Si-C attachment points during sol-gel synthesis of organosilicas from 2,8-bis-silylated Tröger's base as building block precursor

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Supplementary Information

Table S1. Composition the various silicon nucleus species resulting from the signal decompositions of Si-TB-F sample.

Model

Peak	Amplitude	Position (ppm)	Width (ppm)
1	80.47	-61.37	6.15
2	248.16	-69.91	7.96
3	127.69	-78.52	7.20
4	53.80	-92.33	7.61
5	162.61	-100.56	6.82
6	105.73	-108.87	7.72

Integration

Peak	%
1	8.64
2	34.50
3	16.07
4	7.16
5	19.38
6	14.26

Sum of T-sites:
(8.64+34.50+16.07)% = 59.21%

Table S2. Composition the various silicon nucleus species resulting from the signal decompositions of Si-TB-A sample.
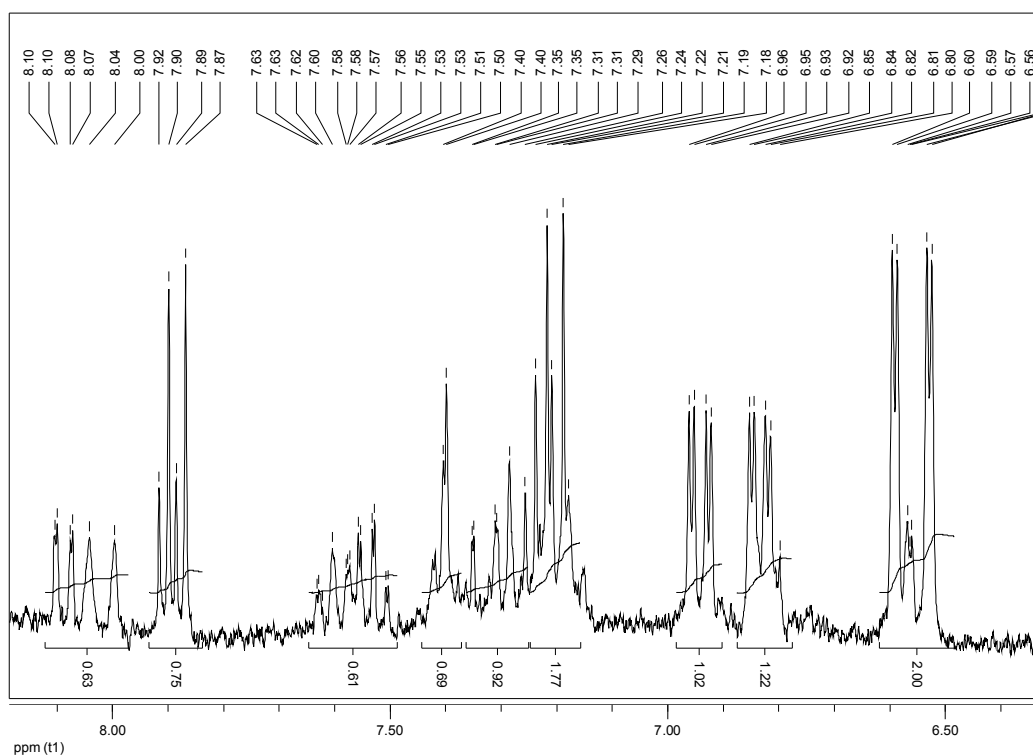
Peak	Amplitude	Position (ppm)	Width (ppm)
1	70.98	-61.52	6.56
2	117.10	-69.83	7.02
3	146.41	-78.39	8.04
4	38.21	-91.79	6.24
5	110.18	-100.65	7.26
6	86.95	-109.22	8.11

Model Integration

Peak	%
1	10.06
2	26.86
3	25.42
4	5.15
5	17.27
6	15.24

Sum of T-sites:
(10.06+26.86+25.42)% = 62.34%

Figure S3. ^{1}H NMR spectra of the recovered organics in solution in deuterated methanol after oxidative treatment of S-TB-F sample.

S4. Method of calculation of the one-point attachment (O) content

The average value of TB content versus pure silica weight determined from elemental and ATG analyses correspond to the sum of the contents Σ (O) +(T).

The value of TB content versus pure silica weight obtained by ^{29}Si OP MAS NMR spectroscopy correspond to the sum of the content Σ (O) /2 + (T).

Then the difference, Δ between these two values corresponds to the contribution of (O) content according to $\Delta = $ (O) /2, then the one-point TB content is equal to 2 Δ.

For Si-TB-100-F: $\Delta = $ 6.30- 4.95 = 1.35, then the (O) contribution is 2.7 mmol / g^{-1} versus the total TB loading of 6.30 mmol / g^{-1} *ie*, 43% of the anchored TB.

For Si-TB-100-A: $\Delta = $ 5.80- 5.20 = 0.6, then the (O) contribution is 1.2 mmol / g^{-1} versus the total TB loading of 5.80 mmol / g^{-1}, *ie*, 21 % of the anchored TB.