

## CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

The synonyms, trade names, chemical formulas, and identification numbers of silica and selected forms of silica are provided in Table 4-1.

**Table 4-1. Chemical Identity of Silica and Compounds<sup>a</sup>**

Characteristic	Information		
Chemical form	Various crystalline and amorphous silica forms		
Chemical name	Silica		
Synonym(s)	Silicon dioxide; diatomaceous earth; diatomaceous silica; diatomite, precipitated amorphous silica; silica gel, silicon dioxide (amorphous); silica colloidal <sup>b,c</sup>		
Registered trade name(s)	No data		
Chemical formula	SiO <sub>2</sub>		
Chemical structure	Not applicable		
CAS Registry Number	7631-86-9		
Chemical form	Crystalline silica		
Chemical name	Quartz	Cristobalite	Tridymite
Synonym(s)	α-Quartz; quartz; agate; chalcedony; chert; flint; jasper; novaculite; quartzite; sandstone; silica sand; tripoli	Silica, crystalline-cristobalite; α-cristobalite; β-cristobalite	Silica, crystalline-tridymite; α-tridymite; β1-tridymite; β2-tridymite
Registered trade name(s)	CSQZ; DQ 12; Min-U-Sil; Sil-Co-Sil; Snowit; Sykron F300; Sykron F600	No data	No data
Chemical formula	SiO <sub>2</sub>	SiO <sub>2</sub>	SiO <sub>2</sub>
Chemical structure	α-Quartz: trigonal crystal	α-Cristobalite: tetragonal crystal	α-Tridymite: orthorhombic crystal
CAS Registry Number	14808-60-7	14464-46-1	15468-32-3

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**Table 4-1. Chemical Identity of Silica and Compounds<sup>a</sup>**

Characteristic	Information			
Chemical form	Natural amorphous silica <sup>d</sup>			
Chemical name	Diatomaceous earth, uncalcined	Diatomaceous earth, flux-calcined	Diatomaceous earth, calcined	Vitreous silica <sup>e</sup>
Synonym(s)	Kieselguhr; Diatomite; Siliceous earth; diatomaceous earth, natural	Kieselguhr, soda ash flux-calcined; Diatomite	Kieselguhr, calcined; Calcined diatomite	Fused silica, quartz glass, volcanic glass, silica glass
Registered trade name(s)	Extrelut; Celatom; Celite; Chromaton; Chromosorb; Clarcel; Decalite; Fina/Optima; Skamol	Celite; Clarcel; Decalite; Chromosorb	Celite; Claracel; Decalite	Accusand, Admafine, Borsil P, Denka F, Fusiflex, Optosil, Rancosil, Siltex, Spectrosil, Suprasil, TAFQ, Vitreosil IR,
Crystalline content (%)	2	2.2 – 10.3	58.1 – 62.7	No data
Chemical formula	SiO <sub>2</sub>	SiO <sub>2</sub>	SiO <sub>2</sub>	SiO <sub>2</sub>
Chemical structure	Not applicable <sup>f</sup>	Not applicable <sup>f</sup>	Not applicable <sup>f</sup>	Not applicable <sup>f</sup>
CAS Registry Number	61790-53-2	68855-54-9	91053-39-3	60676-86-0
Chemical form	Amorphous silica byproduct <sup>d</sup>			
Chemical name	Silica fume <sup>g</sup>			
Synonym(s)	Amorphous silica fume			
Crystalline content (%)	6–8 <sup>h</sup>			
Registered trade name(s)	Not applicable			
Chemical formula	SiO <sub>2</sub>			
Chemical structure	Not applicable <sup>f</sup>			
CAS Registry Number	69012-64-2			

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**Table 4-1. Chemical Identity of Silica and Compounds<sup>a</sup>**

Characteristic		Information		
Chemical form		Synthetic amorphous silica		
Chemical name	Pyrogenic silica	Precipitated silica	Silica gel	Colloidal silica
Synonym(s)	Fumed silica	Silica, amorphous-precipitated silica		Silica sol <sup>i</sup>
Registered trade name(s)	Aerosil, Cab-O-Sil, HKD, Reosil	FK; Hi-Sil; Ketjensil; Neosyl; Nipsil; Sident; Sipernat; Spherosil; Tixosil; Ultrasil; Zeosil <sup>j</sup> ; Zeofree <sup>k</sup>	Art Sorb; Britesorb; Diamantgel; Gasil; KC-Trockenperlen; Lucilite; Silcron; Silica-Perlen; Silica-Pulver; Sylobloc; Syloid; Sylopute; Trisyl	Baykisol, Bindzil, Hispacil, Ludox, Nalcoag, Nyacol, Seahostar, Snowtex, Syton
Chemical formula	SiO <sub>2</sub>	SiO <sub>2</sub>	SiO <sub>2</sub>	SiO <sub>2</sub>
Chemical structure	Not applicable <sup>f</sup>	Not applicable <sup>f</sup>	Not applicable <sup>f</sup>	Not applicable <sup>f</sup>
CAS Registry Number	112945-52-5	112926-00-8	63231-67-4	NA <sup>l</sup>

<sup>a</sup>All information obtained from IARC (1997) and ChemID (2019) except where noted.

<sup>b</sup>Associated chemical (HSDB 2009, 2012).

<sup>c</sup>NIOSH 2015a, 2015b.

<sup>d</sup>Natural  $\alpha$ -Silica and silica fume may contain c-silica; c-silica content varies based on methods of preparation and purification (IARC 1997).

<sup>e</sup>Vitreous silica can be formed naturally (volcanic glass, fusion of siliceous earth following meteorite or lightening impact), unintentionally as a by-product during certain industrial processes, or intentionally as a synthetic  $\alpha$ -silica by heating c-silica and then cooling it rapidly to avoid recrystallization. Both natural and synthetic forms may contain small amounts of c-silica. (Fruijtier-Polloth 2012; Arts et al. 2007; Smith 2006; IARC 1997)

<sup>f</sup>Amorphous, randomly linked silicon and oxygen tetrahedral units with no defined pattern.

<sup>g</sup>By-product formed unintentionally during certain industrial processes (e.g., manufacture of ferrosilicon and silicon). (Fruijtier-Polloth 2012; Arts et al. 2007; IARC 1997). Silica fume produced as a by-product can then be used in certain manufacturing processes (Florke et al. 2008).

<sup>h</sup>Swensson et al. 1971.

<sup>i</sup>Florke et al. 2008.

<sup>j</sup>Arts et al. 2007.

<sup>k</sup>Warheit et al. 1995.

<sup>l</sup>Colloidal silica does not have a unique CAS Registry Number; it is included in the general silicon dioxide CAS Registry Number (7631-86-9).

CAS = Chemical Abstracts Service; NA = not applicable

## 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of selected c-silica, natural  $\alpha$ -silica, and synthetic  $\alpha$ -silica compounds is provided in Tables 4-2, 4-3, and 4-4, respectively.

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**Table 4-2. Physical and Chemical Properties of Crystalline Silica Compounds<sup>a</sup>**

Property	Information		
Chemical name	Quartz	Cristobalite	Tridymite
Molecular weight	60.1	60.1	60.1
Color	Colorless, white, black, purple, or green solid	Colorless, white, or yellowish solid	Colorless or white solid
Physical state	Solid	Solid	Solid
Melting point (°C) <sup>b</sup>	573 ( $\alpha$ -quartz converts to $\beta$ -quartz); 870 ( $\beta$ -quartz converts to tridymite)	1,713	1,470 (tridymite converts to cristobalite)
Boiling point (°C)	2,230	2,230	2,230
Density (g/cm <sup>3</sup> ) at 20°C <sup>c</sup>	2.648 ( $\alpha$ -quartz)	2.334	2.265
Odor	Odorless	Odorless	Odorless
Odor threshold:			
Water	Not applicable	Not applicable	Not applicable
Air	Not applicable	Not applicable	Not applicable
Solubility:			
Water at 20°C	Insoluble	Insoluble	Insoluble
Other solvents	Dissolves in hydrofluoric acid but insoluble in most other acids and organic solvents <sup>d</sup>	Dissolves in hydrofluoric acid	Dissolves in hydrofluoric acid
Partition coefficients:			
Log K <sub>ow</sub>	No data	No data	No data
Log K <sub>oc</sub>	No data	No data	No data
Vapor pressure (mmHg) at 20°C	Negligible at 20°C	No data	No data
Henry's law constant at 25°C	No data	No data	No data
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Conversion factors (ppm to mg/m <sup>3</sup> )	No data	No data	No data
Explosive limits	No data	No data	No data

<sup>a</sup>All information obtained from HSDB (2009, 2012) except where noted.

<sup>b</sup>IARC 1997.

<sup>c</sup>Haynes et al. 2014.

<sup>d</sup>EPA 1996.

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**Table 4-3. Physical and Chemical Properties of Natural Amorphous Silica Compounds<sup>a,b</sup>**

Property	Information			
Chemical name	Diatomaceous earth, uncalcined	Diatomaceous earth, flux-calcined	Diatomaceous earth, calcined	Vitreous silica <sup>c</sup>
Molecular weight	60.1	60.1	60.1	60.1
Color	Colorless crystals or white powder	Colorless crystals or white powder	Colorless crystals or white powder	Colorless crystals or white powder
Physical state	Solid	Solid	Solid	Solid
Melting point (°C)	1,710	1,710	1,710	1,713 <sup>d</sup>
Boiling point (°C)	2,230	2,230	2,230	2,230
Density (g/cm <sup>3</sup> ) at 20°C	2.2 at 25°C	2.2 at 25°C	2.2 at 25°C	2.196 <sup>d</sup>
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water at 20°C	Poorly to insoluble	Poorly to insoluble	Poorly to insoluble	Poorly to insoluble
Other solvents	No data	No data	No data	Dissolves in hydrofluoric acid
Partition coefficients:				
Log K <sub>ow</sub>	No data	No data	No data	No data
Log K <sub>oc</sub>	No data	No data	No data	No data
Vapor pressure (mmHg) at 20°C	Negligible at 20°C	Negligible at 20°C	Negligible at 20°C	Negligible at 20°C
Henry's law constant at 25°C	No data	No data	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors (ppm to mg/m <sup>3</sup> )	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data

<sup>a</sup>All information obtained from HSDB (2009, 2012) except where noted.

<sup>b</sup>Natural forms of a-silica may contain c-silica; c-silica content varies based on methods of preparation and purification (IARC 1997).

<sup>c</sup>Vitreous silica can be formed naturally (volcanic glass, fusion of siliceous earth following meteorite or lightning impact), unintentionally as a by-product during certain industrial processes, or intentionally as a synthetic a-silica by heating c-silica and then cooling it rapidly to avoid recrystallization. (Frujtier-Polloth 2012; Arts et al. 2007; Smith 2006; IARC 1997)

<sup>d</sup>IARC 1997.

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**Table 4-4. Physical and Chemical Properties of Synthetic Amorphous Silica Compounds<sup>a</sup>**

Property	Information			
Chemical name	Precipitated silica	Pyrogenic silica	Silica gel	Colloidal
Molecular weight	60.1	60.1	60.1	60.1
Color	Colorless crystals or white powder	Colorless crystals or white powder	Colorless crystals or white powder	Colorless crystals or white powder
Physical state	Solid	Solid	Solid	Dispersion in aqueous solution <sup>b</sup>
Melting point (°C)	1,710	1,710	1,710	1,710
Boiling point (°C)	2,230	2,230	2,230	2,230
Density (g/cm <sup>3</sup> ) at 25°C	2.2 at 25°C	2.2 at 25°C	2.2 at 25°C	2.2 at 25°C
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility <sup>c</sup> :				
Water at 20°C	Poorly to insoluble 80–130 ppm <sup>d</sup>	Poorly to insoluble	Poorly to insoluble	Colloidal dispersions with water <sup>e</sup>
Other solvents	No data	No data	No data	No data
Partition coefficients:				
Log K <sub>ow</sub>	No data	No data	No data	No data
Log K <sub>oc</sub>	No data	No data	No data	No data
Vapor pressure (mmHg) at 20°C	Negligible at 20°C	Negligible at 20°C	Negligible at 20°C	Negligible at 20°C
Henry's law constant at 25°C	No data	No data	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors (ppm to mg/m <sup>3</sup> )	No data	No data	No data	No data

<sup>a</sup>All information obtained from HSDB (2009, 2012) except where noted.

<sup>b</sup>IARC 1997.

<sup>c</sup>The solubility of silica is influenced by several factors including temperature and pH; it is affected by the presence of trace metals and the rate of solubility is dependent on the particle size and presence of an external α-silica layer on the particle surface (IARC 1997).

<sup>d</sup>EPA 1996.

<sup>e</sup>Frujtier-Polloth 2012.

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Silica occurs naturally in crystalline and amorphous (or non-crystalline) forms, herein referred to as c-silica and a-silica, respectively. Silica has one general Chemical Abstract Service registry number (CASRN 7631-86-9) and more specific CASRNs for individual silica forms and preparations. Both the crystalline and amorphous forms of silica are composed of a 1:2 net ratio of silicon atoms to oxygen atoms, corresponding to an empirical formula of  $\text{SiO}_2$  and the chemical name silicon dioxide (IARC 1997). All silica compounds are silicon dioxide. The internal chemical structure of most forms of silica consists of each silicon atom bonded to four oxygen atoms in a silicon and oxygen tetrahedral ( $\text{SiO}_4$ ) or pyramidal unit with four triangular sides. Crystalline forms of silica have regular, repeating three-dimensional patterns with internal oxygen atoms shared between two tetrahedral silicon atoms. Terminal oxygen atoms are negatively charged ions at environmentally relevant pH (OSHA 2013c). Amorphous forms of silica are composed of highly disordered, randomly linked silicon and oxygen tetrahedral units with no defined pattern. X-ray diffraction patterns distinguish crystalline polymorphs from each other and c-silica from a-silica.

The surface properties of silica compounds, even the same polymorph, vary. Both c- and a- forms of silica have surfaces composed of siloxane (covalently bonded silicon and oxygen; Si-O-Si) and silanol groups (Si-OH) (Rimola et al. 2013; Zhuravlev 2000). Exposure to water will break silicon-oxygen bonds on the surface of silica to form silanols. In contrast, heating silica results in condensation of pairs of silanols to form siloxane bridges. In general, c-silica surfaces tend to have more order, although some c-silica is found with an outer layer of a-silica. Naturally occurring a-silica may contain a c-silica component from exposure to high temperatures and pressures (e.g., flux calcination). Grinding silica results in either heterolytic cleavage or homolytic cleavage of silicon-oxygen bonds at the surface interfaces producing  $\text{Si}^+$  and  $\text{SiO}^-$  surface charges or surface radicals, respectively (Fubini et al. 1995). The total concentration and arrangement of silanol on the surface of c- and a-silica can vary greatly. Thus, for a single polymorph of c- or a-silica, surface chemistry of the compound may vary, depending upon production method and degree of hydration. As discussed in Sections 1.2 and 2.20.2, the biological activity of both c-silica and a-silica polymorphs is affected by surface chemistry of the silica particle (Donaldson and Borm 1998; Greenberg et al. 2007; Guthrie 1995; Mossman and Churg 1998; Mossman and Glenn 2013).

c-Silica is polymorphic, meaning that there are several distinctly different crystalline forms with the same chemical composition. c-Silica polymorphs have regular, repeating three-dimensional patterns with long-range order; however, discernable variations in tetrahedral orientation and crystal symmetry differentiate the polymorphs. c-Silica is often referred to as quartz. Quartz is the most common naturally occurring

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form of silica and is the second most common mineral in the world (USGS 1992). Other common forms of c-silica are tridymite and cristobalite, and less common forms of c-silica are keatite, coesite, stishovite, amethyst, and moganite (NIOSH 2002). Interconversion of the silica polymorphs occurs upon heating or cooling (see Section 5.4.2 for additional information).

The term 'free silica' refers to pure c-silica. Major impurities in c-silica polymorphs include aluminum, iron, titanium, lithium, sodium, potassium, and calcium ions (IARC 1997). The concentration of these impurities varies depending on the sample source, but is generally <1.0% in weight as oxide. Natural quartz may contain elemental impurities that are substitutions for silicon. Elemental impurities may also be present as internal or surface defects (Guthrie 1995). c-Silica substances containing other elements, such as sodium, potassium, calcium, magnesium, iron, and aluminum substituted into the crystalline matrix, are referred to as silicates (EPA 1996; USGS 1992).

a-Silica is composed of a random network of tetrahedral silica, and does not display long-range order. a-Silica forms are classified as natural or synthetic a-silica based on their origin. Natural a-silica, such as raw diatomaceous earth, contains small amounts of c-silica (mostly quartz); however, calcined and flux calcined diatomaceous earth can have cristobalite concentrations up to approximately 10 and 60%, respectively (IARC 1997). Sometimes, a-silica (silica fume, vitreous silica) is unintentionally formed during certain industrial processes, such as manufacture of ferrosilicon and silicons; these forms of a-silica are also often contaminated with c-silica (Arts et al. 2007; Fruijtier-Polloth 2012; IARC 1997). Vitreous silica can also be intentionally produced synthetically by melting c-silica and rapidly cooling to prevent recrystallization (Smith 2006). In general, other forms of synthetic a-silica are free of c-silica. They are further classified by their preparation method; there are wet process silica forms, which include precipitated silica, silica gels, and colloidal silica, and thermal process silica forms, including pyrogenic (or fumed) silica (Fruijtier-Polloth 2012; IARC 1997). Surface-modified silica is physically or chemically treated a-silica (IARC 1997).

Silica is a stable oxide of silicon. c-Silica does not readily react with most acids, but does react with hydrofluoric acid to produce silicon tetrafluoride gas (IARC 2012; OSHA 2013c). c-Silica also reacts with alkaline aqueous solutions and catechol (IARC 2012). a-Silica will react with mineral acids and alkaline solutions (OSHA 2013c).

In general, silica is considered poorly water soluble and chemically unreactive in the environment (EPA 1991; IARC 1997). The water solubility of silica has some variation due to differences in trace metal

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impurities and hydration (OSHA 2013c). Solubility is lower for c-silica polymorphs than for a-silica, and anhydrous a-silica dissolves less rapidly than hydrated a-silica (IARC 1997). a-Silica dissolves in water to form monosilicic acid (Waddell 2006). External conditions such as higher temperatures and pH increase the water solubility of silica. The hydrophilicity of c-silica particles increases in humid conditions because an external layer of hydroxylated silica (silanol; SiOH) forms on the surface of the particles. Fresh surfaces of silica exposed by fracture are highly reactive and have a propensity to produce surface radicals; however, the surface is inactivated once hydrated (Costa et al. 1991; Fubini et al. 1995). Aged quartz has an external amorphous layer, referred to as a Beilby layer. The Beilby layer is more water soluble than the underlying c-silica (IARC 1997; OSHA 2013c).

Particle size has also been found to influence the rate of solubility. Silica particulate surface areas and sizes are distinguishable based on their source. Ground vitreous silica and c-silica particles have acute edges and heterogeneous particle sizes; surface areas range from 0.1 and 10 to 15 m<sup>2</sup>/g (IARC 1997). Diatomaceous earth and cristobalite particles from diatomaceous earth are found in a variety of shapes and surface areas. Calcinated diatomaceous earth particles have surface areas that range from 2 to 20 m<sup>2</sup>/g. Pyrogenic a-silica particles are nonporous, smooth, round aggregates with surface areas that range from 50 to 400 m<sup>2</sup>/g. Precipitated a-silica particles have sizes and porous structures that vary in surface area from 50 to approximately 1,000 m<sup>2</sup>/g, depending on the procedure used in their preparation. Nanoscale forms of silica with a mean particle size in the nanoparticle range ( $\leq 100$  nm) are not included in this profile. However, while synthetic a-silica compounds have initial particle sizes in the nanoparticle range, these particles covalently bond during the manufacturing process to form indivisible aggregates in the respirable range, which can further combine to form micron-sized agglomerates (Fruijtier-Polloth 2012, 2016; IARC 1997; Merget et al. 2002; Taeger et al. 2016; Waddell et al. 2006); see Table 4-5. Of the synthetic a-silica compounds, only colloidal dispersions have been shown to contain stable isolated nanoparticles in addition to aggregates in the respirable range (Fruijtier-Polloth 2012, 2016).

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**Table 4-5. Particle Size Data for Synthetic Amorphous Silica Compounds<sup>a</sup>**

Property	Information			
Chemical name	Precipitated silica	Pyrogenic silica	Silica gel	Colloidal
Average primary particle size (nm)	5–100	5–50	1–100	4–60
Aggregate size (µm)	0.1–40	0.1–1	0.1–25	0.1–1
Agglomerate size (µm)	1–250	1–250	NA	1–250

<sup>a</sup>Particle size ranges combined from several sources to be inclusive of reported data (Fruijtier-Polloth 2012; IARC 1997; Merget et al. 2002; Waddell et al. 2006).