Supporting Information

Novel Single-source Precursors for $SiB_xC_yN_z$ Film Deposition

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List of considered phases, scheme of reactor, molecular structure of TSABA, experimental tensimetry data, experimental and calculated IR and Raman wavenumbers of the most intense bands of TSABA are available here.

In the process of thermodynamic computation we considered a possibility for the following condensed phases to depose: Si (l), Si (s), α-quartz (s), β-quartz (s), α-tridymite (s), β-tridymite (s), γ-tridymite (s), α-cristobalite (s), β-cristobalite (s), silica glass (s), Si_3N_4 (s), H_2O (l), H_2O (s), α-SiC (s), β-SiC (s), graphite (s), diamond (s), α- B_2O_3 (s), β-B_2O_3 (s), B_2O_3 (l), h-BN (s), c-BN (s), w-BN (s), B (s), HBO_2 (s), HBO_2 (l).

The gas phase was assumed to contain the following spices: Si_3, Si_2, SiO_2, SiO, O_3, O_2, SiN, N_2O_4, N_2O_3, N_2O, NO, NO_2, N_2, SiH_2, SiH, H_2O_2, H_2O, HO_2, OH, HNO_2, HNO, HN_3, N_2H_2, H_3N, H_2N, HN, H_2, SiC_2, Si_2C, C_2O, CO, CO_2, C_2N_2, C_2N, CN_2, CN, CHO_2, CHO, HCN, C_2H_6, C_2H_5, C_2H_4, C_2H_3, C_2H_2, C_2H, CH_4, CH_3, CH_2, CH, B_2O_3, B_2O_2, B_2O, BO_2, BO, BN, BHO, B_2H_6, BH_3, BH_2, BH, B_2C, BC_2, BC, B, C, N, H, O, Si.

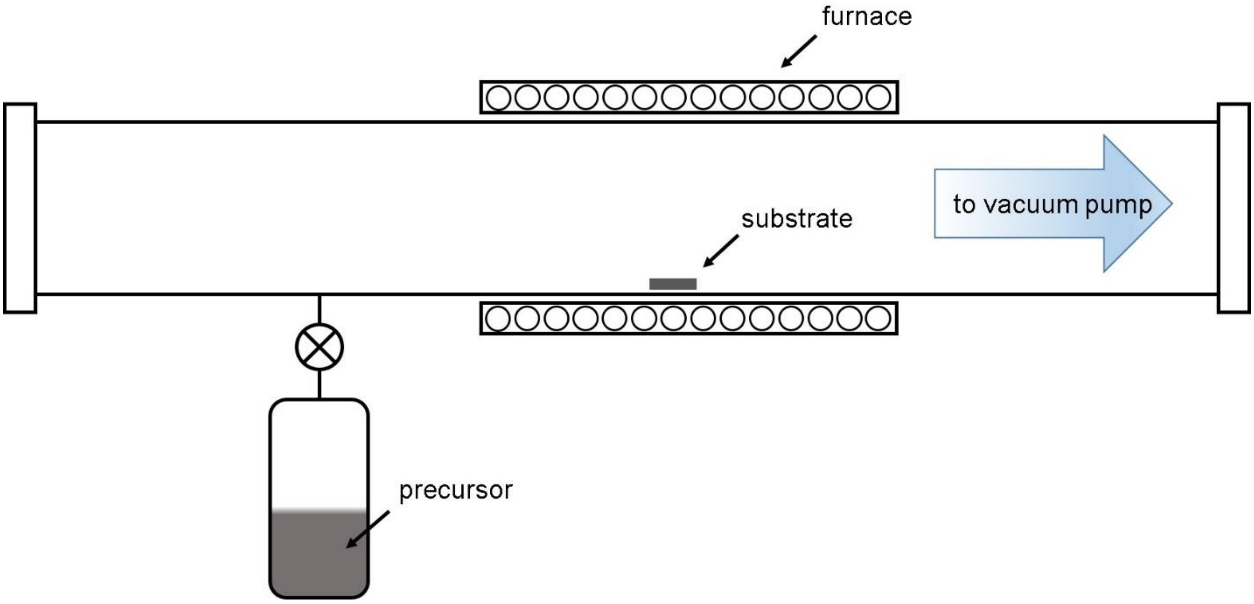

Figure S1. Scheme of reactor

Table S1. Experimental tensimetry data of $HC{\equiv}CB[N(SiMe_3)_2]_2$

Series		Temperature, K	Saturated vapor pressure, Pa
I	heating	340.3	56
		350.0	73
		369.5	197
		379.4	294
		389.4	442
		398.9	688
		408.8	1004
		419.8	1559
	cooling	408.8	1025
		398.9	698
		389.1	430
		379.4	321
II	heating	399.0	762
		409.0	1129
		419.5	1458
		429.6	2172
		439.2	3103
	cooling	429.7	2233
		409.3	1044
III	heating	429.4	2217
		439.2	3183
		449.4	4304
		459.3	5968
		469.0	8088
	cooling	459.6	6023
		449.4	4384

Table S2. Experimental tensimetry data of $MeB[N(SiMe_3)_2]_2$

Series		Temperature, K	Saturated vapor pressure, Pa
I	heating	329.4	129
		348.9	297
		368.5	713
	cooling	349.2	282
		329.5	111
II	heating	345.7	270
		365.5	704
		388.2	1386
		398.1	2074
		408.2	2943
	cooling	398.2	2013
		388.5	1475
		378.8	1101
III	heating	329.5	95

		349.2	357
		368.7	767
		398.1	2065
		418.9	4044
		428.8	5570
	cooling	419.5	4274
		400.8	2222

Table S3. Experimental tensimetry data of $Me_3SiC{\equiv}CB[N(SiMe_3)_2]_2$

Series		Temperature, K	Saturated vapor pressure, Pa
I	heating	300.5	135
		310.2	176
		320.3	219
		330.2	352
		349.3	665
		368.8	1201
		389.5	2145
II	heating	310.4	179
		321.2	275
		330.7	337
		350.3	784
		370.0	1275
		389.5	2136
		399.4	2808
		409.5	3566
		419.8	4526
	cooling	410.0	3384
		399.4	3041
III	heating	310.2	157
		329.9	353
		398.3	2790
		419.2	4456
		429.1	5526
		439.6	6935
		449.6	8742
	cooling	439.9	6866
		430.5	5780
		419.8	4749
IV	heating	399.0	2849
		419.0	4598
		429.0	5682
		438.9	6917
	cooling	430.1	5654
		420.2	4642
		398.8	2825

Table S4. Standard thermodynamic characteristics of compounds **(1)** and **(2)**.

Compound	$\ln P/P^0 = A–B/T$		$\Delta H(T_*)$ $kJ \times mol^{-1}$	$\Delta S°(T_*)$ $J \times mol^{-1}$	Temperature range, K
	A	B			
(1)	9.85	5470	46.0 ± 0.7	81.2 ± 1.8	309 - 429
(2)	11.45	6557	54.5 ± 0.5	94.9 ± 1.2	340 - 470
(3)	6.35	3966	33.0 ± 0.4	52.8 ± 0.8	300 - 450

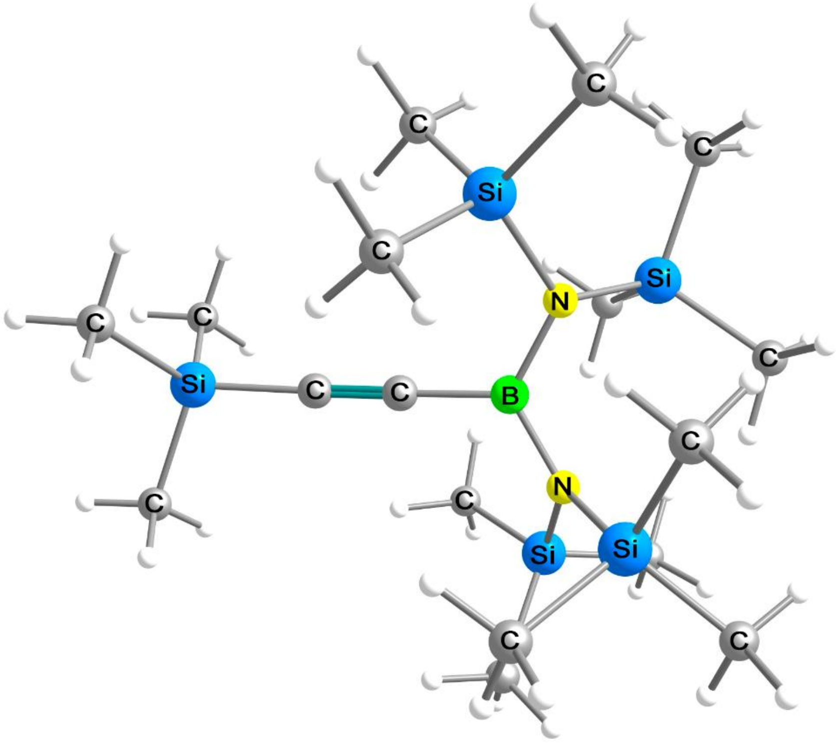

Figure S2. Molecular structure of TSABA

Table S5. NMR spectroscopic data of the compounds **(1)** and **(2)**.

Nucleus	Compound **(1)** δ, ppm	Compound **(2)** δ, ppm	Assignment
^{1}H	0.27 (36H)	0.21 (36H)	$(\mathrm{C}\mathbf{H}_3)_3\mathrm{Si}$
		0.56 (3H)	$\mathrm{BC}\mathbf{H}_3$
	2.81 (1H)		**H**C≡
^{13}C		3.38	$\mathrm{H}_3\mathbf{C}\mathrm{B}$
	4.32	4.74	$\mathrm{H}_3\mathbf{C}\mathrm{Si}$
	93.58		H**C**≡
	94.64		B**C**≡
^{29}Si	2.85	0.51	N**Si**C
^{11}B	32.07	49.20	C**B**N

Table S6. Elemental analysis data of the compounds **(1)** and **(2)**.

Element	Compound **(1)**		Compound **(2)**	
	Calculated	Experimental	Calculated	Experimental
C	47.15	47.31	45.05	45.08
H	10.46	10.37	11.34	11.28
N	7.85	7.65	8.08	8.12
Si	31.50	31.76	32.41	32.37
B	3.03	3.10	3.12	3.15

Based on the elemental analysis and NMR spectroscopy, the purity of the obtained precursors were more 99.6%.

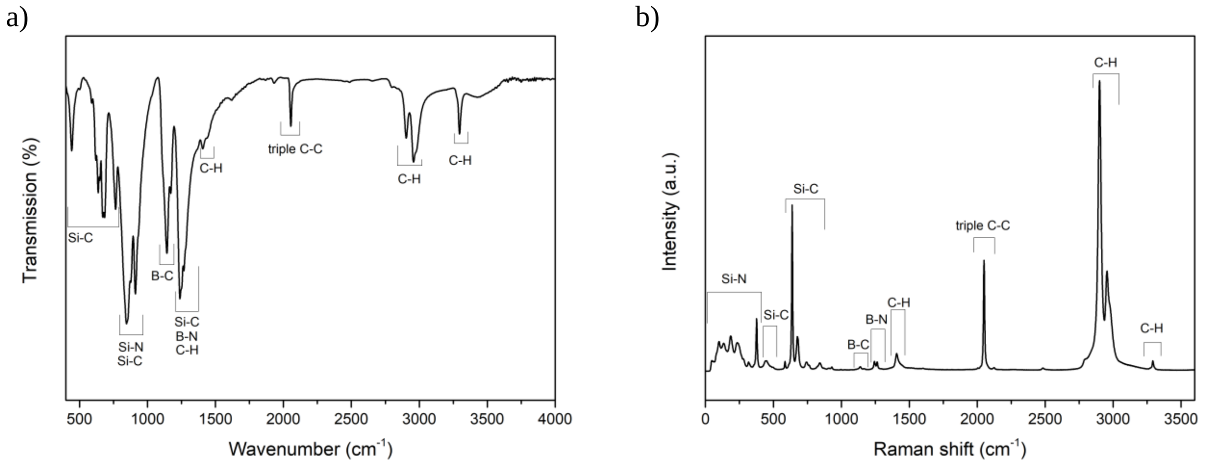

Figure S3. (a) FTIR and (b) Raman spectra of $HC\equiv CB[N(SiMe_3)_2]_2$

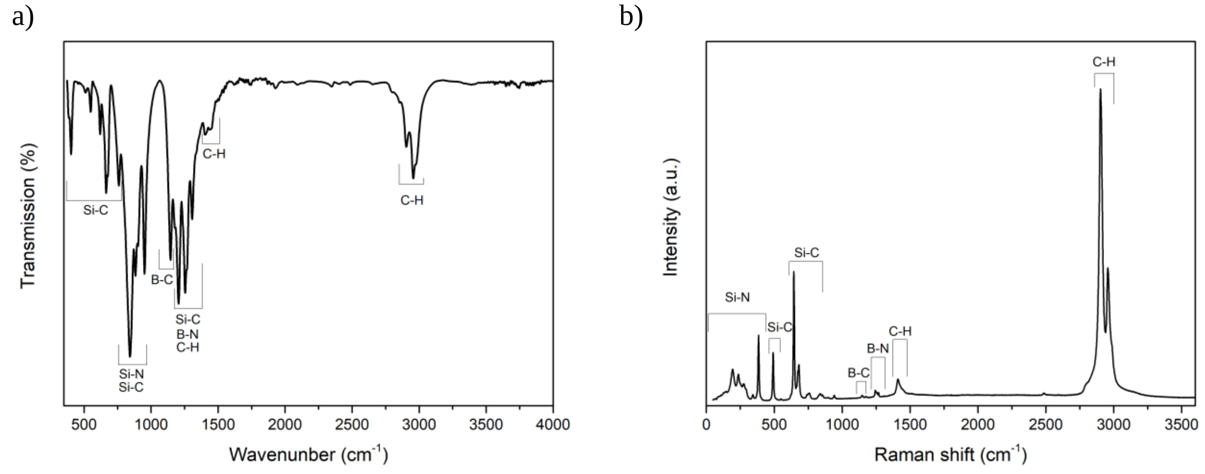

Figure S4. (a) FTIR and (b) Raman spectra of $MeB[N(SiMe_3)_2]_2$

Table S7. Experimental and calculated IR wavenumbers of the most intense bands of TSABA

Experimental IR wavenumber, cm^{-1}	Calculated IR wavenumber, cm^{-1}	Calculated IR intensity, a.u.	Assignment
2959 s	3070 - 3109	255.4	ν(C-H)
2901 s	2959 - 3068	98.9	ν(C-H)
2102 w	2149	0.2	ν(C≡C), δ(N-B-N)
1408 m	1412	8.9	δ(H-C-H)
1252 s	1250	799.6	ν(B-N), δ(C-B-N), δ(H-C-H), δ(Si-N-Si)
	1207 - 1230	350.4	δ(H-C-H), ν(Si-C in Si-CH$_3$)
1175 s	1176	583.3	ν(C-B), ν(B-N), ν(Si-C≡), ν(Si-N), δ(Si-N-B)
943 m	956	75.2	δ(N-B-N), ν(C-B), ν(Si-C≡), δ(Si-C-H), δ(Si-N-Si), δ(Si-N-B)
910 s	906	445.0	ν(N-Si), δ(Si-N-B), ν(C-B), ν(Si-C≡),
889 s	884	153.8	ν(Si-N), δ(N-B-N), ν(C-B), δ(Si-C-H), ν(Si-C), δ(Si-N-B)
849 s	843	602.0	δ(Si-C-H), ν(Si-C in Si-CH$_3$)
	840	485.1	δ(Si-C-H), ν(Si-C≡)
762 s	747	32.2	δ(Si-C-H), ν(Si-C in Si-CH$_3$)
	745	33.8	
667 s	670	10.4	ν(Si-C), δ(Si-C-H)
	655	15.3	δ(Si-C-H), ν(Si-C in Si-CH$_3$)
	649	17.3	ν(Si-C), δ(Si-C-H)
	646	16.0	δ(Si-C-H), δ(N-B-C), δ(C≡C-B)
619 m	615	4.3	ν(Si-C), ν(B-C)
592 w	597	3.8	ν(Si-C in Si-CH$_3$), δ(C≡C-B), δ(Si-N-Si)
577 w	579	0.8	ν(Si-C in Si-CH$_3$), δ(C≡C-B), δ(N-B-C)
465 m	463	18.7	δ(C≡C-B), δ(C≡C-Si), δ(Si-N-B)
388 m	393	27.6	δ(Si-N-B), δ(C-Si-C)
	388	5.5	δ(C≡C-Si), δ(Si-C-H)

Table S8. Experimental and calculated Raman wavenumbers of the most intense bands of TSABA

Experimental Raman wavenumber, cm^{-1}	Calculated Raman wavenumber, cm^{-1}	Calculated Raman intensity, a.u.	Assignment
2963 m	3051 - 3109	2248.8	ν(C-H)
2901 s	2959 - 2972	2411.4	ν(C-H)
2125 s	2149	998.7	ν(C≡C), δ(N-B-N)
1411 w	1370 - 1412	304.1	δ(H-C-H)
1261w	1250	2.7	ν(B-N), δ(C-B-N), δ(H-C-H), δ(Si-N-Si)
1252 w	1207 - 1230	24.4	δ(H-C-H), ν(Si-C in Si-CH$_3$)

1175 w	1176	46.3	ν(C-B), ν(B-N), ν(Si-C≡), ν(Si-N), δ(Si-N-B)
843 w	840	3.2	δ(Si-C-H), ν(Si-C≡)
	834	7.8	δ(Si-C-H), ν(Si-C)
761 w	740	3.8	δ(Si-C-H), ν(Si-C in Si-CH$_3$)
	730	3.4	δ(Si-C-H)
683 m	677	10.3	δ(Si-C-H), ν(Si-C)
638 s	649	3.2	ν(Si-C), δ(Si-C-H)
593 w	597	2.4	ν(Si-C in Si-CH$_3$), δ(C≡C-B), δ(Si-N-Si)
465 w	463	4.8	δ(C≡C-B), δ(C≡C-Si), δ(Si-N-B)
381 s	393	4.2	δ(Si-N-B), δ(C-Si-C)
	370	5.5	δ(Si-N-Si), δ(C≡C-Si), δ(Si-C-H)
	362	9.6	δ(Si-N-Si), δ(C≡C-B), δ(C≡C-Si)
192 m	187	1.5	δ(C-Si-C), δ(Si-C-H)
108 w	110	0.9	δ(Si-N-B)