

A simple method to control the microstructure and their properties of sol-gel silica antireflective coating

PMHS was purchased from Chengguang Research Institute of Chemical Industry (Chengdu, China). The hydrogen content of PMHS is 1.5%, 1.0% and 0.2%, and named as 0.2PMHS, 1.0PMHS and 1.5PMHS, respectively. PMHS is commonly used as vulcanizing and foaming agent in silicone rubber and foam, in which the key parameter of PMHS is the hydrogen content. Most of the PMHS manufacturer do not character and notify the molecule weight of PMHS. However, the theoretical molecule weight of PMHS can be calculated.

The general molecule formula of PMHS is shown in Figure S1. 1.5PMHS is the concentrated hydrogen silicone oil or high hydrogen silicone oil, in which there is no $-\text{Si}(\text{CH}_3)_2\text{O}-$ unit. So, the molecule weight can be calculated as Figure S2. As shown in Figure S2, the molecule weight of 1.5PMHS is about 1602.

According to the synthesis method of PMHS with hydrogen content lowers than 1.5%, the molecule weight of 1.0PMHS and 0.2PMHS can be also calculated. The synthesis process of 1.0PMHS and 0.2PMHS and the calculation of molecule weight are shown in Figure S3. As shown in Figure S3, the molecule weight of 1.0PMHS and 0.2PMHS is 2416 and 12036.

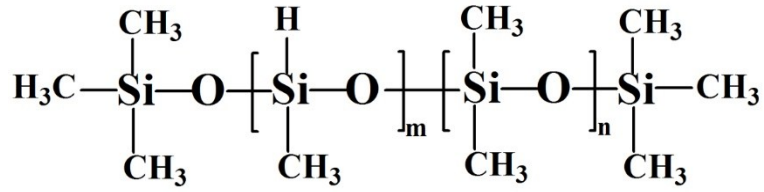
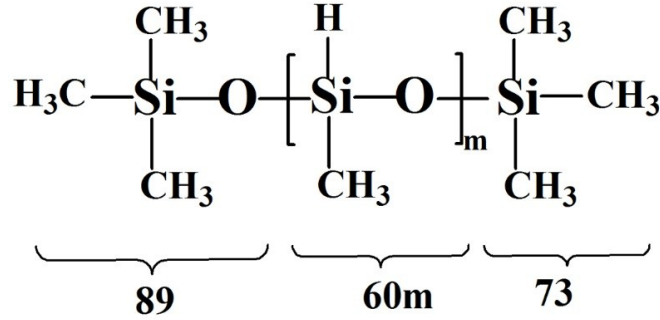
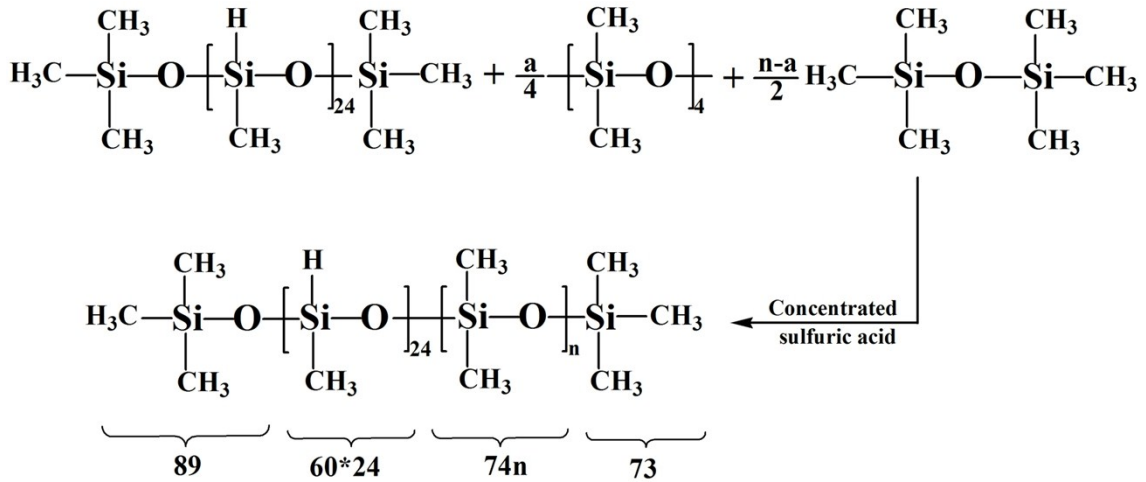


Figure S1 General molecule formula of PMHS



$$\frac{m}{89+60m+73}=0.015 \Rightarrow m=24 \Rightarrow M=1602$$

Figure S2 Molecule formula and molecule weight calculation of 1.5PMHS



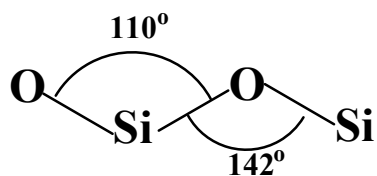
$$1.0\text{PMHS: } \frac{24}{1602+74n}=0.01 \Rightarrow n=11 \Rightarrow M=2416$$

$$0.2\text{PMHS: } \frac{24}{1602+74n}=0.002 \Rightarrow n=141 \Rightarrow M=12036$$

Figure S3 Molecule formula and molecule weight calculation of 1.0PMHS and 0.2PMHS

The bond length of Si-O is 0.164 nm, and the bond angle value of O-Si-O and Si-O-Si is 110° and 142°, respectively. To estimate the chain length of PMHS, the

PMHS chain is considered as the extended-chain, and the bond angle value of O-Si-O and Si-O-Si is approximated to be 120° . Finally, the chain length of 1.5PMHS, 1.0PMHS and 0.2 PMHS is calculated approximately to be 7 nm, 10 nm and 47 nm, respectively.



Si-O bond length: 0.164 nm

Figure S4 Bond angle of O-Si-O and Si-O-Si