5926	0.0062	-0.7144	1.5908	-0.0098	-0.7191	
C	2.5557	1.0916	-0.0239	2.5509	1.0625	-0.0224	
C	2.0640	2.5362	-0.1924	2.0518	2.4994	-0.1985	
H	-0.6929	-0.7755	-0.2738	-0.6943	-0.7616	-0.2571	
H	-0.3123	0.9324	-0.3172	-0.2912	0.9313	-0.3342	
H	0.5833	0.8610	2.0287	0.6015	0.8957	1.9880	
H	0.3267	-0.8890	2.1099	0.3720	-0.8437	2.0939	
H	-1.0638	0.2026	2.0054	-1.0247	0.2201	2.0021	
C	1.3069	-0.0021	-2.2932	1.3011	-0.0041	-2.2898	
H	2.1061	-1.1633	-0.4245	2.0588	-1.1805	-0.4235	
H	1.1244	-0.9574	-0.0365	1.0940	-0.9482	-0.0456	
H	3.5579	1.0065	-0.4749	3.5448	0.9816	-0.4686	
H	2.7065	0.8770	1.0467	2.6927	0.8510	1.0398	
H	1.9374	2.7951	-1.2540	1.9260	2.7434	-1.2538	

H	2.7667	3.2631	0.2399		2.7453	3.2253	0.2252	
H	1.0912	2.6993	0.2967		1.0869	2.6538	0.2869	
C	2.5694	-0.0874	-3.1605		2.5729	-0.0555	-3.1393	
H	2.3394	-0.0570	-4.2357		2.3556	-0.0324	-4.2070	
H	3.2567	0.7450	-2.9491		3.2242	0.7901	-2.9183	
H	3.1232	-1.0185	-2.9670		3.1411	-0.9637	-2.9358	
H	0.6211	-0.8230	-2.5644		0.6435	-0.8323	-2.5685	
H	0.7590	0.9232	-2.5481		0.7446	0.9062	-2.5366	
TS-H2BB2				-184.8350				-184.5715
C	-0.1635	-0.0045	-0.0280		-0.1676	-0.0156	-0.0088	
B	-0.1538	0.4369	1.7024		-0.1628	0.4446	1.7140	
C	1.2526	0.0878	2.3844		1.2505	0.1017	2.3707	
C	1.5711	-1.4136	2.3781		1.5699	-1.3950	2.3338	
C	1.0473	0.3763	-0.8798		1.0591	0.3540	-0.8352	
H	-1.1082	0.2113	-0.5499		-1.0913	0.2065	-0.5469	
H	-0.1747	-1.0848	0.1653		-0.1892	-1.0827	0.1988	
H	1.9847	0.0790	-0.3921		1.9730	0.0359	-0.3387	
H	1.1014	1.4612	-1.0591		1.1286	1.4316	-0.9926	
H	1.0101	-0.1156	-1.8616		1.0258	-0.1190	-1.8152	
H	-1.2009	0.0310	2.1360		-1.1975	0.0459	2.1512	
H	-0.3036	1.7218	1.7205		-0.3021	1.7196	1.6777	
H	-0.2823	1.2374	0.7406		-0.2939	1.2086	0.7340	
H	1.2270	0.4391	3.4284		1.2331	0.4297	3.4118	
H	2.0820	0.6421	1.9146		2.0621	0.6617	1.9012	
H	0.7638	-1.9920	2.8517		0.7685	-1.9737	2.7940	
H	2.5012	-1.6400	2.9194		2.4924	-1.6268	2.8652	
H	1.6917	-1.8041	1.3559		1.6872	-1.7576	1.3119	
TS-H2BB3				-106.2805				-106.1184
C	0.0389	0.1552	0.0006		0.0374	0.1591	-0.0052	
C	-0.0160	-0.0157	1.5172		-0.0081	-0.0218	1.5071	
B	1.6441	0.0296	-0.7572		1.6458	0.0352	-0.7552	
H	-0.7709	-0.4014	-0.4973		-0.7629	-0.3960	-0.4983	
H	-0.1114	1.2032	-0.2828		-0.1032	1.2004	-0.2789	
H	2.4060	0.5798	-0.0146		2.3889	0.5886	-0.0149	
H	0.7482	0.6027	2.0056		0.7507	0.5930	1.9859	
H	0.1641	-1.0582	1.8206		0.1796	-1.0574	1.7932	
H	-0.9983	0.2756	1.9144		-0.9808	0.2583	1.9073	
H	1.5326	0.2903	-1.9211		1.5346	0.2715	-1.9123	
H	1.9814	-1.2027	-0.7136		1.9418	-1.1992	-0.6738	
H	0.9624	-0.9260	-0.3334		0.9574	-0.8995	-0.3166	
TS-HB2				-104.9874				-104.8257
B	-0.2787	-0.4260	0.0067		-0.3608	-0.3822	-0.0126	
C	-0.0582	-0.1098	1.5134		-0.0364	-0.0907	1.4980	
H	1.0407	0.0711	1.5487		1.0418	0.1217	1.5283	
H	-0.1937	-1.0682	2.0442		-0.1628	-1.0362	2.0264	
C	-0.8096	1.0204	2.2342		-0.8108	1.0218	2.2168	

H	-0.2732	1.4098	-0.3957		-0.1977	1.2621	-0.2663	
H	-0.5823	1.0390	3.3094		-0.5998	1.0239	3.2845	
H	-1.8962	0.9017	2.1289		-1.8853	0.8941	2.0958	
H	-0.5393	1.9958	1.8058		-0.5449	1.9990	1.8153	
H	-0.3360	0.6933	-0.8978		-0.3700	0.7136	-0.8883	
TS-HB5								-26.3667
B					-0.7546	-0.0732	0.5107	
H					0.3351	-0.1408	1.0652	
H					0.5781	0.0936	-0.8618	
H					-0.1659	0.1204	-1.0811	
TS-LB5a				-262.1758				-261.8139
B	0.4028	0.1707	0.2784		0.3750	0.1611	0.2784	
C	0.2254	-0.0681	2.0953		0.2231	-0.0722	2.0795	
H	0.8174	-0.9146	2.4717		0.8248	-0.8983	2.4621	
H	-0.7962	-0.4345	1.9465		-0.7878	-0.4456	1.9428	
C	0.2283	1.1203	3.0565		0.2264	1.1311	3.0166	
C	-0.4623	1.3830	-0.2860		-0.4788	1.3794	-0.2702	
C	0.1937	2.7698	-0.2116		0.2113	2.7445	-0.1933	
H	-1.4491	1.4157	0.2107		-1.4478	1.4289	0.2378	
H	-0.6920	1.1564	-1.3412		-0.7184	1.1657	-1.3157	
C	0.7329	-1.2098	-0.4147		0.7343	-1.2026	-0.4132	
C	1.8834	-0.2463	-0.3295		1.8710	-0.2197	-0.3024	
H	0.2865	-1.3530	-1.3999		0.3212	-1.3397	-1.4031	
H	0.8165	-2.1369	0.1552		0.8283	-2.1218	0.1494	
H	2.1712	0.3133	-1.2213		2.1598	0.3369	-1.1843	
H	2.7383	-0.5292	0.2880		2.7078	-0.5009	0.3249	
H	1.1897	0.3789	1.2504		1.1671	0.3536	1.2390	
H	1.2362	1.5360	3.2001		1.2237	1.5567	3.1269	
H	-0.1523	0.8179	4.0415		-0.1267	0.8419	4.0047	
H	-0.4152	1.9269	2.6825		-0.4314	1.9104	2.6386	
H	0.4180	3.0616	0.8252		0.4692	3.0065	0.8328	
H	-0.4432	3.5577	-0.6411		-0.4139	3.5454	-0.5889	
H	1.1487	2.7799	-0.7571		1.1404	2.7343	-0.7627	
TS-BB1				-262.177159				
B	-0.512828	0.31557	0.05737					
C	-0.135754	0.07483	1.583212					
C	1.866335	0.063908	-0.774849					
C	-1.098862	-0.837746	-0.855979					
C	1.51232	1.327526	-1.054586					
H	2.327468	-0.203936	0.175533					
H	1.736467	-0.738183	-1.501625					
H	1.081518	1.6023	-2.017571					
H	-0.814259	1.453531	-0.247762					
H	1.667653	2.137237	-0.341494					
C	-1.283228	-0.552897	-2.350239					

H	-2.101931	-0.997759	-0.405327
H	-0.581679	-1.799863	-0.70246
H	-1.835342	-1.353278	-2.864659
H	-1.832387	0.386711	-2.508334
H	-0.314624	-0.45025	-2.863714
C	-1.396982	0.265462	2.454872
H	0.272676	-0.933693	1.763333
H	0.628635	0.791269	1.9264
H	-1.17269	0.136802	3.523942
H	-1.825161	1.27009	2.322811
H	-2.181483	-0.460769	2.196015

[a] Total SCF-Energies E in E_h and cartesian coordinates in Å
[b] Reaction index referring to the reaction catalogue.
[c] β-H elimination analogue to BB1 and BB3 with *tert*-butyl substituents instead of ethyl substituents.

References:

(1) H. Pedersen, C. Höglund, J. Birch, J. Jensen, A. Henry, *Chem. Vap. Deposition.,* 2012, **18**, 221-224.