Simethicone

1 Nonproprietary Names

BP: Simeticone

PhEur: Simeticone

USP–NF: Simethicone

2 Synonyms

Dow Corning Q7-2243 LVA; *Dow Corning Q7-2587*; polydimethylsiloxane–silicon dioxide mixture; *Sentry Simethicone*; *Silfar*; simeticonum.

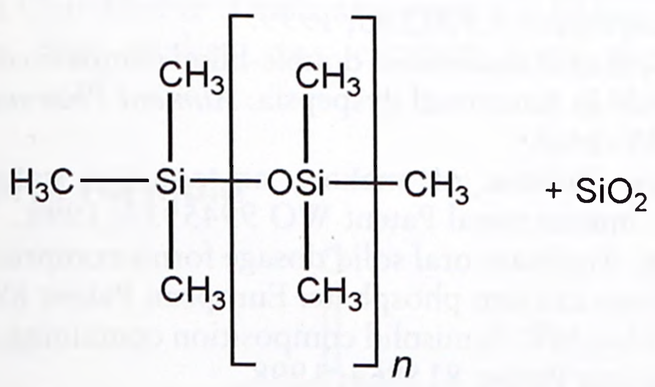
3 Chemical Name and CAS Registry Number

α-(Trimethysilyl-ω-methylpoly[oxy(dimethylsilylene)], mixture with silicon dioxide [8050-81-5]

4 Empirical Formula and Molecular Weight

See Section 8.

5 Structural Formula



where n = 200–350

6 Functional Category

Antifoaming agent; tablet and capsule diluent; water-repelling agent.

7 Applications in Pharmaceutical Formulation or Technology

The main use of simethicone as an excipient is as an antifoaming agent in pharmaceutical manufacturing processes, for which 1–50 ppm is used. It is also included in antacid products such as tablets or capsules.[1–6]

When simethicone is used in aqueous formulations, it should be emulsified to ensure compatibility with the aqueous system and components.

In the US, up to 10 ppm of simethicone may be used in food products.

8 Description

The PhEur 9.2 and USP 40–NF 35 S1 describe simethicone as a mixture of fully methylated linear siloxane polymers containing repeating units of the formula $[-(CH_3)_2SiO-]_n$, stabilized with trimethylsiloxy end-blocking units of the formula $[(CH_3)_3\ SiO-]$, and silicon dioxide. It contains not less than 90.5% and not more than 99.0% of the polydimethylsiloxane $[-(CH_3)_2SiO-]_n$, and not less than 4.0% and not more than 7.0% of silicon dioxide. The PhEur 9.2 additionally states that the degree of polymerization is between 20–400.

Simethicone occurs as a translucent, gray-colored, viscous fluid. It has a molecular weight of 14 000–21 000.

9 Pharmacopeial Specifications

See Table I.

Table I: Pharmacopeial specifications for simethicone.

Test	PhEur 9.2	USP 40–NF 35 S1
Identification	+	+
Characters	+	–
Production	+	–
Acidity	+	–
Defoaming activity	≤15 seconds	≤15 seconds
Loss on heating	–	≤18.0%
Volatile matter	≤1.0%	–
Heavy metals	–	≤5 µg/g
Mineral oils	+	–
Phenylated compounds	+	–
Assay (silicon dioxide)	–	4.0–7.0%
Assay (silica)	4.0–7.0%	–
Assay (polydimethylsiloxane)	90.5–99.0%	90.5–99.0%

10 Typical Properties

Boiling point 35°C

Refractive index n_D^{20} = 0.965–0.970

Solubility Practically insoluble in ethanol (95%) and water. The liquid phase is soluble in benzene, chloroform, and ether, but silicon dioxide remains as a residue in these solvents.

Specific gravity 0.95–0.98 at 25°C

Spectroscopy

IR spectrum *see* Figure 1.

Raman spectrum *see* Figure 2.

Viscosity (kinematic) 370 mm^2/s (370 cSt) at 25°C for *Dow Corning Q7-2243 LVA*.

11 Stability and Storage Conditions

Simethicone is generally regarded as a stable material when stored in the original unopened container. A shelf-life of 18 months from the date of manufacture is typical. However, some simethicone products have a tendency for the silicon dioxide to settle slightly and containers of simethicone should therefore be shaken thoroughly to ensure uniformity of contents before sampling or use. Simethicone should be stored in a cool, dry location away from oxidizing materials.

Simethicone can be sterilized by dry heating or autoclaving. With dry heating, a minimum of 4 hours at 160°C is required.

12 Incompatibilities

Simethicone as supplied is not generally compatible with aqueous systems and will float like an oil on a formulation unless it is first emulsified. It should not be used in formulations or processing conditions that are very acidic (below pH 3) or highly alkaline (above pH 10), since these conditions may have some tendency to break the polydimethylsiloxane polymer. Simethicone cannot normally be mixed with polar solvents of any kind because it is very minimally soluble. Simethicone is incompatible with oxidizing agents.