Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Second Order Nonlinear Optical Properties of Eight-Membered Centrosymmetric Cyclic Borasiloxanes

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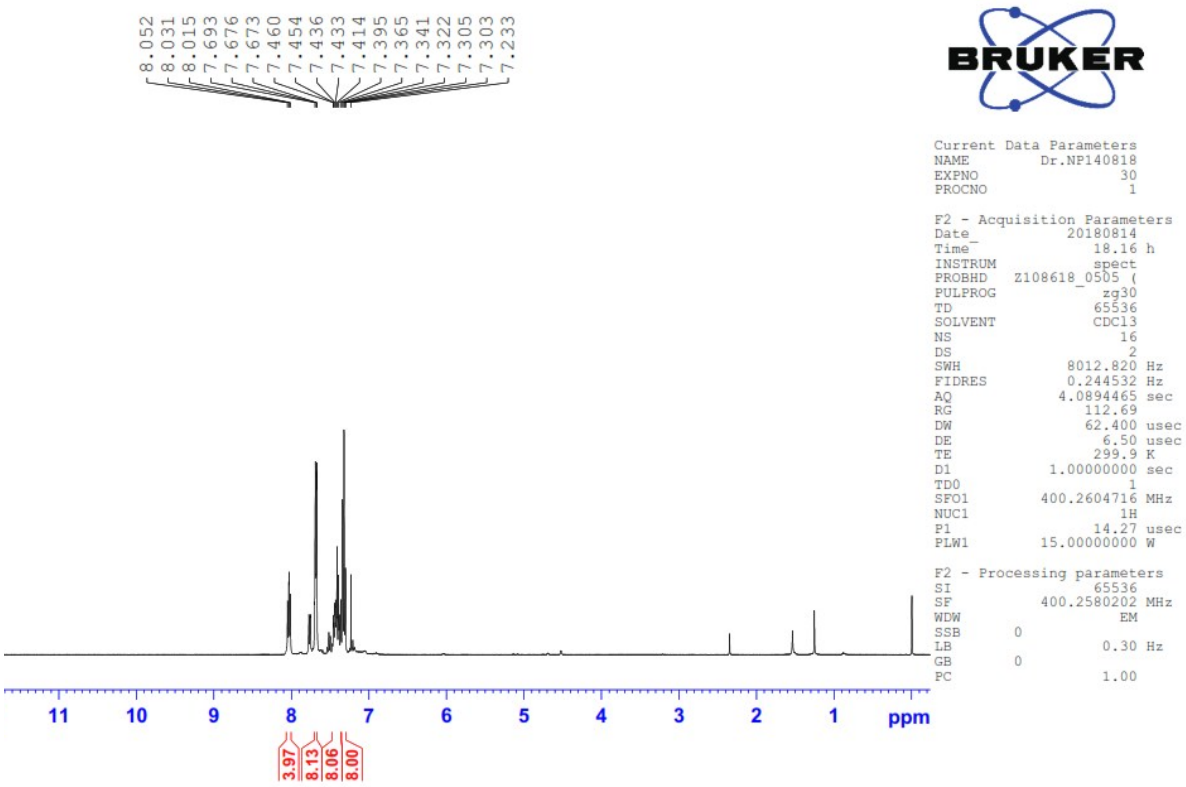


Fig. S1. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

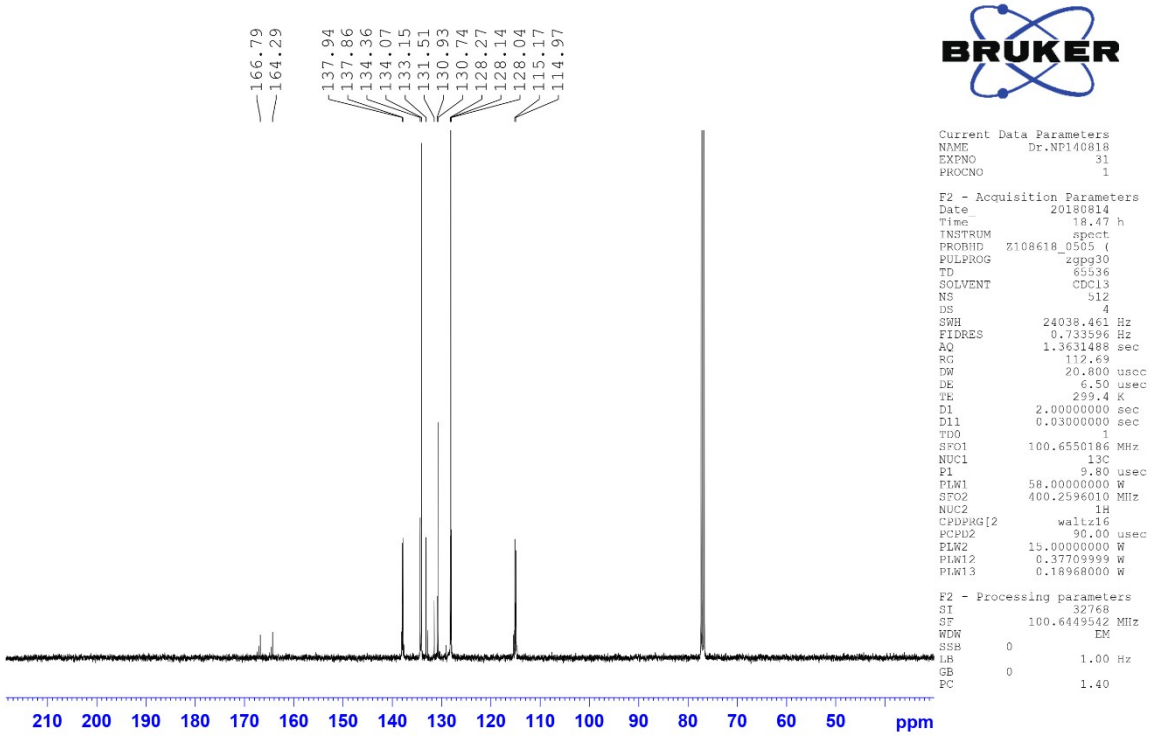


Fig. S2. ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

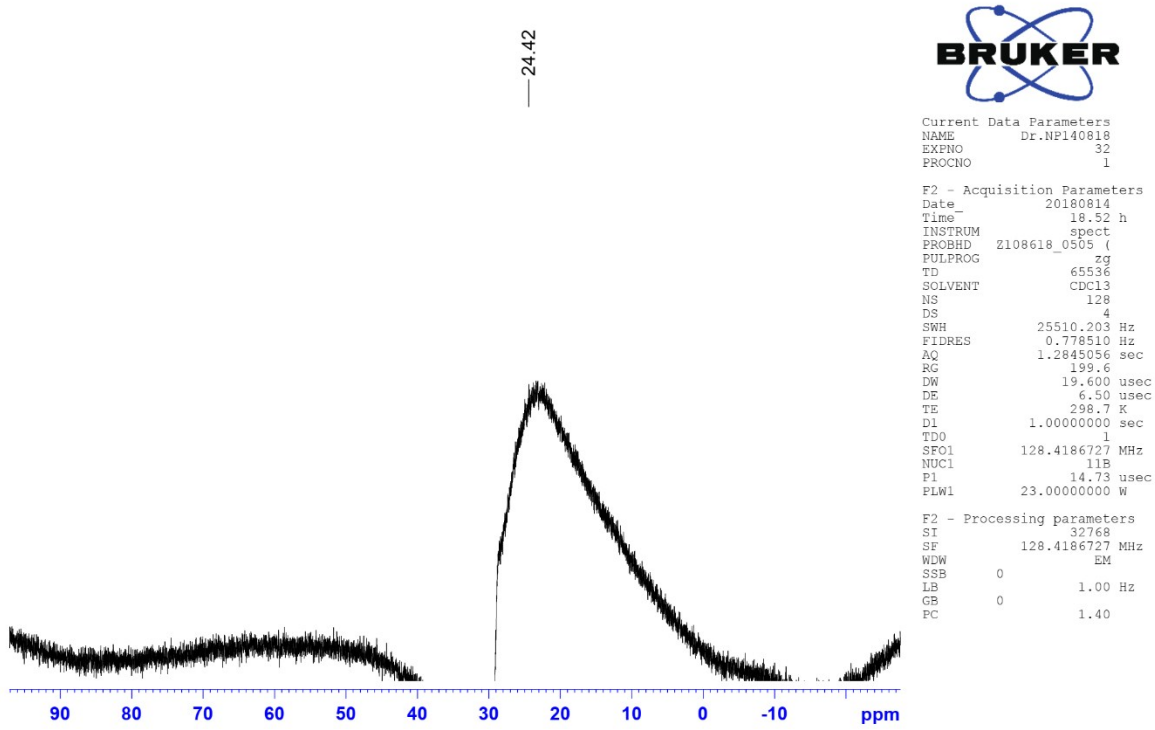


Fig. S3. ^{11}B NMR spectrum of compound **1** in $CDCl_3$.

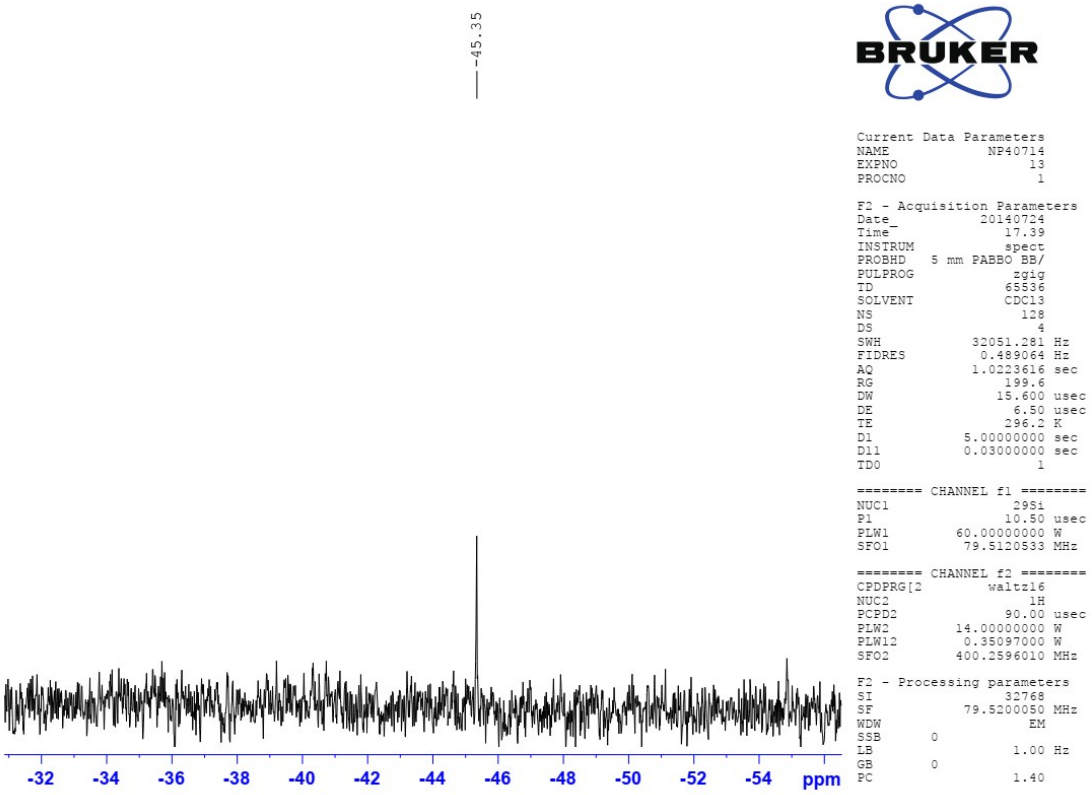


Fig. S4. ^{29}Si NMR spectrum of compound **1**in $CDCl_3$.

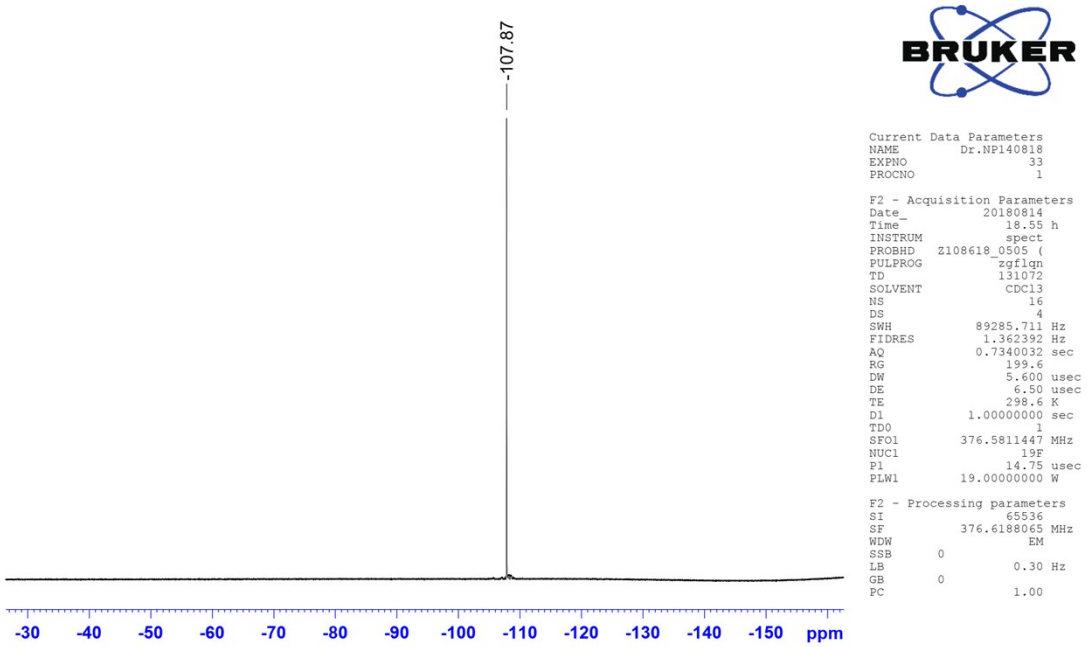


Fig. S5. ^{19}F NMR spectrum of compound **1** in $CDCl_3$. E

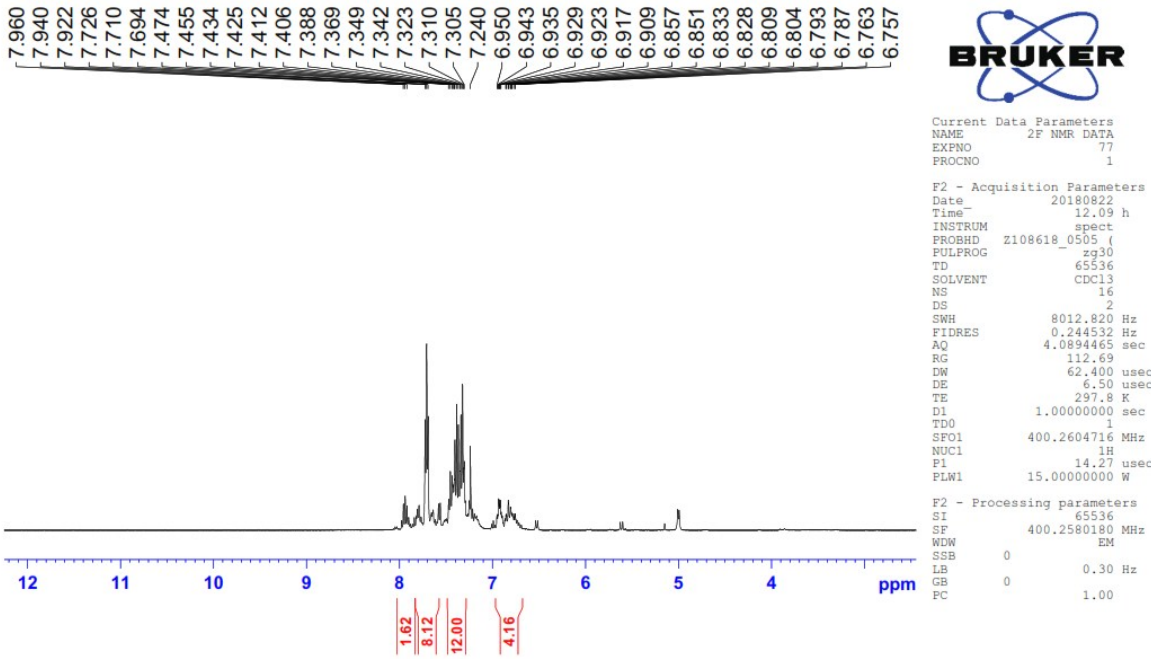
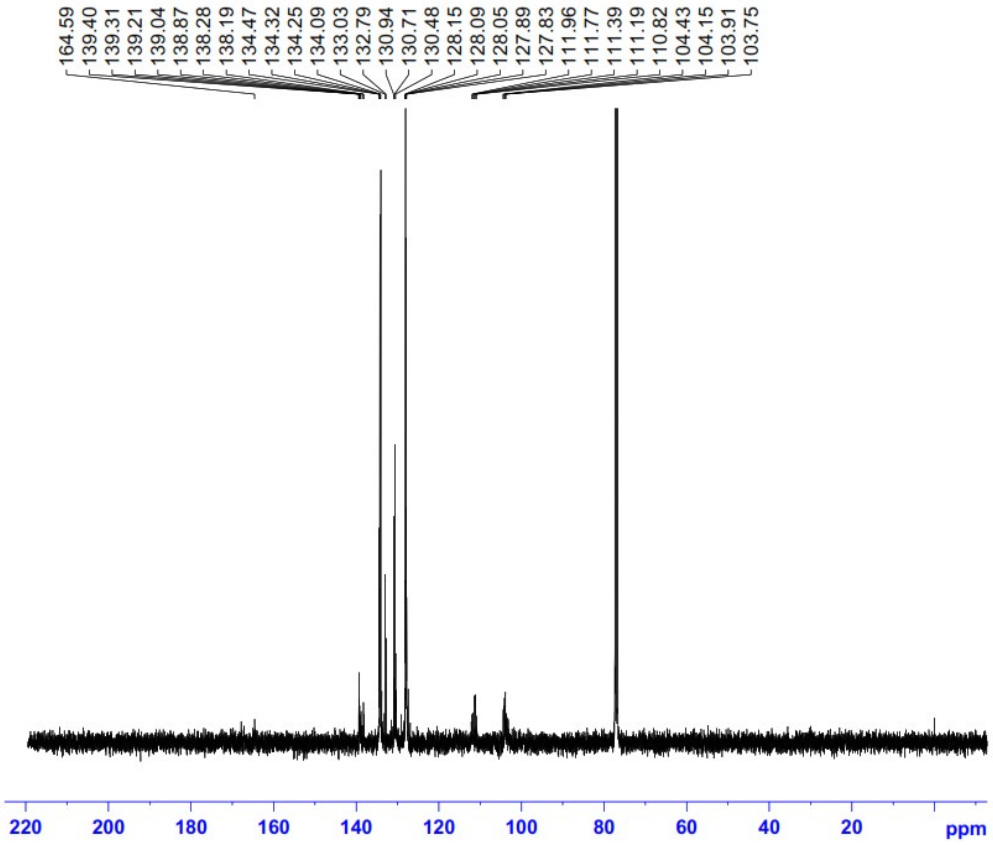


Fig. S6. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

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PROCNO                 1

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DS                    4
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FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                143.73
DW                20.800 usec
DE                 6.50 usec
TE                298.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6550186 MHz
NUC1                13C
P1                 9.80 usec
PLW1        58.00000000 W
SFO2        400.2596010 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        15.00000000 W
PLW12        0.37709999 W
PLW13        0.18968000 W

F2 - Processing parameters
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LB                 1.00 Hz
GB        0
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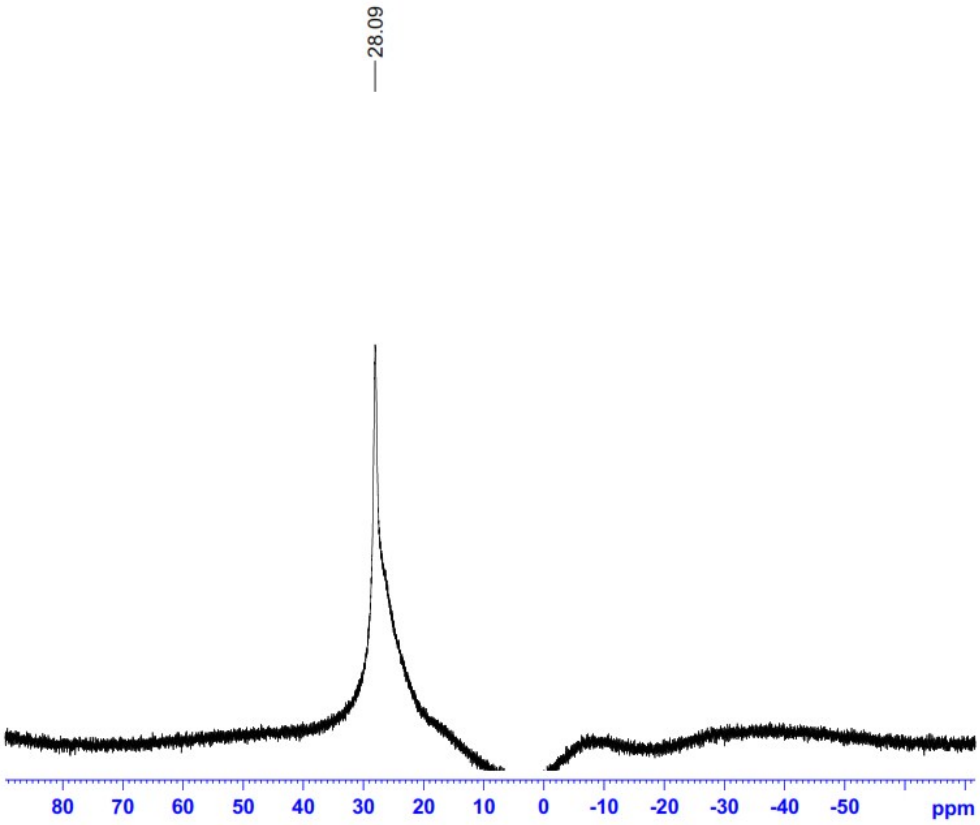
Fig. S7. ^{13}C NMR spectrum of compound **2** in $CDCl_3$.

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DS                    4
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RG                199.6
DW                19.600 usec
DE                 6.50 usec
TE                298.5 K
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TD0                   1
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NUC1                11B
P1                14.73 usec
PLW1        23.00000000 W

F2 - Processing parameters
SI                32768
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LB                 1.00 Hz
GB        0
PC                 1.40
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Fig. S8. ^{11}B NMR spectrum of compound **2** in $CDCl_3$.

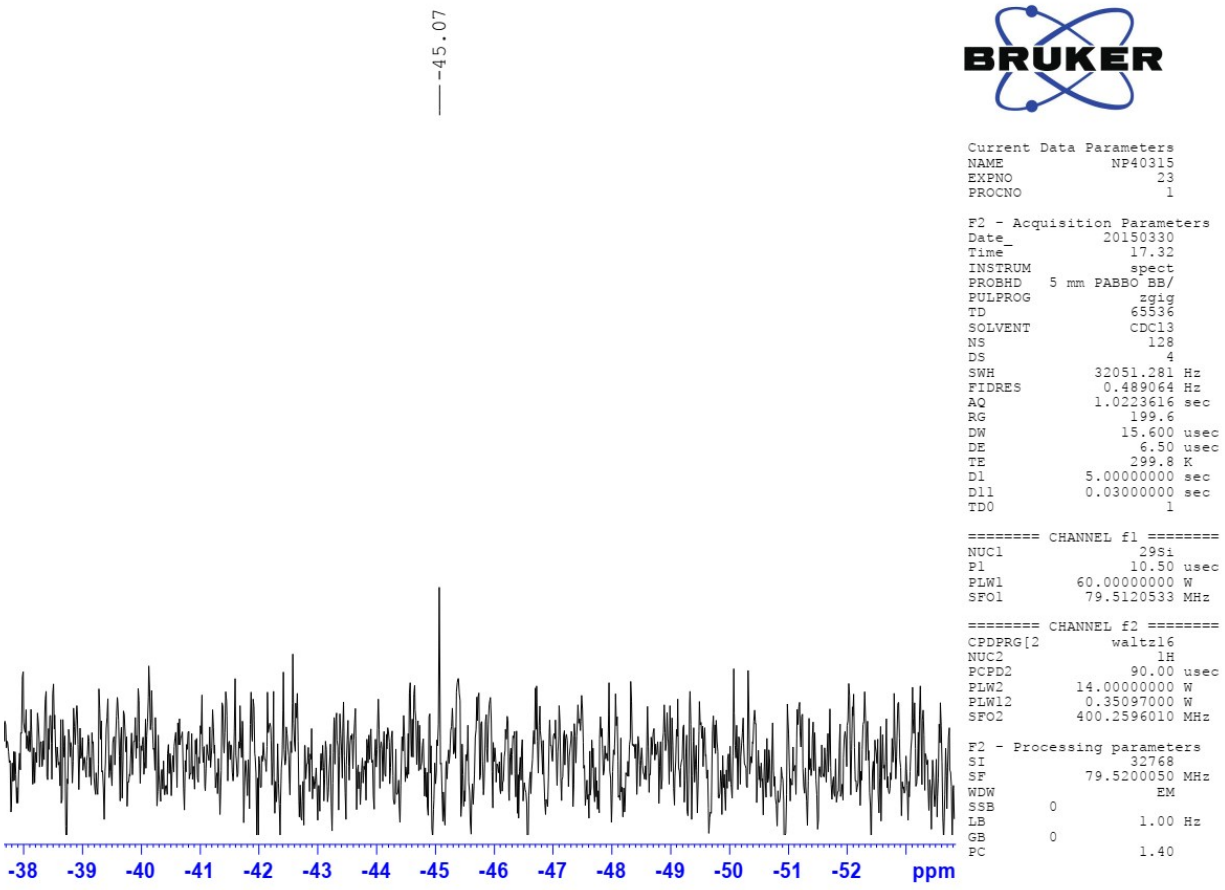


Fig. S9. ^{29}Si NMR spectrum of compound **2** in $CDCl_3$.

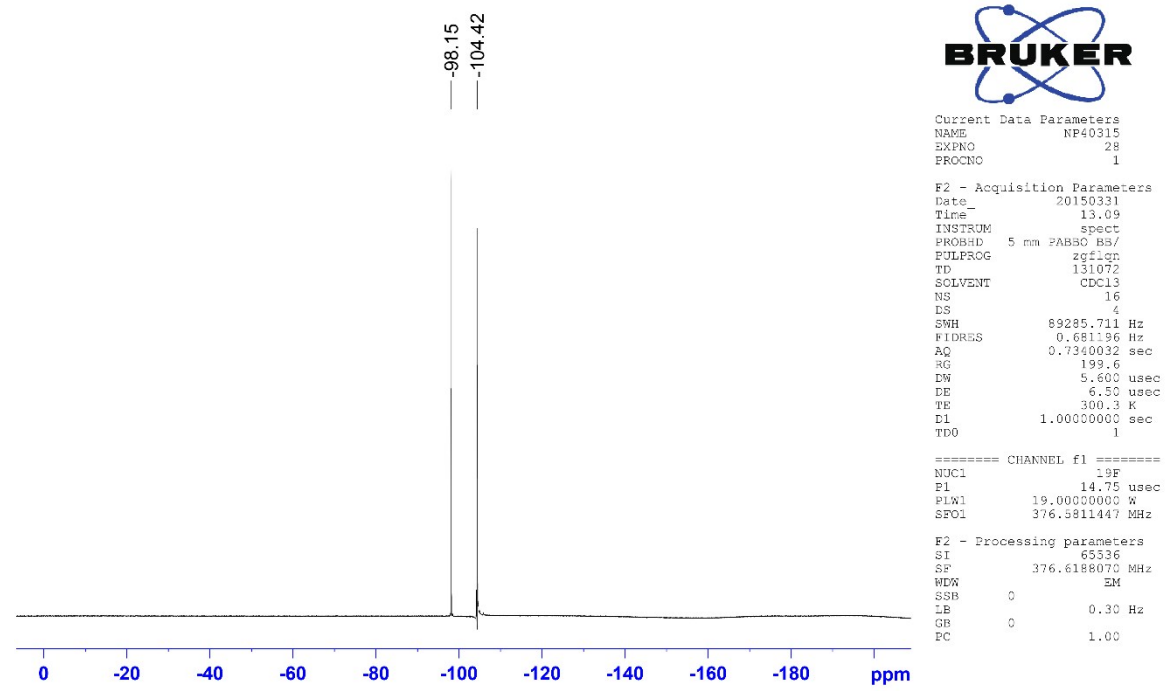


Fig. S10. ^{19}F NMR spectrum of compound **2** in $CDCl_3$

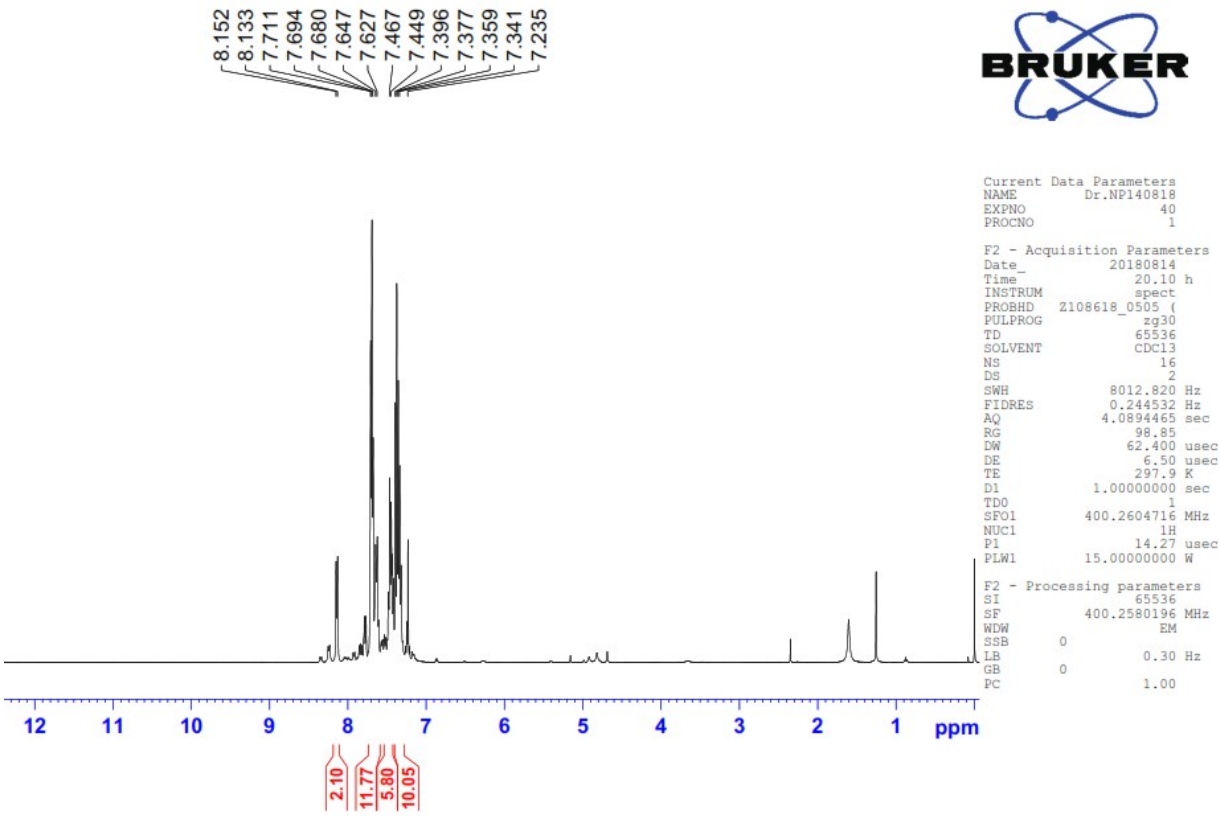


Fig. S11. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

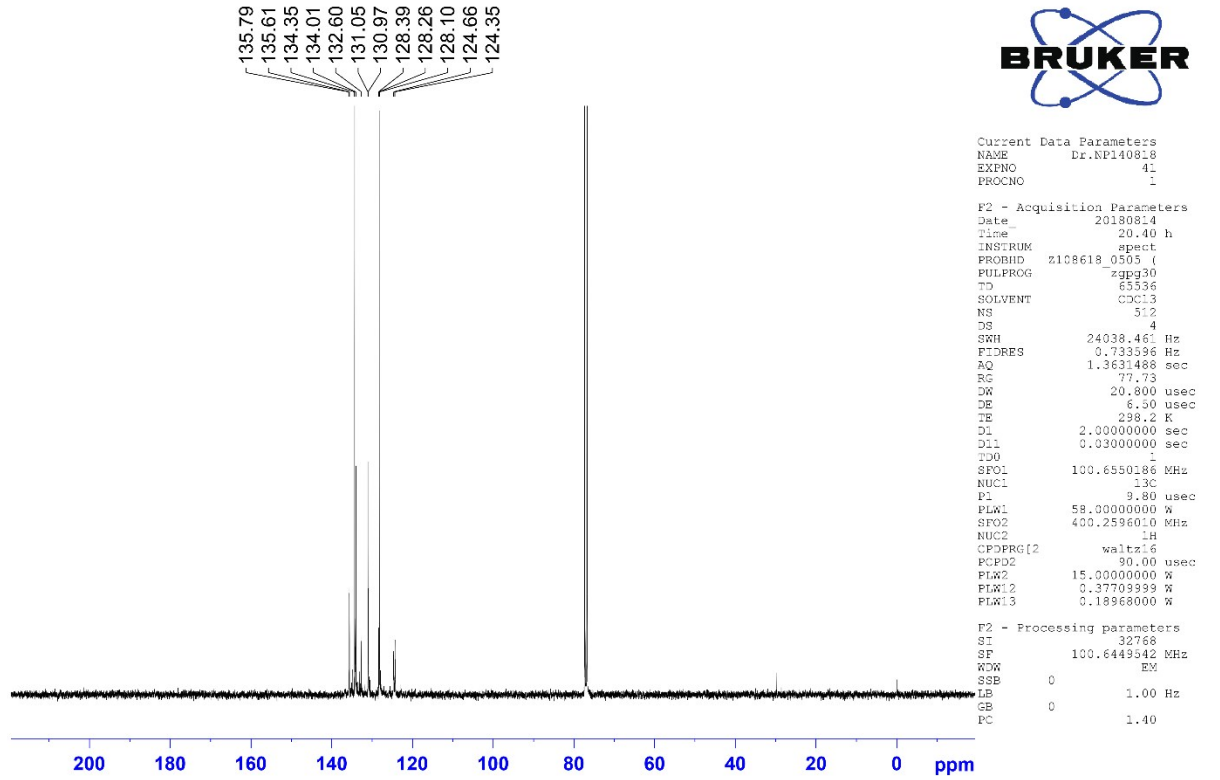


Fig. S12. ^{13}C NMR spectrum of compound **3** in $CDCl_3$**.**

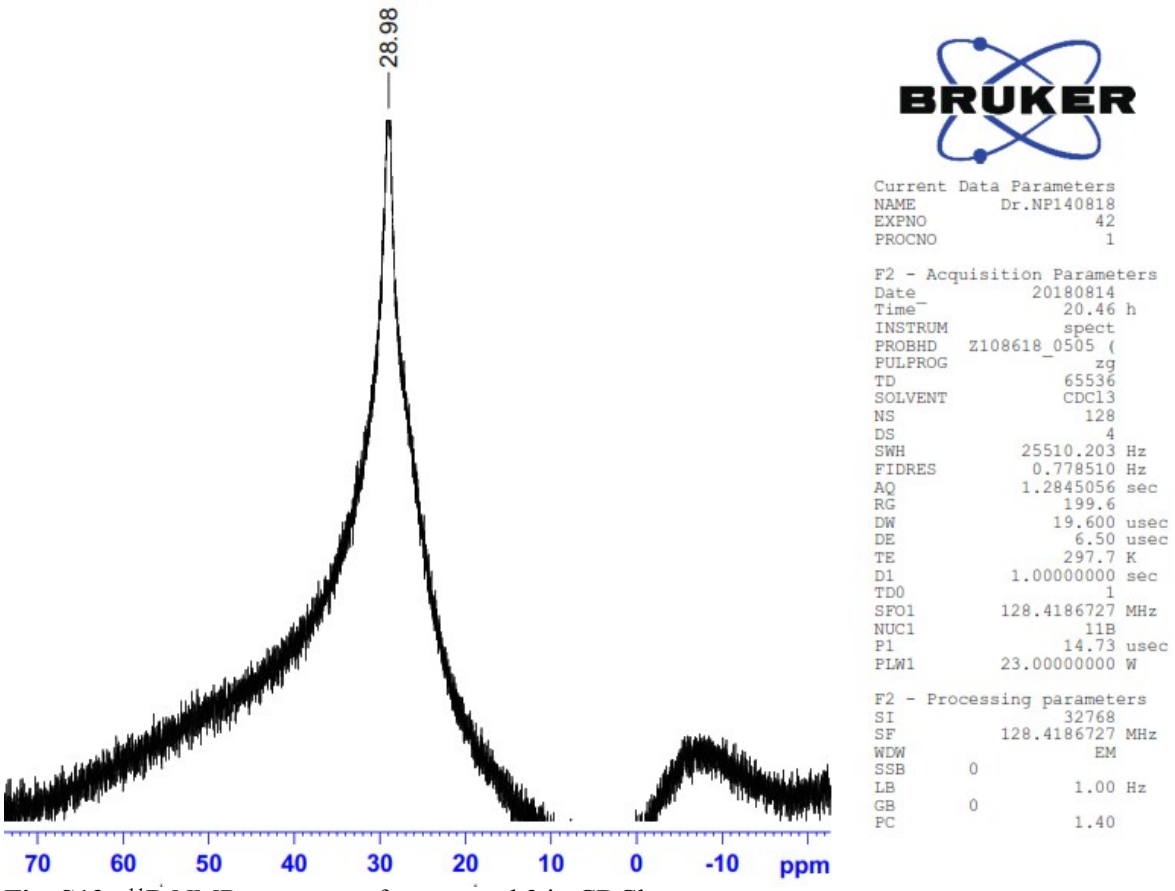


Fig. S13. ^{11}B NMR spectrum of compound **3** in $CDCl_3$.

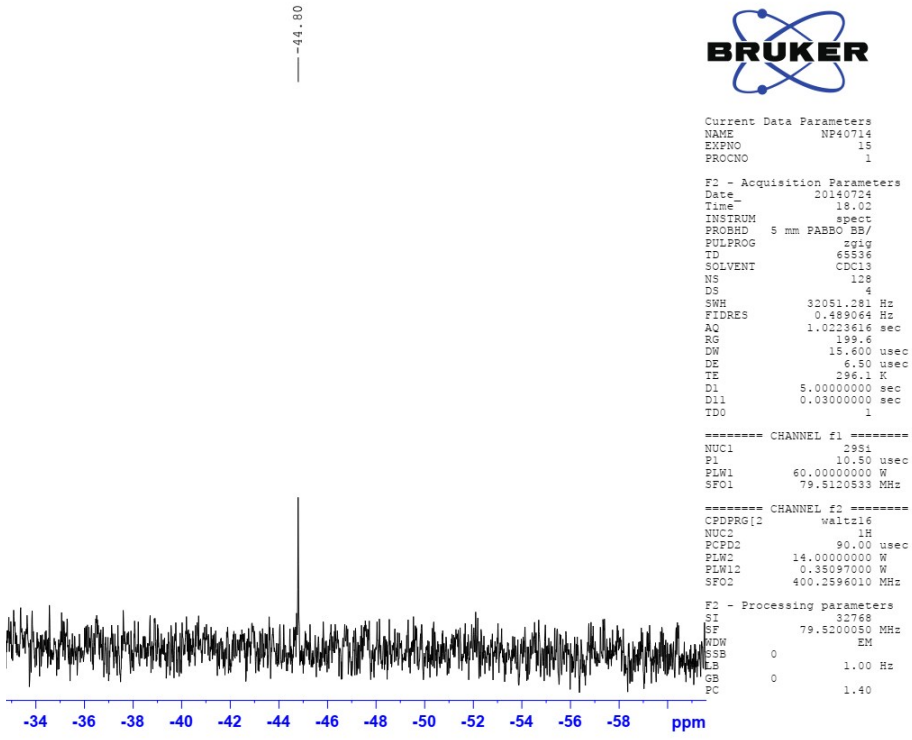


Fig. S14. ^{29}Si NMR spectrum of compound **3** in $CDCl_3$.

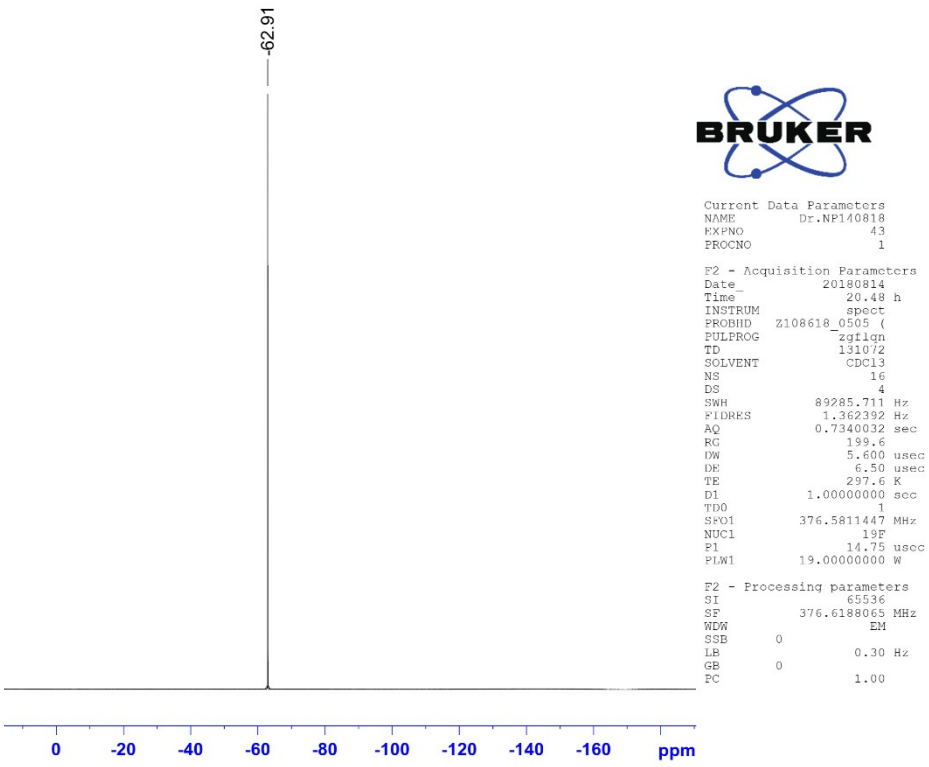


Fig. S15. ^{19}F NMR spectrum of compound **3** in $CDCl_3$.

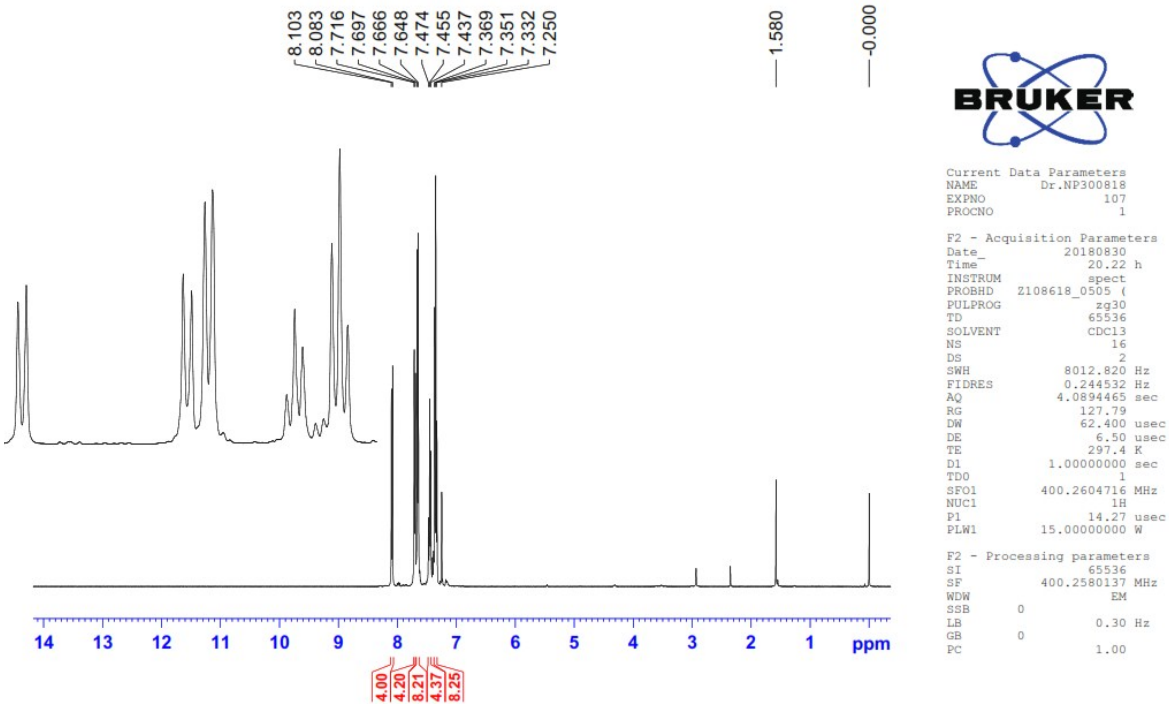


Fig. S16. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

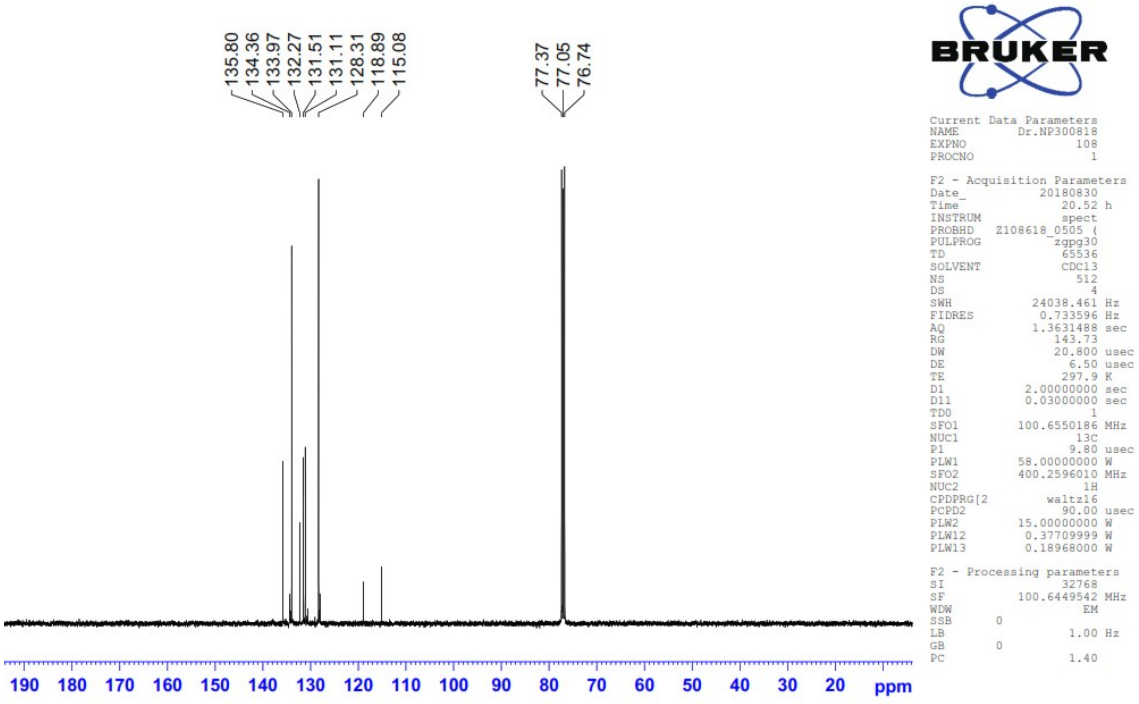


Fig. S17. ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

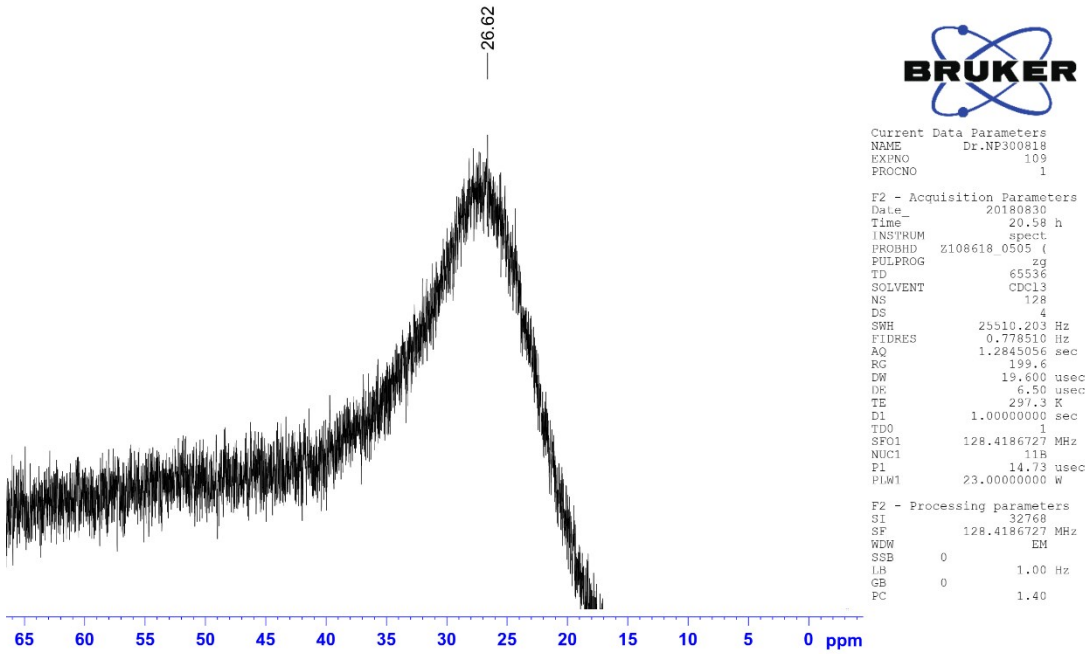
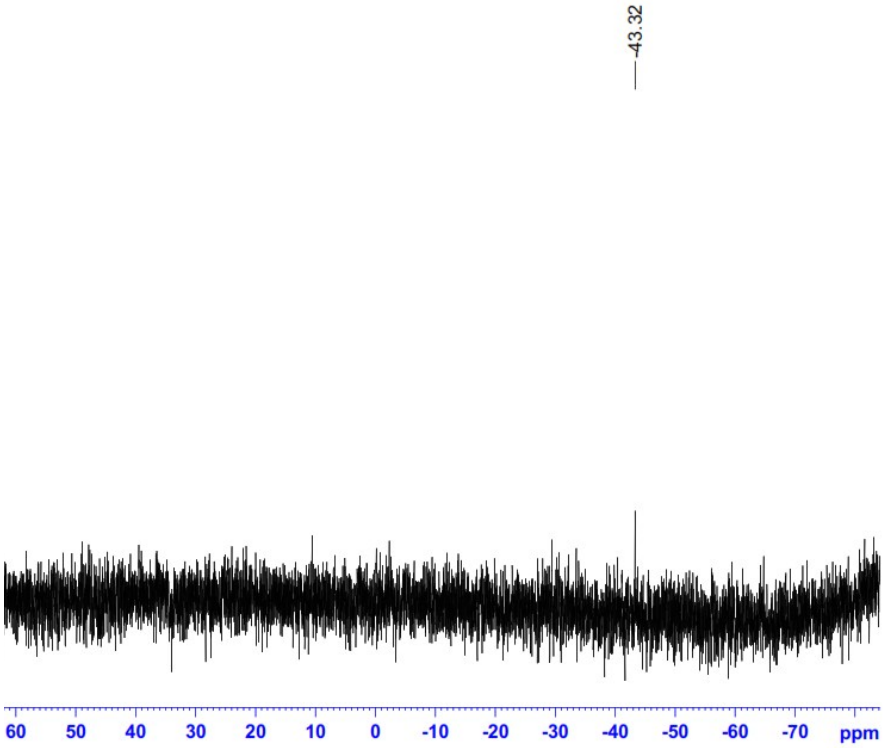


Fig. S18. ^{11}B NMR spectrum of compound **4** in $CDCl_3$.

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SOLVENT           CDCl3
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FIDRES         0.978127 Hz
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RG                199.6
DW               15.600 usec
DE                6.50 usec
TE                297.2 K
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TD0                   1
SFO1         79.5120533 MHz
NUC1                29Si
P1                10.38 usec
PLW1        60.00000000 W
SFO2        400.2596010 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        15.00000000 W
PLW12        0.37709999 W

F2 - Processing parameters
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PC                1.40
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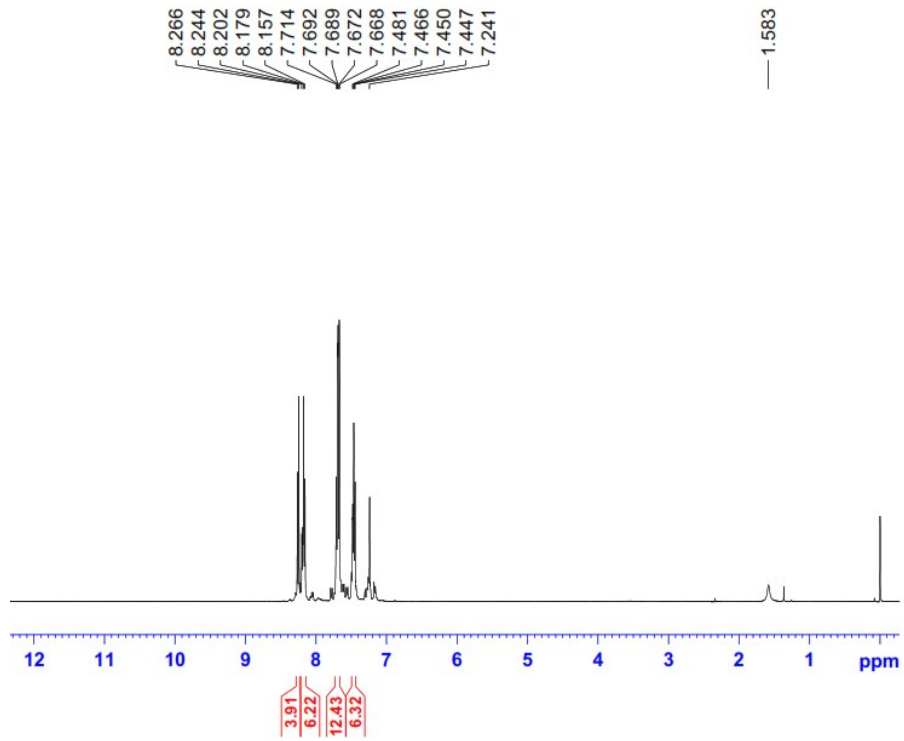
Fig. S19. ^{29}Si NMR spectrum of compound **4** in $CDCl_3$.

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SOLVENT           CDCl3
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DS                    2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                 98.85
DW               62.400 usec
DE                6.50 usec
TE                299.3 K
D1           1.00000000 sec
TD0                   1
SFO1        400.2604716 MHz
NUC1                1H
P1                14.27 usec
PLW1        15.00000000 W

F2 - Processing parameters
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SF          400.2580172 MHz
WDW                  EM
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LB                0.30 Hz
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Fig. S20. ^{1}H NMR spectrum of compound **5** in $CDCl_3$.

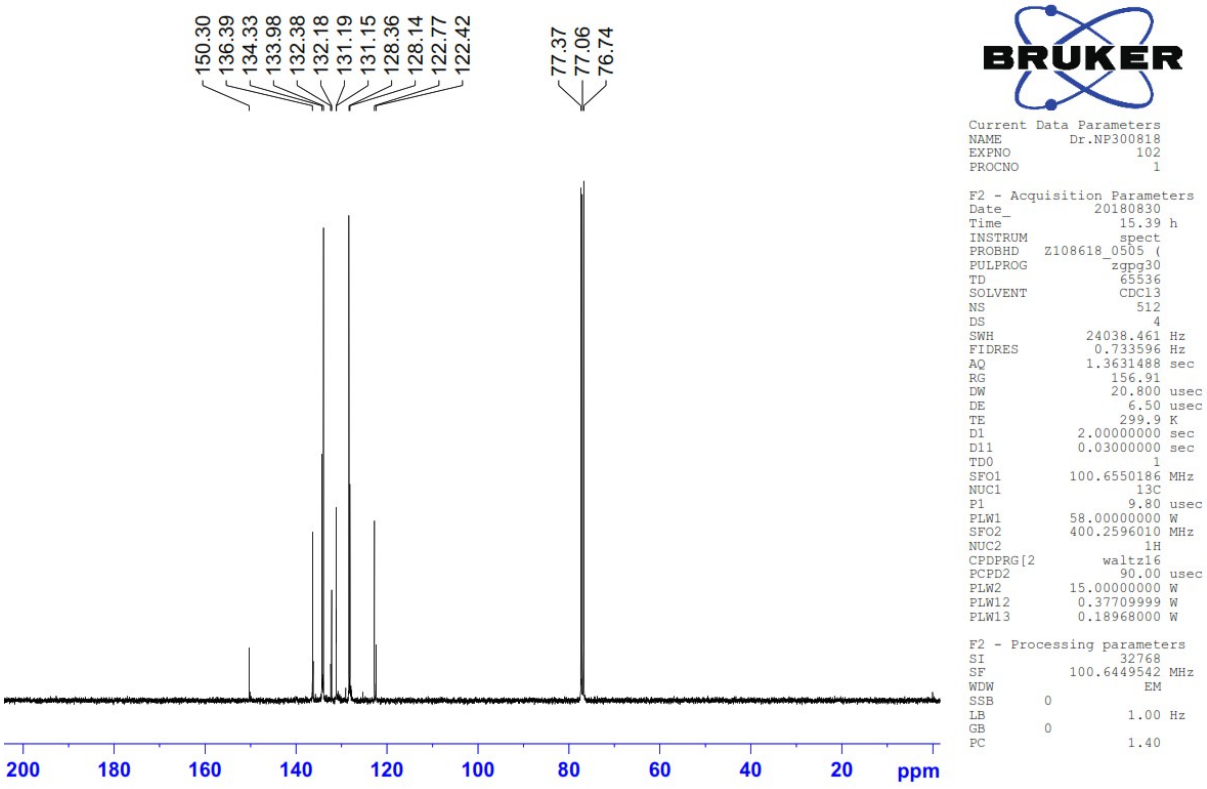


Fig. S21. ^{13}C NMR spectrum of compound **5** in $CDCl_3$.

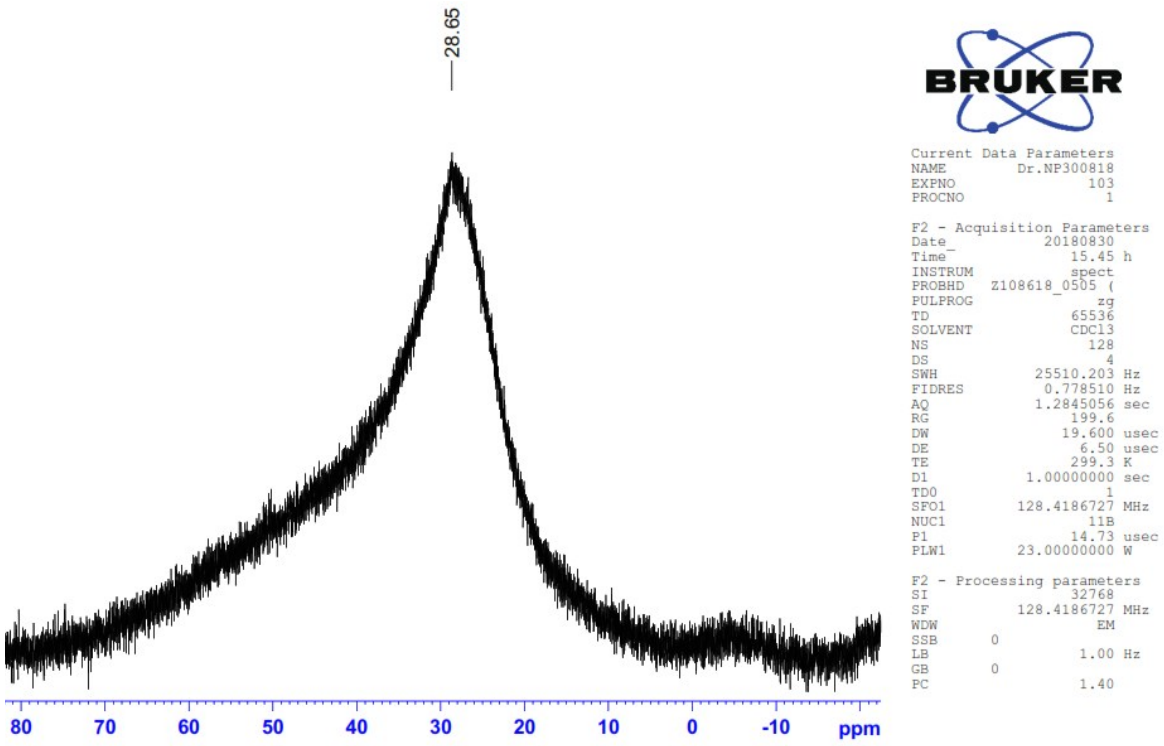


Fig. S22. ^{11}B NMR spectrum of compound **5** in $CDCl_3$.

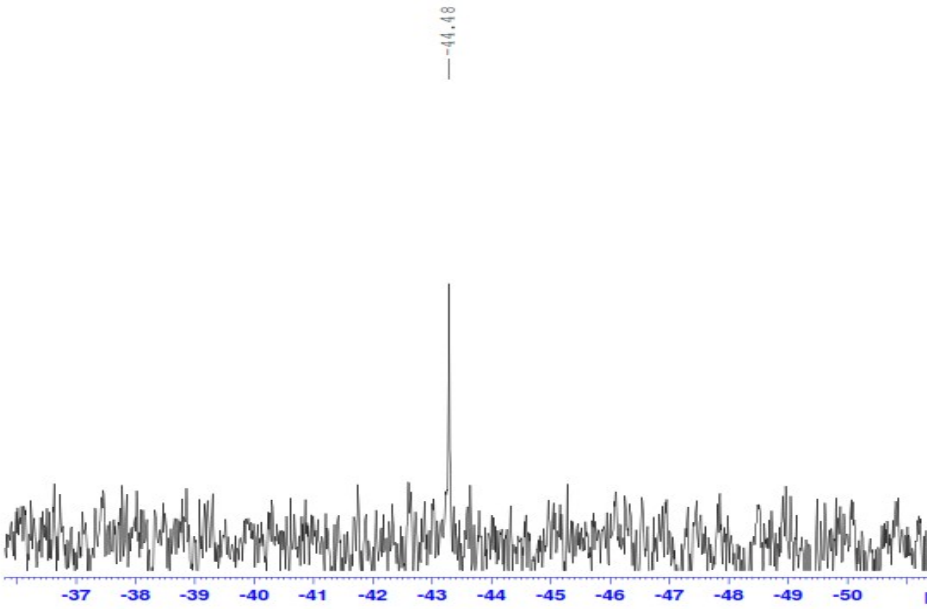
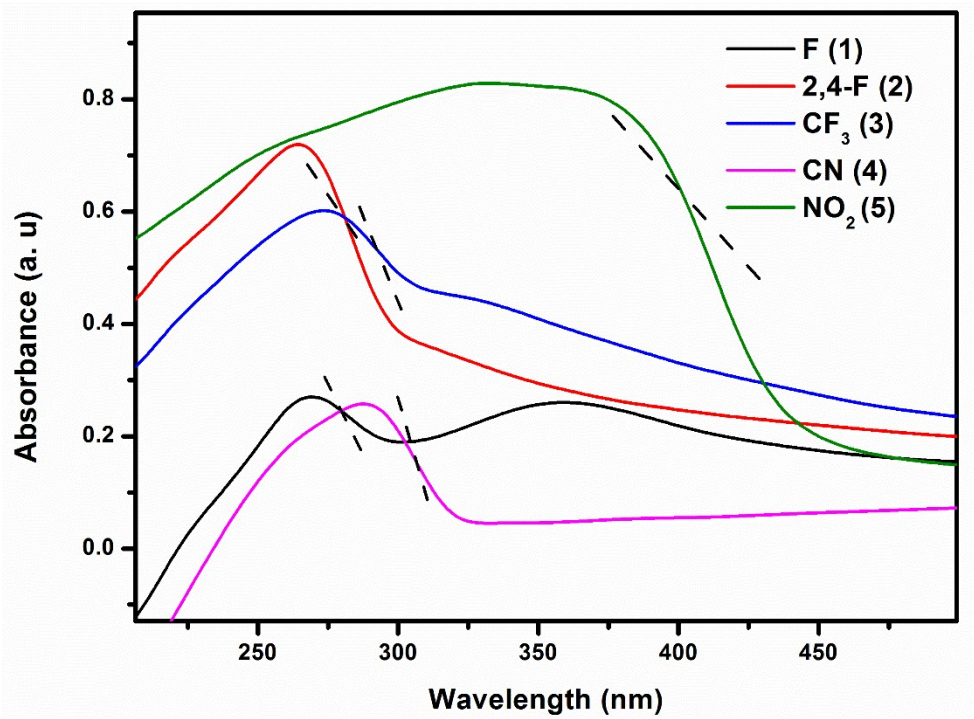


Fig. S23. ^{29}Si NMR spectrum of compound **5** in $CDCl_3$.



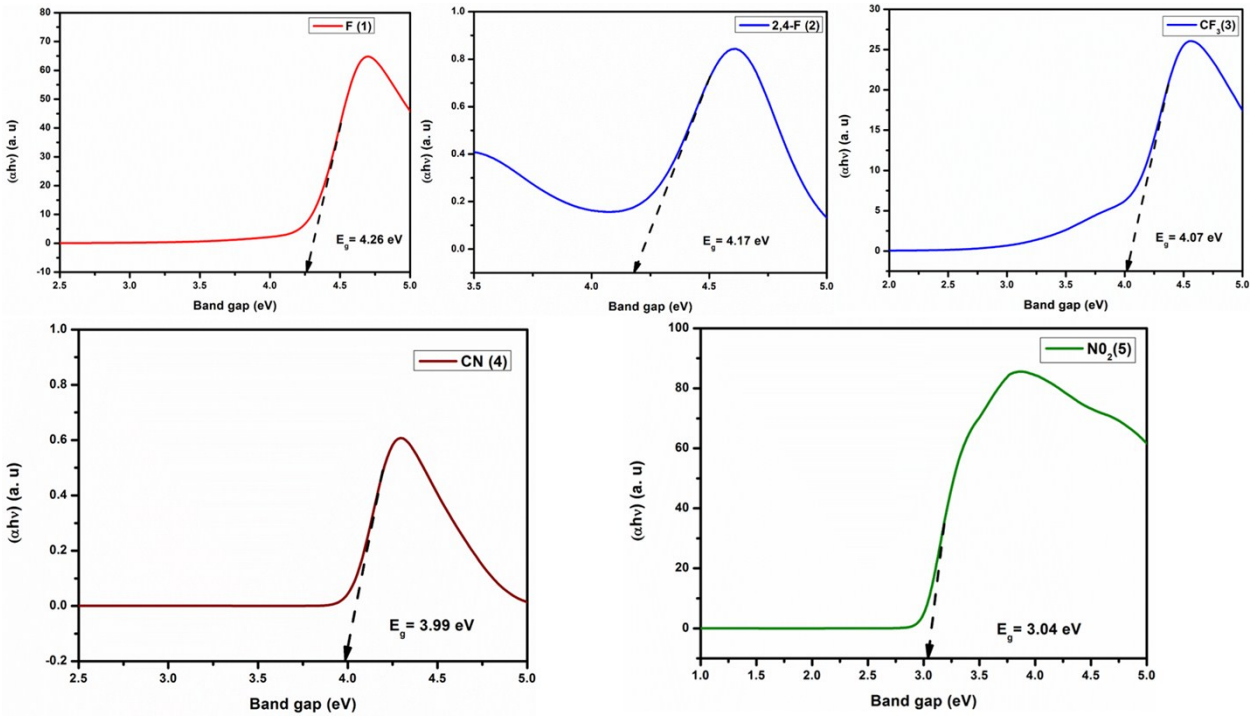


Fig. S24. UV-visible transmission spectra of borasiloxanes **1-5** and Tauc plot of (αhν) *versus* Photon energy (hν) for borasiloxanes **1-5.**

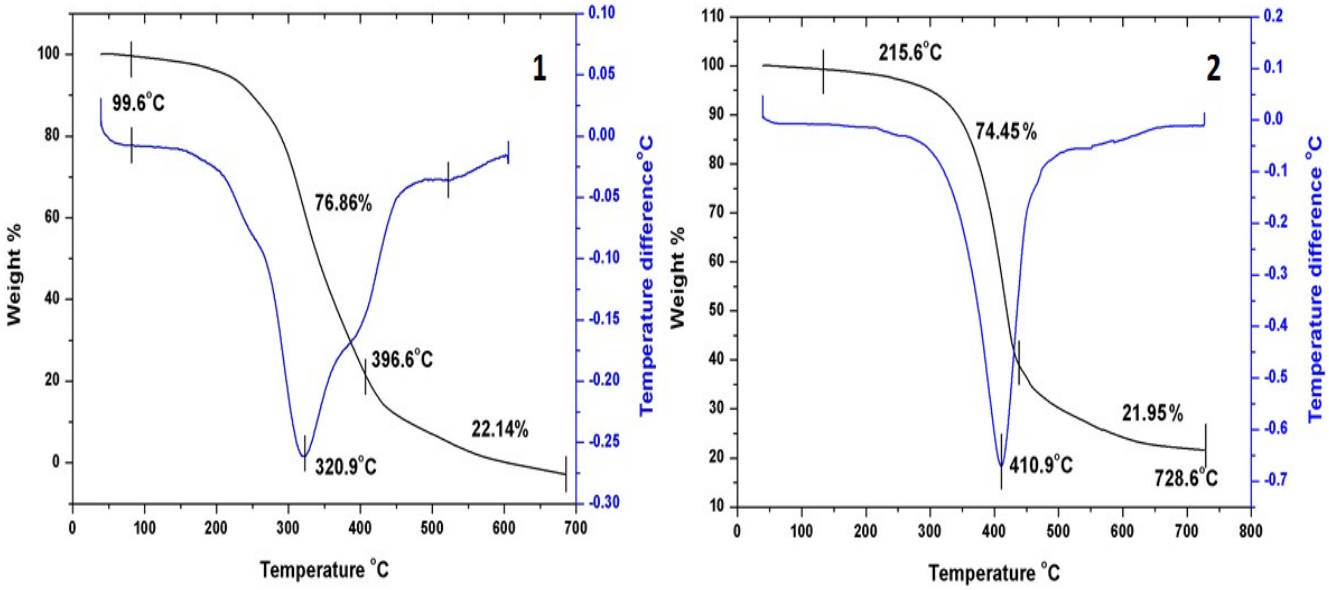


Fig. 25. TGA/DTG spectrum of borasiloxanes **4** and **5**.

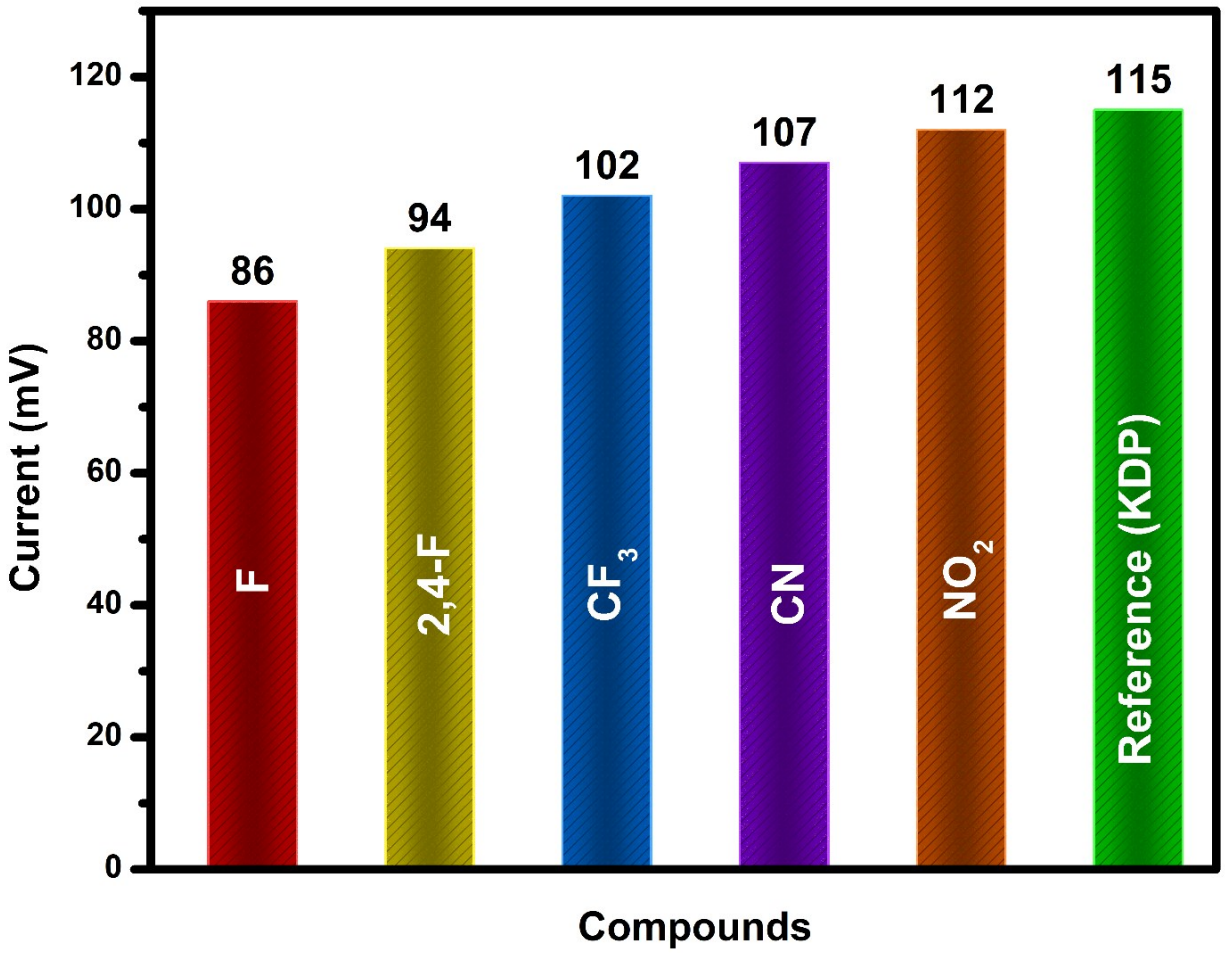


Fig. 26. Second harmonic generation (SHG) efficiency of borasiloxanes **1-5.**

Table. S1. Crystallographic data for the compounds **1- 5.**

	Compound-1	**Compound-2**	**Compound-3**	**Compound-4**	**Compound-5**
Empirical formula	C36 H28 B2 F2 O4 Si2	C36 H26 B2 F4 O4 Si2	C38 H28 B2 F6 O4 Si2	C38 H28 B2 N2 O4 Si2	C36 H28 B2 N2 O8 Si2
Formula weight	640.38	676.37	740.40	654.42	694.40
Temperature	150.15 K	150.15 K	150.15 K	150.15 K	150.15 K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	P-1	P-1	P 1 21/n 1	P-1	P-1
Unit cell dimensions	a = 8.543(3) Å	a = 8.562(3) Å	a = 12.184(3) Å	a = 8.287(2) Å	a = 8.030(3) Å
	b = 9.812(3) Å	b = 9.842(3) Å	b = 7.791(2) Å	b = 10.295(3) Å	b = 10.958(4) Å
	c = 11.326(4) Å	c = 11.327(4) Å	c = 18.420(5) Å	c = 11.708(3) Å	c = 11.633(5) Å
Volume	819.1(5) $Å^3$	821.8(4) $Å^3$	1724.4(8) $Å^3$	869.3(4) $Å^3$	870.2(6) $Å^3$
Z	1	1	2	1	1
Density (calculated)	1.298 Mg/m^3	1.367 Mg/m^3	1.426 Mg/m^3	1.250 Mg/m^3	1.325 Mg/m^3
Absorption coefficient	0.158 mm^{-1}	0.170 mm^{-1}	0.177 mm^{-1}	0.145 mm^{-1}	0.157 mm^{-1}
F(000)	332	348	760	340	360
Crystal size	0.57 x 0.56 x 0.56 mm^3	0.54 x 0.54 x 0.52 mm^3	0.46 x 0.27 x 0.13 mm^3	0.58 x 0.32 x 0.2 mm^3	0.3 x 0.21 x 0.12 mm^3
Theta range for data collection	2.083 to 27.482°.	2.088 to 27.530°.	1.871 to 27.500°.	1.980 to 27.588°.	2.051 to 27.520°.

Index ranges	-11<=h<=11, -12<=k<=12, -14<=l<=14	-11<=h<=11, -12<=k<=12, -14<=l<=14	-15<=h<=15, -10<=k<=9, -23<=l<=23	-10<=h<=10, -13<=k<=13, -14<=l<=15	-10<=h<=10, -14<=k<=14, -15<=l<=15
Reflections collected	9545	9465	16295	9085	16230
Independent reflections	3690 [R(int) = 0.0370]	3702 [R(int) = 0.0505]	3898 [R(int) = 0.0353]	3923 [R(int) = 0.0488]	3960 [R(int) = 0.0265]
Completeness to theta = 25.242°	99.5 %	99.6 %	99.6 %	99.4 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7455 and 0.5812	0.7456 and 0.5003	0.7456 and 0.6545	0.7456 and 0.5347	0.7456 and 0.6849
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3690 / 0 / 208	3702 / 0 / 227	3898 / 0 / 235	3923 / 0 / 217	3960 / 0 / 226
Goodness-of-fit on F^2	1.046	1.029	1.035	1.043	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0383, wR2 = 0.1001	R1 = 0.0408, wR2 = 0.1094	R1 = 0.0414, wR2 = 0.1015	R1 = 0.0412, wR2 = 0.1035	R1 = 0.0328, wR2 = 0.0872
R indices (all data)	R1 = 0.0460, wR2 = 0.1053	R1 = 0.0470, wR2 = 0.1153	R1 = 0.0508, wR2 = 0.1076	R1 = 0.0499, wR2 = 0.1091	R1 = 0.0360, wR2 = 0.0900
Extinction coefficient	n/a	n/a	n/a	n/a	n/a
Largest diff. peak and hole	0.407 and -0.283 e.Å^{-3}	0.445 and -0.480 e.Å^{-3}	0.456 and -0.353 e.Å^{-3}	0.483 and -0.359 e.Å^{-3}	0.347 and -0.331 e.Å^{-3}

Table. S2. Important bond length and angles of borasiloxanes **1- 5.**

Bond length									
Compound-1		**Compound-2**		**Compound-3**		**Compound-4**		**Compound-5**	
Si(1)-O(2)	1.6195(11)	Si(1)-O(1)#1	1.6248(11)	Si(1)-O(1)	1.6340(12)	Si(1)-O(1)#1	1.6234(11)	Si(1)-O(1)	1.6280(9)
Si(1)-O(1)#1	1.6229(11)	Si(1)-O(2)	1.6233(11)	Si(1)-O(2)#1	1.6348(12)	Si(1)-O(2)	1.6221(11)	Si(1)-O(2)#1	1.6197(10)
Si(1)-C(13)	1.8502(14)	Si(1)-C(7)	1.8551(16)	Si(1)-C(8)	1.8419(16)	Si(1)-C(8)	1.8507(15)	Si(1)-C(7)	1.8553(13)
Si(1)-C(7)	1.8547(17)	Si(1)-C(13)	1.8563(14)	Si(1)-C(14)	1.8594(17)	Si(1)-C(14)	1.8525(16)	Si(1)-C(13)	1.8481(13)
O(2)-B(1)	1.3592(18)	F(1A)-C(2)	1.362(4)	F(1)-C(7)	1.324(2)	O(1)-Si(1)#1	1.6234(11)	O(1)-B(1)	1.3575(15)
F(1)-C(4)	1.3609(17)	F(1)-C(6)	1.3548(19)	F(2)-C(7)	1.326(2)	O(1)-B(1)	1.3576(19)	O(2)-Si(1)#1	1.6197(10)
O(1)-Si(1)#1	1.6229(11)	F(2)-C(4)	1.3581(17)	F(3)-C(7)	1.324(2)	O(2)-B(1)	1.359(2)	O(2)-B(1)	1.3536(15)
O(1)-B(1)	1.3595(18)	O(1)-B(1)	1.3569(19)	O(1)-B(1)	1.360(2)	N(1)-C(7)	1.139(2)	O(3)-N(1)	1.2231(14)
C(1)-C(6)	1.394(2)	O(2)-B(1)	1.3617(19)	O(2)-Si(1)#1	1.6348(12)	C(1)-C(2)	1.395(2)	O(4)-N(1)	1.2254(15)
C(1)-C(2)	1.396(2)	C(1)-B(1)	1.564(2)	O(2)-B(1)	1.363(2)	C(4)-C(7)	1.444(2)	N(1)-C(4)	1.4691(15)
C(1)-B(1)	1.558(2)	Si(1)-O(2)	1.6233(11)	C(1)-B(1)	1.563(2)	C(1)-B(1)	1.563(2)	C(1)-B(1)	1.5669(17)
Bond angle									
O(2)-Si(1)-O(1)#1	113.12(6)	O(1)#1-Si(1)-C(7)	109.27(7)	O(1)-Si(1)-O(2)#1	113.30(6)	O(1)#1-Si(1)-C(8)	107.90(7)	O(1)-Si(1)-C(7)	108.13(6)
O(2)-Si(1)-C(13)	108.41(6)	O(1)#1-Si(1)-C(13)	107.84(6)	O(1)-Si(1)-C(8)	107.53(7)	O(1)#1-Si(1)-C(14)	108.80(7)	O(1)-Si(1)-C(13)	108.66(6)
O(2)-Si(1)-C(7)	107.82(7)	O(2)-Si(1)-O(1)#1	112.73(6)	O(1)-Si(1)-C(14)	107.58(7)	O(2)-Si(1)-O(1)#1	113.82(6)	O(2)#1-Si(1)-O(1)	113.02(5)
O(1)#1-Si(1)-C(13)	107.57(6)	O(2)-Si(1)-C(7)	107.60(7)	O(2)#1-Si(1)-C(8)	107.83(7)	O(2)-Si(1)-C(8)	108.48(7)	O(2)#1-Si(1)-C(7)	108.56(6)

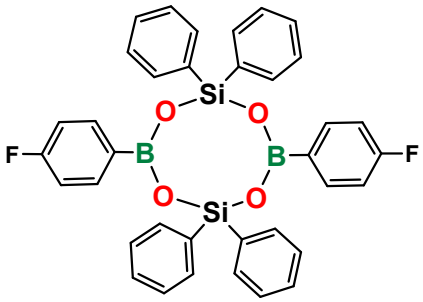
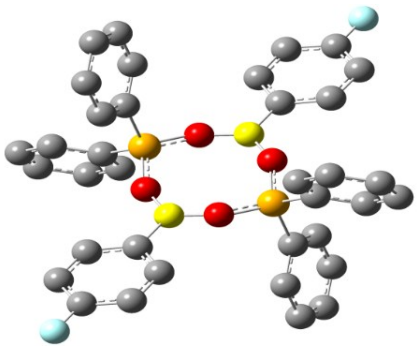
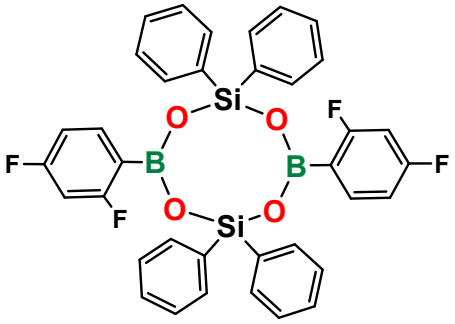
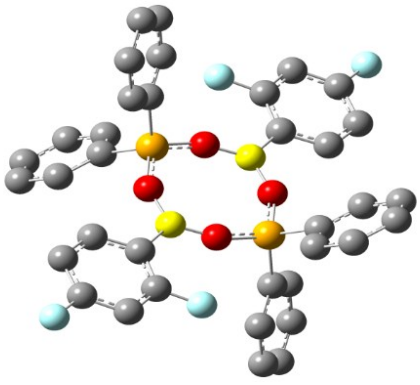
O(1)#1-Si(1)-C(7)	108.85(7)	O(2)-Si(1)-C(13)	108.18(6)	O(2)#1-Si(1)-C(14)	107.02(7)	O(2)-Si(1)-C(14)	107.36(7)	O(2)#1-Si(1)-C(13)	107.87(6)
C(13)-Si(1)-C(7)	111.10(7)	C(7)-Si(1)-C(13)	111.26(7)	C(8)-Si(1)-C(14)	113.73(7)	C(8)-Si(1)-C(14)	110.48(7)	C(13)-Si(1)-C(7)	110.61(6)
B(1)-O(2)-Si(1)	150.41(10)	B(1)-O(1)-Si(1)#1	144.42(10)	B(1)-O(1)-Si(1)	138.67(11)	B(1)-O(1)-Si(1)#1	150.07(11)	B(1)-O(1)-Si(1)	147.85(8)
B(1)-O(1)-Si(1)#1	142.64(10)	B(1)-O(2)-Si(1)	147.21(10)	B(1)-O(2)-Si(1)#1	138.23(11)	B(1)-O(2)-Si(1)	151.89(10)	B(1)-O(2)-Si(1)#1	150.29(8)
C(6)-C(1)-C(2)	117.90(13)	C(2)-C(1)-B(1)	121.04(13)	C(2)-C(1)-B(1)	121.32(14)	C(2)-C(1)-C(6)	117.95(14)	O(3)-N(1)-O(4)	123.97(11)
C(6)-C(1)-B(1)	121.10(13)	C(6)-C(1)-C(2)	115.42(13)	C(6)-C(1)-C(2)	117.78(15)	C(2)-C(1)-B(1)	121.02(13)	O(3)-N(1)-C(4)	117.88(10)
C(2)-C(1)-B(1)	120.98(13)	C(6)-C(1)-B(1)	123.53(13)	C(6)-C(1)-B(1)	120.89(14)	C(6)-C(1)-B(1)	120.98(14)	O(4)-N(1)-C(4)	118.15(1
C(13)-C(14)-H(14)	119.5	F(1A)-C(2)-C(1)	123.4(2)	C(5)-C(6)-H(6)	119.2	N(1)-C(7)-C(4)	178.0(2)	C(2)-C(1)-B(1)	120.79(11)
C(15)-C(14)-H(14)	119.5	F(1A)-C(2)-C(3)	113.0(2)	F(1)-C(7)-F(2)	105.90(17)	C(9)-C(8)-Si(1)	119.26(11)	C(6)-C(1)-B(1)	121.00(10)
C(15)-C(14)-C(13)	121.07(14)	F(2)-C(4)-C(3)	118.33(15)	F(1)-C(7)-F(3)	105.98(17)	(8)-Si(1)	122.57(11)	C(3)-C(4)-N(1)	118.65(10)
C(14)-C(13)-Si(1)	123.15(11)	F(2)-C(4)-C(5)	118.09(15)	F(1)-C(7)-C(4)	113.33(16)	C(13)-C(8)-C(9)	118.05(14)	C(5)-C(4)-N(1)	118.28(11)
C(14)-C(13)-C(18)	117.66(13)	F(1)-C(6)-C(1)	121.17(14)	F(2)-C(7)-C(4)	112.45(15)	C(15)-C(14)-Si(1)	121.67(12)	C(8)-C(7)-Si(1)	119.56(9)

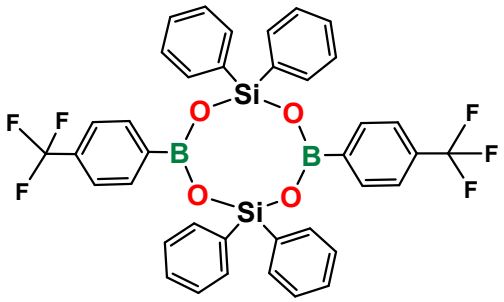
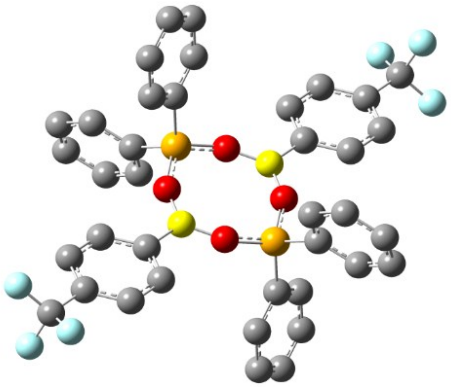
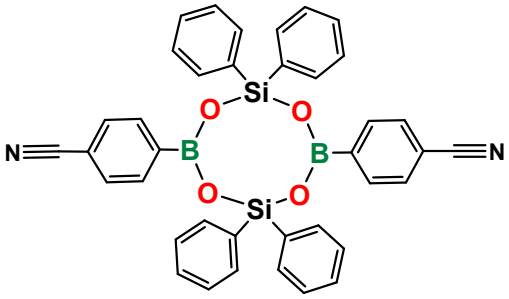
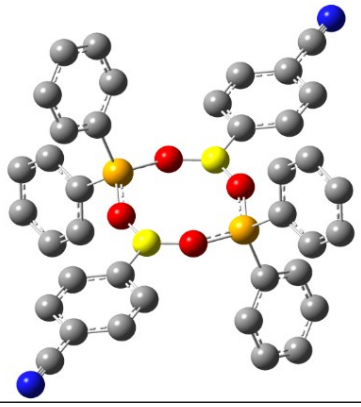
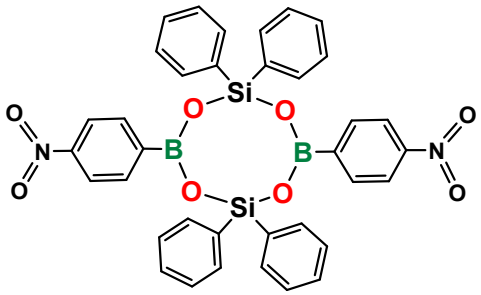
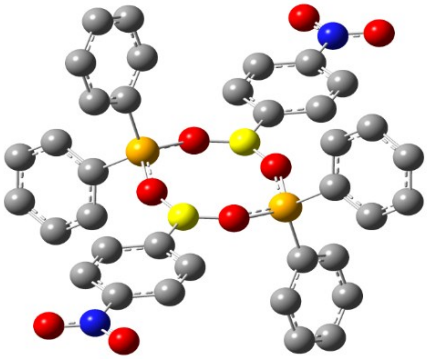
C(18)-C(13)-Si(1)	119.18(11)	F(1)-C(6)-C(5)	114.81(14)	F(3)-C(7)-F(2)	105.55(17)	C(19)-C(14)-Si(1)	120.50(12)	C(12)-C(7)-Si(1)	122.42(10)
C(12)-C(7)-Si(1)	122.33(14)	C(8)-C(7)-Si(1)	122.40(14)	F(3)-C(7)-C(4)	113.00(16)	O(1)-B(1)-O(2)	122.29(14)	C(14)-C(13)-Si(1)	122.68(9)
C(8)-C(7)-Si(1)	119.80(14)	C(12)-C(7)-Si(1)	119.32(13)	C(9)-C(8)-Si(1)	120.58(13)	O(1)-B(1)-C(1)	118.96(14)	C(18)-C(13)-Si(1)	119.22(9)
F(1)-C(4)-C(5)	118.15(15)	C(14)-C(13)-Si(1)	122.98(11)	C(13)-C(8)-Si(1)	122.08(13)	O(2)-B(1)-C(1)	118.74(13)	O(1)-B(1)-C(1)	118.48(10)
F(1)-C(4)-C(3)	118.14(14)	C(18)-C(13)-Si(1)	118.96(11)	C(15)-C(14)-Si(1)	121.26(13)			O(2)-B(1)-O(1)	123.18(11)
O(2)-B(1)-O(1)	122.17(13)	O(1)-B(1)-O(2)	121.86(13)	C(19)-C(14)-Si(1)	121.13(13)			O(2)-B(1)-C(1)	118.34(10)
O(2)-B(1)-C(1)	118.93(12)	O(1)-B(1)-C(1)	120.14(13)	O(1)-B(1)-O(2)	121.80(14)			O(1)-Si(1)-C(7)	108.13(6)
O(1)-B(1)-C(1)	118.90(13)	O(2)-B(1)-C(1)	118.00(13)	O(1)-B(1)-C(1)	119.18(14)			C(2)-C(1)-C(6)	118.21(11)
				O(2)-B(1)-C(1)	119.02(14)			C(3)-C(2)-C(1)	121.36(11)

Table S3. Boron-11 and Silicon-29 NMR Chemical Shift for borasiloxanes in $CDCl_3$ solution; UV (λ_{max}) and Emission (λ_{ex}) values of borasiloxanes **1-5.**

Compound	δ (^{11}B) ppm	δ (^{29}Si) ppm	UV-Vis (nm) ($CHCl_3$)	Solid	Fluorescence (nm) $CHCl_3$	Reference
1	24.42	-45.35	266	280	318	[5,19]
2	28.09	-45.07	258	286	322	[21]
3	28.98	-44.80	273	292	314	[21]
4	26.62	-43.32	302	305	303	[19]
5	28.65	-44.48	308	395	304	[19]

Table S4. Optimized structures of compound **1-5** at B3LYP/6-31+G** level of theory. All hydrogen atoms were omitted for clarity.

Compounds	**Structures**	**Optimized structures**
1		
E **2**		

3		
4		
5		

Electrophilicity Index of Lewis Sites

The electrophilicity index is computed by following equation.[25-27]

$$\omega = \mu^2/2\eta \quad \text{..... (1)}$$

Where μ and η are the chemical potential and chemical hardness, respectively.[27, 20d]

$$\mu = (\text{LUMO}+\text{HOMO})/2 \text{ and } \eta = (\text{LUMO}- \text{HOMO})/2$$

Where LUMO is the energy of the lowest unoccupied molecular orbital and HOMO is the energy of the highest occupied molecular orbital.

Polarizability and Hyperpolarizability

The value of the first hyperpolarizability (β), dipole moment (μ) and polarizability (α) of borasiloxanes are reported in the atomic mass units (a.u) and electrostatic unit (esu). The constituent of β are defined as the coefficients in the Taylor series expansion of the energy in the external electric field. When the external electric field is weak and homogeneous, this expansion becomes.

$$E = E^0-\mu_\alpha F_\alpha-1/2\alpha_\alpha\beta F_\alpha F_\beta-1/6\beta_\alpha\beta_\gamma F_\alpha F_\beta F_\gamma + \text{..... (2)}$$

Where E_0 is the energy of the unperturbed molecules, F_α is the field at the rigid μ_α, $\alpha_{\alpha\beta}$ and $\beta_{\alpha\beta\gamma}$ are the components of dipole moment, polarizability and the first order hyperpolarizabilities respectively. For calculating the magnitude of total static dipole moment (μ_{tot}), the mean polarizability (α_o) and the mean first hyperpolarizability (β_o) are followed as given in the literature.[31, 38] The mean polarizability defined as the following equation,

$$\alpha_o = (\alpha_{xx}+\alpha_{yy}+\alpha_{zz})/3 \text{..... (3)}$$

The components of the first hyperpolarizability can be calculated using the following equation.

$$\beta_0 = (\beta^2_x +\beta^2_y+\beta^2_z)^{1/2} \text{ ..... (4)}$$

Where $\beta_x = \beta_{xxx}+\beta_{yyy}+\beta_{zzz}$; $\beta_y = \beta_{yyy}+\beta_{yzz}+\beta_{yxx}$; $\beta_z = \beta_{zzz}+\beta_{zxx}+\beta_{zyy}$ complete equation for calculating the magnitude of β_0. The total dipole moment can be calculated using the following equation.

$$\mu_t = (\mu_x^2+ \mu_y^2+ \mu_z^2)^{1/2} \text{ ..... (5)}$$