Supplementary Information

A Ring-Strain Model for Predicting ^{29}Si NMR Chemical Shifts in Polyhedral Oligomeric Silsesquioxanes and Siloxanes

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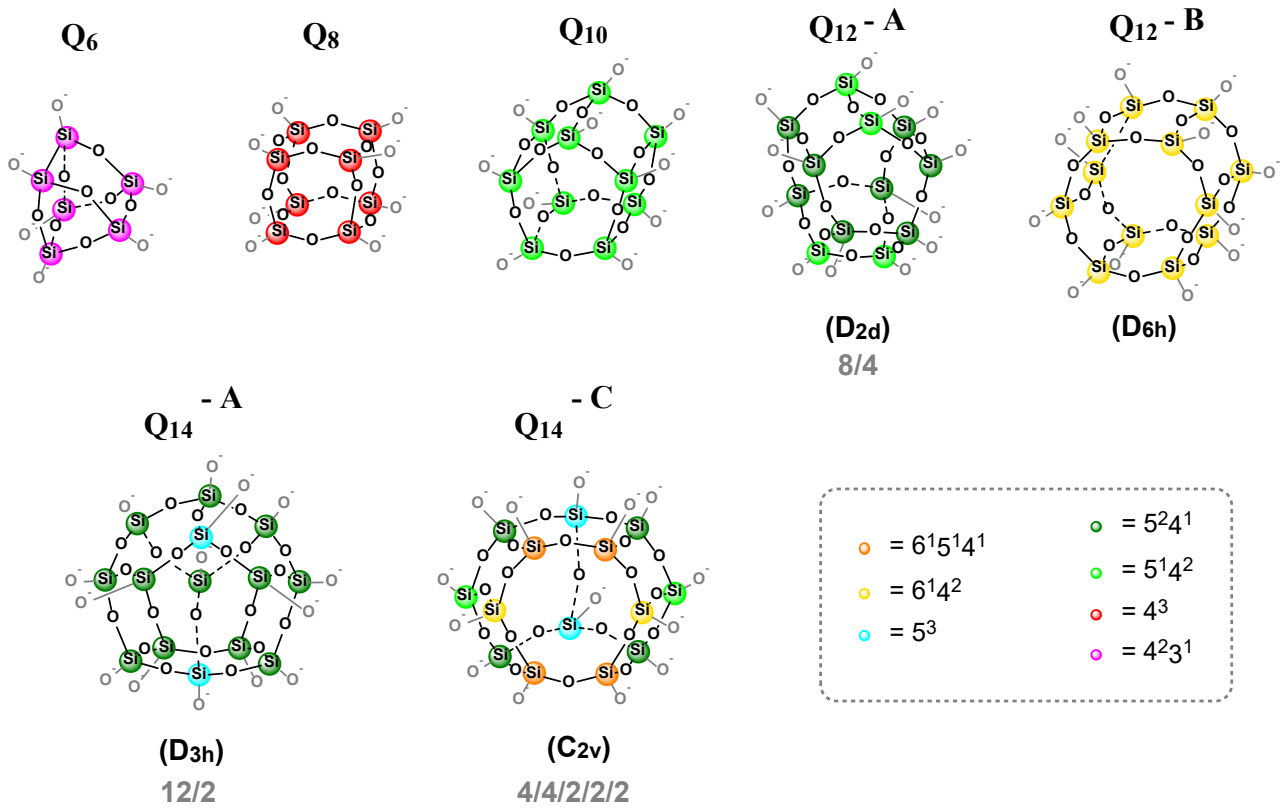


Figure S1. 3D-projection of the unambiguously identified and characterized Q_n POS cages. the proportion of Si-atom contributing to each ^{29}Si NMR resonance observed for the compound is given as ".../.../…"

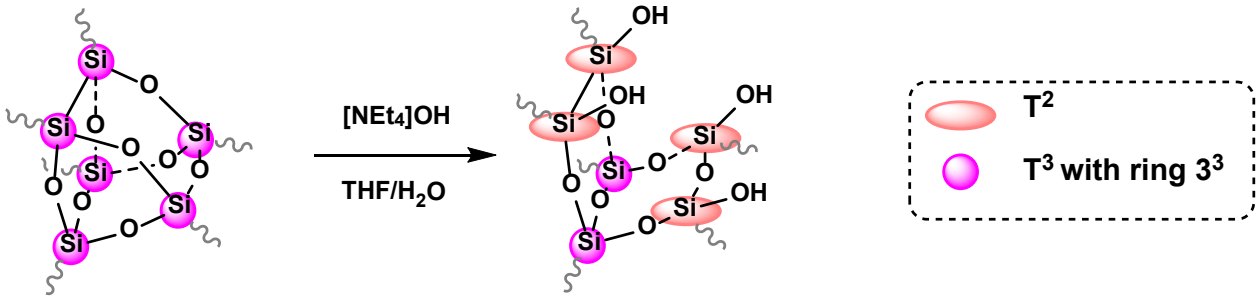
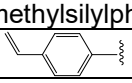
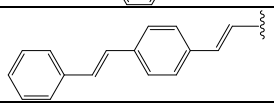


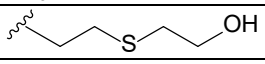
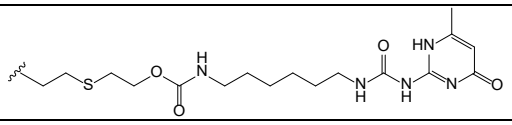
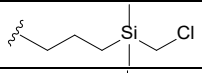
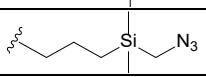
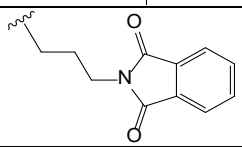
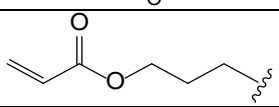
Figure S2. T_6 POSS before and after cleavage of 3-rings

Table S1. Selected ^{29}Si NMR Data for T_6 POSS Compounds with equivalent functional groups on all vertices (all Si atoms located in $4^2 3^1$ positions)

Entry	Functional Group	NMR Solvent	Chemical Shift (ppm)	Ref
T_6-001	vinyl	$CDCl_3$	-71.40	1
T_6-002	phenyl	$CDCl_3$	-66.9	2
T_6-003	ethyl	$CDCl_3$	-56.93	1
T_6-004	isopropyl	$CDCl_3$	-54.16	3
T_6-005	cyclohexyl	$CDCl_3$ $CDCl_3$/Et_3N THF-d_8	-56.6 -56.23 -56.72	2 4 5
T_6-006	octyl	$CDCl_3$	-54.2	2

Table S2. Selected ^{29}Si NMR Data for T_8 POSS Compounds with equivalent functional groups on all vertices (all Si atoms located in 4^3 positions)

Entry	Functional Group	NMR Solvent	Chemical Shift (ppm)	Ref
T_8-001	H	C_6D_6 C_6D_6 $CDCl_3$ $CDCl_3$ $CDCl_3$ $CDCl_3$ $CDCl_3$	-84.45 -84.73 -84.5 -84.7 -84.12 -84.70 -84.70	6 7 8 9 10 11 12
T_8-002	phenyl	Acetone-d_6 Acetone-d_6 THF-d_8 THF-d_8 CD_2Cl_2 $CDCl_3$ $CDCl_3$	-65.78 -79.7 -78.1 -78.3 -78.3 -78.3 -78.07	13 14 15 16 17 18 19
T_8-003	CH_2=CH-	Acetone-d_6 THF-d_8 $CDCl_3$ $CDCl_3$ $CDCl_3$ $CDCl_3$ $CDCl_3$ $CDCl_3$ $CDCl_3$ $CDCl_3$ $CDCl_3$ $CDCl_3$	-80.2 -80.11 -80.19 -79 -87 -80.20 -80 -81.81 -80.2 -79.5 -81.63 -80.19 -79.80 -79.3 -80.0	14, 20, 21 22 21, 23 24 25 26 27 28 29, 30 31 7 32 33 20 15
T_8-004	4-nitrophenyl	Acetone-d_6	-79.22	34
T_8-005	4-trimethylsilylphenyl	$CDCl_3$	-78.4	34
T_8-006		$CDCl_3$	-78.19	35
T_8-007		$CDCl_3$ or DMSO-d_6	-78.15	36
T_8-008	Ethyl	$CDCl_3$	-65.5	37

Entry	Functional Group	NMR Solvent	Chemical Shift (ppm)	Ref
		$CDCl_3$	-65.71	38
		$CDCl_3$	-65.74	11
T_8-009	$^{i}C_3H_7$-	$CDCl_3$	-66.26	3
T_8-010	Cyclohexyl	$CDCl_3$	-68.7	39
			-69.8	40
			-71.19	41
T_8-011	$^{n}C_8H_{17}$-	$CDCl_3$	-66.6	39
			-66.64	11
			-67.16	42
T_8-012	C_8H_{17}-	$CDCl_3$	-66.74	38
T_8-013	$ClCH_2CH_2CH_2$-	C_6D_6	-67.11	43
		$CDCl_3$	-67.07	44
		$CDCl_3$	-67.28	45
		$CDCl_3$	-67.1	46
		$CDCl_3$	-66.2	47
		$CDCl_3$	-67.0	48
		$CDCl_3$	-67.0	49
		$CDCl_3$	-67.1	50
		$CDCl_3$	-67.05	51
		$CDCl_3$	-67.35	52
		$CDCl_3$	-67.35	53
		$CDCl_3$	-60.05	54
		$CDCl_3$	-67.00	55
		$CDCl_3$	-67.08	56
		$CDCl_3$	-67.08	57
		$CDCl_3$	-67.08	38
		$CDCl_3/CD_3OH$	-67.08	58
		DMSO-*d*$_6$	-66.64	59
			-68.00	60, 61
			-67.10	62
			-67.08	63
T_8-014	CF_3-CH_2CH_2-	THF-*d*$_8$	-66.7	15
		DMSO-*d*$_6$	-67.3	64
T_8-015	HOOC-CH_2CH_2-	DMSO-*d*$_6$	-66.5	65
T_8-016	CH_3CH_2OOC-CH_2CH_2-	DMSO-*d*$_6$	-66.8	65
T_8-017		DMSO-*d*$_6$	-68.44	66
T_8-018		DMSO-*d*$_6$	-68.51	66
T_8-019	N_3-$CH_2CH_2CH_2$-	$CDCl_3$	-67.04	67
			-67.1	68
			-69.1	46
			-69.07	52
			-69.07	53
T_8-020	NCS-$CH_2CH_2CH_2$-	C_6D_6	-66.62	[43]
		$CDCl_3$	-67.58	38
T_8-021		$CDCl_3$	-66.52	57
T_8-022		$CDCl_3$	-66.60	57
T_8-023		$CDCl_3$	-67.11	69
T_8-024		$CDCl_3$	-66.81	70

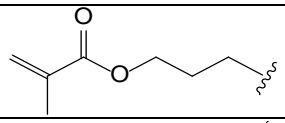
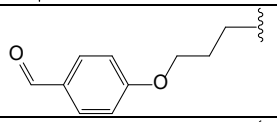
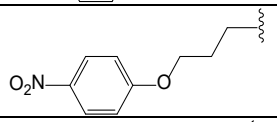
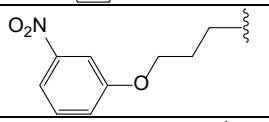
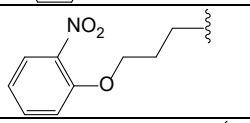
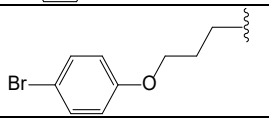
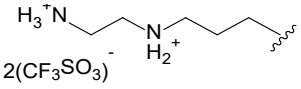
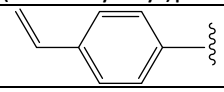
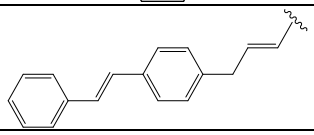
Entry	Functional Group	NMR Solvent	Chemical Shift (ppm)	Ref
T_8-025		$CDCl_3$ $CDCl_3$ DMSO-d_6	-66.79 -68.5 -66.2	70 16 71
T_8-026		$CDCl_3$	-66.76	72
T_8-027		CD_2Cl_2	-66.7	72
T_8-028		$CDCl_3$	-66.70	44
T_8-029		$CDCl_3$	-66.70	44
T_8-030		$CDCl_3$	-66.77	72
T_8-031	3-ammoniumpropyl, trifluoromethanesulfonate salt	DMSO-d_6 DMSO-d_6 DMSO-d_6 DMSO-d_6 DMSO-d_6 D_2O	-66.53 -66 -66.4 -66.63 -66.3 to -66.6 -66.7	73 74 75 76 77 78
T_8-032		DMSO-d_6	-66.7 -66.92 -66.8 to -66.9	75 76 77

Table S3. Selected ^{29}Si NMR Data for T_{10} POSS Compounds with equivalent functional groups on all vertices (all Si atoms located in $5^1 4^2$ positions)

Entry	Functional Group	NMR Solvent	Chemical Shift (ppm)	Ref
T_{10}-001	H	C_6D_6 C_6D_{12} $CDCl_3$	-86.26 -86.50 -86.4	6 7, 79 9
T_{10}-002	vinyl	$CDCl_3$	-81.40 -80.5	17 29
T_{10}-003	phenyl	$CDCl_3$	-79.61	80
T_{10}-004	p-nitrophenyl	Acetone-d_6	-80.92	34
T_{10}-005	p-(trimethylsilyl)phenyl	$CDCl_3$	-79.6	34
T_{10}-006		$CDCl_3$	-79.59	35, 81
T_{10}-007		$CDCl_3$	-78.85	82
T_{10}-008	Ethyl	$CDCl_3$	-67.56	38
T_{10}-009	3-chloropropyl	$CDCl_3$	-68.94 -68.95	44 57

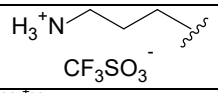
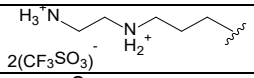
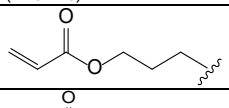
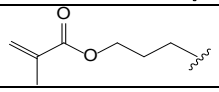
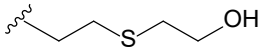
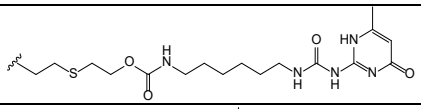
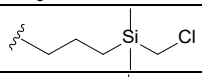
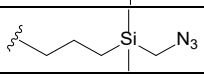
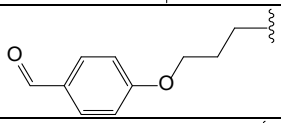
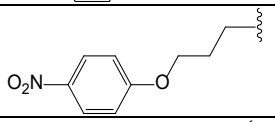
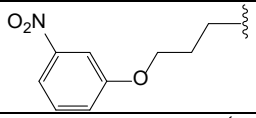
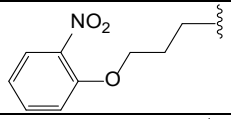
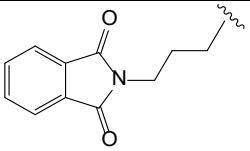
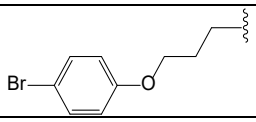
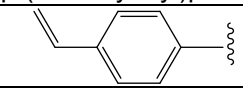
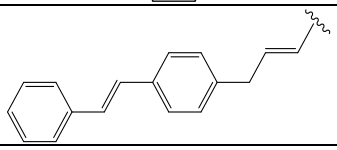
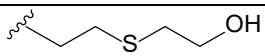
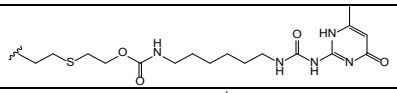
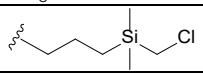
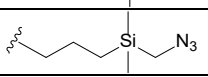
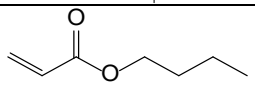
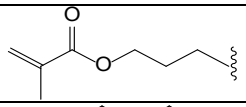
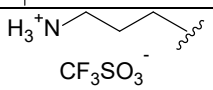
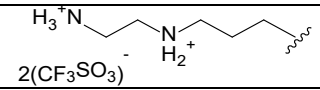
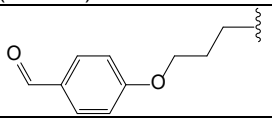
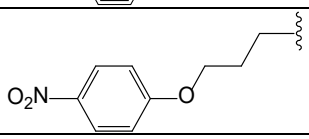
Entry	Functional Group	NMR Solvent	Chemical Shift (ppm)	Ref
T_{10}-010	Cl-C_3H_6-	$CDCl_3$	-68.97	38
T_{10}-011	3-azidopropyl	$CDCl_3$	-68.94	67
T_{10}-012	NCS-C_3H_6-	$CDCl_3$	-69.56	38
T_{10}-013	HOOC-CH_2CH_2-	DMSO-*d*$_6$	-68.7	65
T_{10}-014	CH_3CH_2OOC-CH_2CH_2-	DMSO-*d*$_6$	-68.9	65
T_{10}-015		DMSO-*d*$_6$	-68.3 -68.3 to -68.6	75 77
T_{10}-016		DMSO-*d*$_6$	-68.9 -68.7 to -69.0	75 77
T_{10}-017		$CDCl_3$	-68.70	70
T_{10}-018		$CDCl_3$ DMSO-*d*$_6$	-68.64 -68.1	70 71
T_{10}-019	C_8H_{17}-	$CDCl_3$	-68.68	38
T_{10}-020		DMSO-*d*$_6$	-70.65	66
T_{10}-021		DMSO-*d*$_6$	-70.69	66
T_{10}-022		$CDCl_3$	-68.45	57
T_{10}-023		$CDCl_3$	-68.51	57
T_{10}-024		$CDCl_3$	-68.62	72
T_{10}-025		DMSO-*d*$_6$	-68.1	72
T_{10}-026		$CDCl_3$	-68.53	44
T_{10}-027		$CDCl_3$	-68.41	44
T_{10}-028		$CDCl_3$	-68.95	69
T_{10}-029		$CDCl_3$	-68.6	72

Table S4. Selected ^{29}Si NMR Data for T_{12} POSS Compounds with equivalent functional groups on all vertices

Entry	Functional Group	NMR Solvent	Si Speciation and Chemical Shift (ppm)		Ref
			$5^1 4^2$	$5^2 4^1$	
T_{12}-001	H	C_6D_6	-85.78	-87.76	6
T_{12}-002	Vinyl	$CDCl_3$	-80.24 -81.36	-83.26 -83.37	17 29
T_{12}-003	phenyl	$CDCl_3$ or THF-d_8	-78.2	-80.1	83
T_{12}-004	p-nitrophenyl	Acetone-d_6	-80.34	-82.24	34
T_{12}-005	p-(trimethylsilyl)phenyl	$CDCl_3$	-79.4	-81.5	34
T_{12}-006		$CDCl_3$	-79.45	-81.29	35
T_{12}-007		$CDCl_3$	-78.69	-80.44	82
T_{12}-008	Ethyl	$CDCl_3$	-67.53	-69.79	38
T_{12}-009	Cyclohexyl	$CDCl_3$ or C_6D_6	-71.29	-74.29	40
T_{12}-010	Cl-C_3H_6-	$CDCl_3$	-68.73 -68.71	-71.37 -71.37	38 57
T_{12}-011	NCS-C_3H_6-	$CDCl_3$	-69.27	-72.07	38
T_{12}-012	3-chloropropyl	$CDCl_3$	-68.68	-71.34	44
T_{12}-013	3-azidopropyl	$CDCl_3$	-68.69	-71.36	67
T_{12}-014	$CF_3CH_2CH_2$-	THF-d_8	-69.24	-72.05	84
T_{12}-015		DMSO-d_6	-70.44	-72.89	66
T_{12}-016		DMSO-d_6	-70.48	-72.92	66
T_{12}-017		$CDCl_3$	-68.25	-70.94	57
T_{12}-018		$CDCl_3$	-68.37	-71.04	57
T_{12}-019		$CDCl_3$	-68.47	-71.18	70
T_{12}-020		$CDCl_3$ DMSO-6_6	-68.44 -67.3	-71.14 -70.3	70 71
T_{12}-021		DMSO-d_6	-67.6	-70.7	75
T_{12}-022		DMSO-d_6	-68.0 -68.7 to-69.0	-71.3 -71.2	75 77
T_{12}-023		$CDCl_3$	-68.30	-71.03	72
T_{12}-024		DMSO-d_6	-67.8	-70.3	72

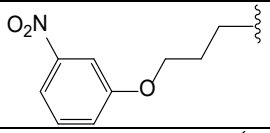
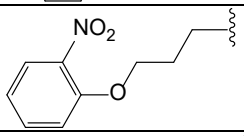
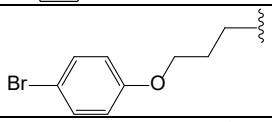
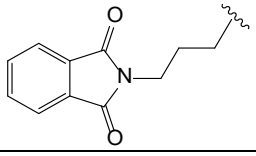
Entry	Functional Group	NMR Solvent	Si Speciation and Chemical Shift (ppm)		Ref
			$5^1 4^2$	$5^2 4^1$	
T_{12}-025		$CDCl_3$	-68.21	-70.90	[44]
T_{12}-026		$CDCl_3$	-67.98	-70.75	[44]
T_{12}-027		$CDCl_3$	-68.30	-70.97	72
T_{12}-028		$CDCl_3$	-68.74	-71.46	69

Table S5. Selected ^{29}Si NMR Data for T_n POSS Compounds with n > 12 and with equivalent functional groups on all vertices

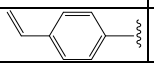
Cage Type	Functional Group	NMR Solvent	Chemical shift (ppm) and silicon speciation								Ref
			$6^2 4^1$	$6^1 4^2$	$6^2 5^1$	$6^1 5^1 4^1$	$5^1 4^2$	$5^2 4^1$	5^3	4^3	
T_{14}, D_{3h}	H	C_6D_6						-87.89 -88.03	-89.71		6
T_{14}, D_{3h}	Ph	$CDCl_3$ C_6D_6	-80.1 -79.1	-78.3 -77.6						-76.9 -76.2	85
T_{14} C_{2v}	H			-85.35		-87.68	-85.76	-87.95	-88.72		6
T_{16} D_{4d}	H							-88.10	-89.27		6
T_{18}		$CDCl_3$	-77.40	-78.35	-79.12	-79.18	-79.35				86

Table S6. Selected ^{29}Si NMR Data for Q_n POS Compounds with equivalent functional groups on all vertices

Entry	Functional Group	NMR Solvent	Cage Chemical Shift (ppm)	Ref
Q_6-001	$OSi(Me)_3$	Heptane	-98.84	87
Q_6-002	$OSi(Me)_2H$	$CDCl_3$	-99.03 -98.94	88 89
Q_6-003	$OSi(Me)_2OH$	THF-d_8	-99.94	88
Q_6-004	-OH [1]	$(CD_3)_2CO$	-90.9	90
Q_8-001	$OSi(Me)_3$	Benzene THF-d_8	-109.3 -108.95	91 92
Q_8-002	$OSiMe_2H$	$CDCl_3$ $CDCl_3$ Heptane	-108.7 -110.6 -109.36	93 7

Entry	Functional Group	NMR Solvent	Cage Chemical Shift (ppm)	Ref
		THF-d_8 $CDCl_3$	-110.34 -108.65	94 92 95
Q_8-003	$OSiMe_2OH$	THF-d_8	-109.42	96
Q_8-004	$OSi(Me)_2CHCH_2$	$CDCl_3$	-109.03	97
Q_8-005	$-OSi(OMe)_3$	CD_3CN	-110.3	98
Q_8-006	$-OSi(Vi)(OMe)_2$	CD_3CN	-110.2	98
Q_8-007	-OH [1]	THF-d_8 $(CD_3)_2CO$	-100.0 -100.2	93 90
Q_8-008	$-OSi(Me)_2CH_2Cl$	$CDCl_3$	-109.32	97
Q_8-009	$-OSi(^iPr)_2H$	$CDCl_3$	-109.02	99
Q_8-010	$-OSi(^iPr)_2OH$	THF-d_8	-109.7	99
Q_8-011	$-OSi(Ph)_2OH$	THF-d_8	-109.9	100
Q_8-013	$-OSi(OEt)_2H$	DMF-d_7	-110.2	101
Q_{10}-001	$-OSi(Me)_3$	Benzene	-110.2	91, 102
Q_{10}-002	$-OSi(Me)_2CHCH_2$	$CDCl_3$	-110.36	97
Q_{10}-003	$-OSiMe_2CH_2Cl$	$CDCl_3$	-110.82	97
Q_{12}-001	$-OSi(Me)_3$	C_6D_6	-108.77 (5^14^2) -110.48 (5^24^1)	103
Q_{12}-002	$-OSi(Me)_2H$ (6^14^2), D_{6h}	$CDCl_3$	-109.58 -109-54	95 104
Q_{12}-003	$-OSi(Me)_2OH$ (6^14^2), D_{6h}	THF-d_8	-110.62	104
Q_{12}-004	-OH, D_{6h} [1]	DMSO-d_6	-101.2	105
Q_{14}-001	$-OSi(Me)_3$ (D_{3h})	C_6D_6	-110.61 (5^24^1) -110.77 (5^24^1) -112.35 (5^3)	103
Q_{14}-002	$-OSi(Me)_3$ (C_{2v})	C_6D_6	-108.75 (6^14^2) -108.96 ($6^15^14^1$) -110.39 (5^14^2) -110.78 (5^24^1) -111.53 (5^3)	103

[1] The Si sites in these compounds are Q^3; all others are Q^4.

Table S7. Functional groups used to derive parameters *A′*, *B′*, *C′* and *D′* in Equation 2 for Q_n compounds, together with the values of k_i obtained via least-squares fitting

Functional Group	Q_n cages used to derive k_i for each functional group (no. chemical shifts shown in parenthesis)							k_i
	Q_6 (1)	Q_8 (1)	Q_{10} (1)	Q_{12} (D_{6h}) (1)	Q_{12} (D_{2d}) (2)	Q_{14} (A) (D_{3h}) (2)	Q_{14} (C) (C_{2v}) (5)	
$-OSi(Me)_3$	X	X	X		X	X	X	-108.6
$-OSi(Me)_2H$	X	X		X				-109.4
$-OSi(Me)_2OH$	X	X		X				-110.0
-OH [1]	X	X						-100.0

[1] The Si sites in these compounds are Q^3; all others are Q^4.

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