

Electronic Supplementary Information

Can Intact and Crystalline Octakis(methacryloxypropyl) Silsesquioxane be Prepared by Hydrolysis-condensation of Trimethoxysilane Precursor?

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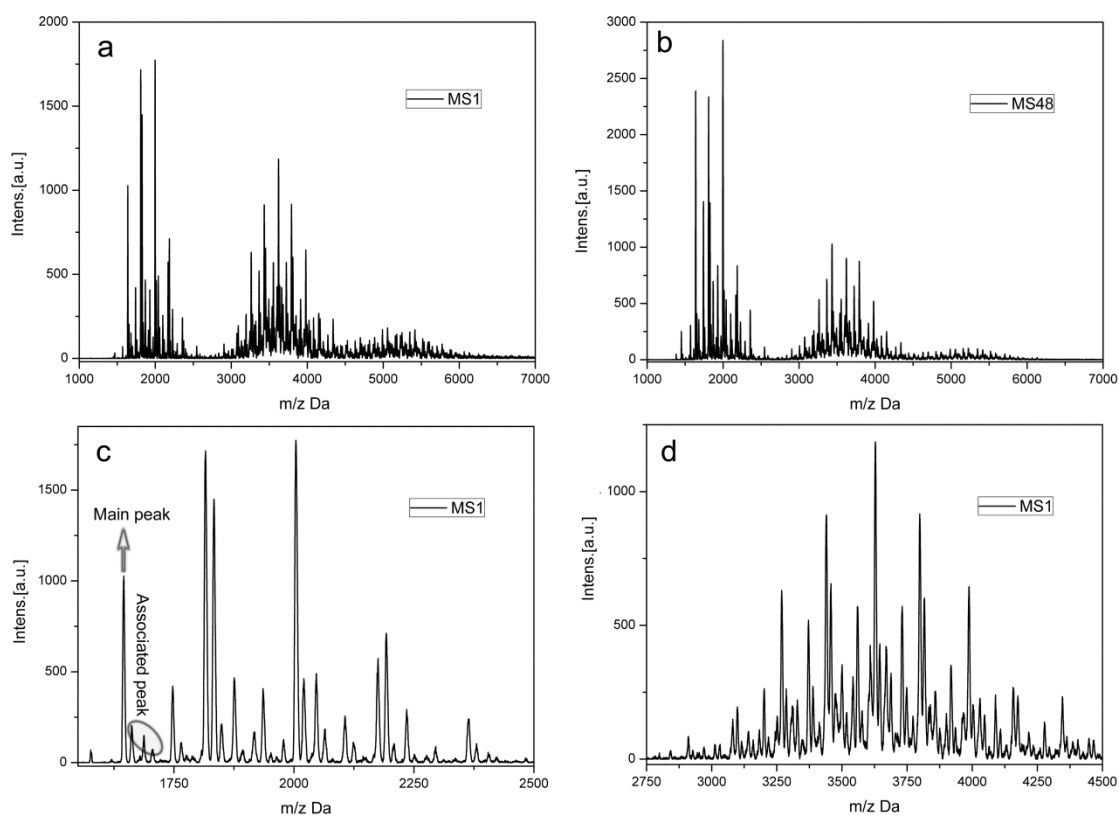


Figure S1. MALDI-TOF mass spectrum of MS1 (a) and MS48 (b) derived from the hydrolysis of (3-methacryloxypropyl)-trimethoxysilane, c and d were enlarged view of MS1 (a), MS1 and MS48 (the numeric suffix represented the hydrolysis time.)

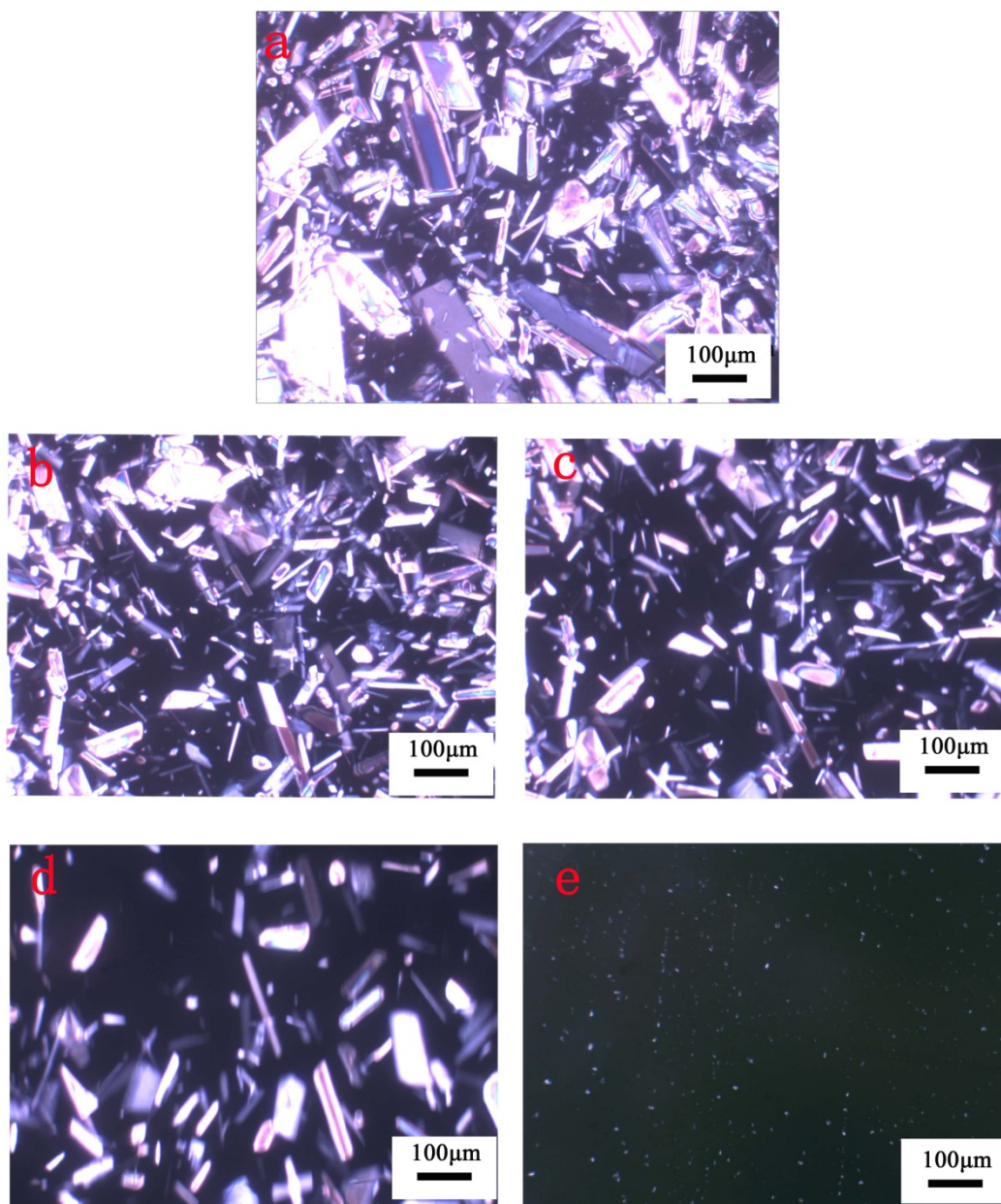


Figure S2. POM of CMSQ-T₈ with a heating rate of 1 °C/5 s, 20-60 °C (a), 62 °C (b), 64 °C (c), 68 °C (d), 72 °C (e).

Table S1. Assignment of peaks of MS MALDI-TOF mass spectrum, T represented [SiO_{1.5}(CH₂)₃OCOCCH₃CH₂] section.

MS Experimental and Predicted Values Corresponding to Ionization with Na ⁺			
m/z(exp)	Species (m/z)	m/z(exp)	Species (m/z)
1645	T ₉ (HO) ₁ (1645)	3099	T ₁₇ (HO) ₃ (3097)
1662	T ₉ (HO) ₃ (1663)	3201	T ₁₇ [SiO _{1.5} (CH ₂) ₃ (OH)](HO) ₂ (3199)
1687	T ₉ (HO) ₅ (1681)	3268	T ₁₈ (HO) ₂ (3267)
1706	T ₉ (HO) ₇ (1699)	3494	T ₁₉ (HO) ₇ (3491)
1747	T ₉ [SiO _{1.5} (CH ₂) ₃ (OH)](HO) ₁ (1747)	3541	T ₁₉ (HO) ₁₃ (3545)
1765	T ₉ [SiO _{1.5} (CH ₂) ₃ (OH)](HO) ₃ (1765)	3561	T ₁₉ (HO) ₁₅ (3563)
1816	T ₁₀ (1815)	3609	T ₂₀ (3607)
1833	T ₁₀ (HO) ₂ (1833)	3627	T ₂₀ (HO) ₂ (3625)
1849	T ₁₀ (HO) ₄ (1851)	3645	T ₂₀ (HO) ₄ (3643)
1875	T ₁₀ (HO) ₆ (1869)	3671	T ₂₀ (HO) ₆ (3661)
1892	T ₁₀ (HO) ₈ (1887)	3689	T ₂₀ (HO) ₈ (3679)
1917	T ₁₀ (HO) ₁₀ (1905)	3730	T ₂₀ (HO) ₁₄ (3733)
1935	T ₁₀ [SiO _{1.5} (CH ₂) ₃ (OH)](HO) ₁ (1936)	3749	T ₂₀ (HO) ₁₆ (3751)
1951	T ₁₀ [SiO _{1.5} (CH ₂) ₃ (OH)](HO) ₃ (1954)	3798	T ₂₁ (HO) ₁ (3796)
2004	T ₁₁ (HO) ₁ (2003)	3815	T ₂₁ (HO) ₃ (3814)
2020	T ₁₁ (HO) ₃ (2021)	3838	T ₂₁ (HO) ₅ (3832)
2040	T ₁₁ (HO) ₅ (2039)	3859	T ₂₁ (HO) ₇ (3850)
2058	T ₁₁ (HO) ₇ (2057)	3901	T ₂₁ (HO) ₁₃ (3904)
2106	T ₁₁ [SiO _{1.5} (CH ₂) ₃ (OH)] (2105)	3918	T ₂₁ (HO) ₁₅ (3922)
2175	T ₁₂ (2173)	3967	T ₂₂ (3966)
2124	T ₁₁ [SiO _{1.5} (CH ₂) ₃ (OH)](HO) ₂ (2123)	3988	T ₂₂ (HO) ₂ (3984)
2192	T ₁₂ (HO) ₂ (2191)	4004	T ₂₂ (HO) ₄ (4002)
2208	T ₁₂ (HO) ₄ (2209)	4029	T ₂₂ (HO) ₆ (4020)
2234	T ₁₂ (HO) ₆ (2226)	4049	T ₂₂ (HO) ₈ (4038)
2250	T ₁₂ (HO) ₈ (2244)	4088	T ₂₂ (HO) ₁₂ (4072)
2264	T ₁₂ (HO) ₁₀ (2262)	4156	T ₂₃ (HO) ₁ (4154)
2280	T ₁₂ (HO) ₁₂ (2280)	4345	T ₂₄ (HO) ₂ (4342)
3080	T ₁₇ (HO) ₁ (3079)		

Table S2. MM2 calculations of the minimization energies of CMSQ-T₈, T₁₀ and T₁₂ cage silsesquioxanes.

Energy Parameters*	T ₈	T ₁₀	T ₁₂
Stretch	7.1618	51.2374	9.6608
Bend	24.5503	135.7256	35.2502
Stretch-Bend	-0.1763	9.7302	0.5639
Torsion	-1.5293	3.9275	1.3665
Non-1,4 VDW	-39.3756	-12.4928	-68.9255
1,4 VDW	50.7130	93.8165	79.9198
Dipole-Dipole	48.0409	48.8186	48.1490
Total Energy	89.3848	330.7628	105.9847

*Units of energy are kcal/mol