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Theoretical and experimental investigations on mono-substituted and multi-substituted functional polyhedral oligomeric silsesquioxanes

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Tabel 1S The geometrical parameters $H_8Si_8O_{12}$ and $(CH_3)_8Si_8O_{12}$, the experimental values are shown in brackets

	Bond length (Å)			Angle (°)		
	R_{Si-O}	R_{Si-H}	R_{Si-C}	∠Si-O-Si	∠O-Si-O	∠O-Si-C
$H_8Si_8O_{12}$	1.643 (1.620)	(1.450)	/	147.5-148.9 (147.5)	109.5-109.7 (109.6)	/
$(CH_3)_8Si_8O_{12}$	1.647	/	1.856	148.2	109.3	109.6

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Table 2S The related vibration frequencies of $H_8Si_8O_{12}$ and $(CH_3)_8Si_8O_{12}$ calculated (DFT), experimentally measured (Expt), and reference data (RD) in cm^{-1}

	DFT[a]	Expt[b]	RD[c]
		$H_8Si_8O_{12}$	
Si-O-Si (ring-asym)	1139	1140	1155
Si-H (stretch)	2274	2277	2375
Si-H (wag)	883	881	898
O-Si-O (bend)	543	531	559
Si-O-Si (bend)	451	465	451-453
		$(CH_3)_8Si_8O_{12}$	
Si-O-Si (ring-asym)	1120	1117	1138
Si-C (stretch)	1314	1270	1345-1347
Si-C (wag)	843	824	856
Si-C (wag)	770	773	781
O-Si-O (bend)	503	518	510-512
Si-O-Si (bend)	451	464	450

[a] our work; [b] data are from reference 49; [c] data are from reference 50.

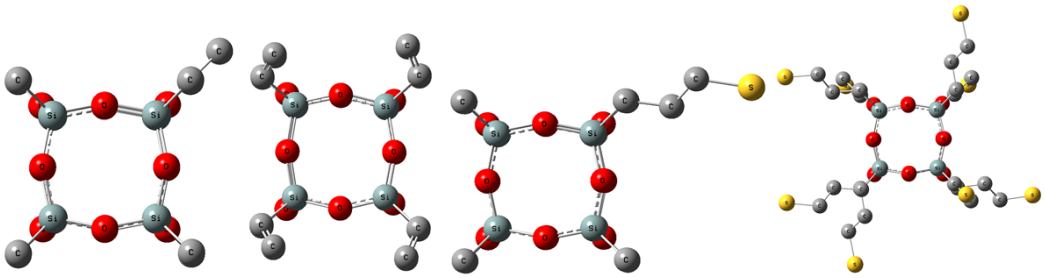

Fig. 1S The obtained optimized geometry of $(C_2H_3)(CH_3)_7Si_8O_{12}$, $(C_2H_3)_8Si_8O_{12}$, $(C_3H_6SH)(CH_3)_7Si_8O_{12}$, and $(C_3H_6SH)_8Si_8O_{12}$ (from left to right).