CB4REACH Consortium

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Carbon Black Information Letter 2- revised
Boundary composition - carbon black

This letter gives information on the boundary compositions for the forms of carbon black covered by the joint submission for carbon black.

Overall information on composition.

	Bulk form	**Nanoform 1**	**Nanoform 2**
Name of boundary composition	BC_non nano	BC_set_not treated	BC_set_treated
Designation of set	Carbon black (solid: particulate/powder) - non nanoform	(Set of) carbon black (solid: nanoform, no surface treatment)	(Set of) carbon black (solid: nanoform, surface-treated)

Carbon black is an engineered material, primarily composed of elemental carbon, obtained from the partial combustion or thermal decomposition of hydrocarbons. It exists as aggregates of aciniform morphology (i.e. shaped like a cluster of grapes) which are composed of spheroidal primary particles. While the fundamental building block of carbon black is the primary particle, these never exist in isolation, but are strongly fused by covalent bonds into aggregate. The primary particles are thus conceptual in nature since once the aggregate is formed the primary particles no longer exist as discrete entities and have no physical boundaries among them. Once produced, individual aggregates are joined by van der Waals forces to form agglomerates. Agglomerates do not break down into smaller components unless adequate force is applied (for example, shear force). Primary particle and aggregate sizes are distributional properties and vary depending on the carbon black grade. Transmission electron micrographs demonstrate that while primary particle and aggregate sizes vary greatly within a given grade of carbon black, the primary particle size is essentially uniform within an individual aggregate.

Post-production, some nanoforms of the set carbon black (solid: nanoform, no surface treatment) are subjected to oxidative after-treatment; giving rise to nanoforms of the set carbon black (solid: nanoform, surface-treated). The treatment augments the level of already present acidic and polar oxides on the surface of carbon black. These functional groups renders these forms slightly more hydrophilic in comparison to the corresponding virgin non-oxidized form; meaning that the carbon black particles becomes better dispersible and wettable in polar solutions but are still completely insoluble. Surface treatment does not affect the morphological features i.e. primary particles, aggregates, and agglomerates of carbon black.

Name: BC_non nano

State/form: solid: particulate/powder
Degree of purity: 100 % (w/w)

Table 1. Constituents (BC_non nano)

Constituent	Typical concentration	Concentration range	Remarks

Carbon black
EC no.: 215-609-9
	99 % (w/w)	>= 95 - <=99.6 % (w/w)	carbon black contains
			
			oxygen (EC no.: 231-956-9), ca. 0.5 %w/w (range >=0.2 - <= 3.5 % w/w);
			
			sulphur (EC no.: 231-722-6), ca. 0.3 % w/w (range >=0.02 - <= 1.0 % w/w);
			
			nitrogen (EC no.: 231-783-9), ca. 0.2 % w/w (range >0 - <= 1.5 % (w/w);
			
			hydrogen EC no.: 215-605-7, ca. 0.8 % w/w (range >=0.2 - <=1.1 % w/w).

Table 2. Impurities (BC_non nano)

Constituent	Typical concentration	Concentration range	Remarks
selenium EC no.:	5 ppm	>=0 - <=10 ppm	
mercury EC no.:	5 ppm	>=0 - <=10 ppm	
nickel EC no.:	5 ppm	>=0 - <=10 ppm	
lead EC no.:	5 ppm	>=0 - <=10 ppm	
copper EC no.:	5 ppm	>=0 - <=10 ppm	
cobalt EC no.:	5 ppm	>=0 - <=10 ppm	
chromium EC no.:	5 ppm	>=0 - <=10 ppm	
cadmium EC no.:	5 ppm	>=0 - <=10 ppm	
barium EC no.:	5 ppm	>=0 - <=10 ppm	
arsenic EC no.:	5 ppm	>=0 - <=10 ppm	
antimony EC no.:	5 ppm	>=0 - <=10 ppm	
extractable polycyclic aromatic hydrocarbons (PAHs) EC no.:	12 ppm	>=0.001 - <=33 ppm	Typical concentration and concentration range refer to the sum of REACH PAH8 (cf Annex XVII to REACH - Entry #50 on Polycyclic-aromatic hydrocarbons, PAH)

Name: BC_set_not treated

State/form: solid: nanoform
Degree of purity: 100 % (w/w)

Table 3. Constituents (BC_set_not treated)

Constituent	Typical concentration	Concentration range	Remarks

Carbon black
EC no.: 215-609-9
	98 % (w/w)	>=96 - <=99.9 % (w/w)	carbon black contains
			oxygen EC no.: 231-956-9, ca. 0.8 %w/w (range >=0.1 - <= 4.9 % w/w);
			sulphur EC no.: 231-722-6, ca. 0.8 % w/w (range >=0.02 - <= 1.8 % w/w);
			nitrogen EC no.: 231-783-9, ca. 0.3 % w/w (range >0.1 - <= 1.0 % (w/w);
			hydrogen EC no.: 215-605-7, ca. 0.1 % w/w (range >=0.1 - <= 0.7 % w/w).

Table 4. Impurities (BC_set_not treated)

Constituent	Typical concentration	Concentration range	Remarks
selenium EC no.:	5 ppm	>=0 - <=10 ppm	
mercury EC no.:	5 ppm	>=0 - <=10 ppm	
nickel EC no.:	5 ppm	>=0 - <=10 ppm	
lead EC no.:	5 ppm	>=0 - <=10 ppm	
copper EC no.:	5 ppm	>=0 - <=10 ppm	
cobalt EC no.:	5 ppm	>=0 - <=10 ppm	
chromium EC no.:	5 ppm	>=0 - <=10 ppm	
cadmium EC no.:	5 ppm	>=0 - <=10 ppm	
barium EC no.:	5 ppm	>=0 - <=10 ppm	
arsenic EC no.:	5 ppm	>=0 - <=10 ppm	
antimony EC no.:	5 ppm	>=0 - <=10 ppm	
extractable polycyclic aromatic hydrocarbons (PAHs) EC no.:	15 ppm	>=0.1 - <=120 ppm	Typical concentration and concentration range refer to the sum of REACH PAH8 (cf Annex XVII to REACH - Entry #50 on Polycyclic-aromatic hydrocarbons, PAH)

Characterisation of set of carbon black (solid: nanoform, no surface treatment)
Type of information reported: set of nanoforms

Shape
Shape description: spheroidal, spherical, Pure shape: yes - typical composition: - range: 100 %

Particle size distribution and range
Shape category: spheroidal
(D10, Typical value: , Range of typical value:>6 - <71 nm)
(D50, Typical value: , Range of typical value:>7 - <101 nm)
(D90, Typical value: , Range of typical value:>21 - <178 nm)

Fraction of constituent particles in the size range 1-100nm (%): >=50 - <=100 %

Crystallinity structures:

amorphous (amorphous carbon black) Pure Structure: yes

(range of typical composition: 100 %)
Crystal system: not applicable

Specific surface area
(range: ca.18 - <1200 m²/g)

Surface functionalisation / treatment
Surface treatment applied: (The set does not contain both treated and non-surface treated nanoforms)

Name: BC_set_treated

State/form: solid: nanoform
Degree of purity: 100 % (w/w)

Table 5. Constituents (BC_set_treated)

Constituent	Typical concentration	Concentration range	Remarks

Carbon black
EC no.: 215-609-9
	99 % (w/w)	>=80 - <=99.9 % (w/w)	carbon black contains
			
			oxygen EC no.: 231-956-9, ca. 9 %w/w (range >= 0.2 - <= 14 % w/w);
			
			sulphur EC no.: 231-722-6, ca. 0.8 % w/w (range >=0.02 - <= 1.8 % w/w);
			
			nitrogen EC no.: 231-783-9, ca. 0.3 % w/w (range >0.1 - <= 1% (w/w);
			
			hydrogen EC no.: 215-605-7, ca. 0.1 % w/w (range >=0.1 - <= 0.6 % w/w).

Table 6. Impurities (BC_set_treated)

Constituent	Typical concentration	Concentration range	Remarks
selenium EC no.:	5 ppm	>=0 - <=10 ppm	
mercury EC no.:	5 ppm	>=0 - <=10 ppm	
nickel EC no.:	5 ppm	>=0 - <=10 ppm	
lead EC no.:	5 ppm	>=0 - <=10 ppm	
copper EC no.:	5 ppm	>=0 - <=10 ppm	
cobalt EC no.:	5 ppm	>=0 - <=10 ppm	
chromium EC no.:	5 ppm	>=0 - <=10 ppm	
cadmium EC no.:	5 ppm	>=0 - <=10 ppm	
barium EC no.:	5 ppm	>=0 - <=10 ppm	
arsenic EC no.:	5 ppm	>=0 - <=10 ppm	
antimony EC no.:	5 ppm	>=0 - <=10 ppm	
extractable polycyclic aromatic hydrocarbons (PAHs) EC no.:	0.5 ppm	>=0.01 - <=20 ppm	Typical concentration and concentration range refer to the sum of REACH PAH8 (cf Annex XVII to REACH - Entry #50 on Polycyclic-

			aromatic hydrocarbons, PAH)

Characterisation of set of carbon black (solid: nanoform, surface-treated)
Type of information reported: set of nanoforms

Shape
Shape description: spheroidal, spherical, Pure shape: yes - typical composition: - range: 100 %

Particle size distribution and range
Shape category: spheroidal
(D10, Typical value: , Range of typical value:>3 - <71 nm)
(D50, Typical value: , Range of typical value:>7 - <87 nm)
(D90, Typical value: , Range of typical value:>15 - <178 nm)

Fraction of constituent particles in the size range 1-100nm(%): >=50 - <=100 %

Crystallinity structures:

amorphous (amorphous carbon black) Pure Structure: yes

(range of typical composition: 100 %)
Crystal system: not applicable

Specific surface area
(range: >=35 - <600 m^2/g)

Surface functionalisation / treatment
Surface treatment applied: (The set does not contain both treated and non-surface treated nanoforms)

Surface treatment: Oxidisation with ozone;
External Layer: hydrophobic
- Main features of the surface treatment/functionalisation process: Carried out at room temperature by passing a gas produced in an ozonizer through a layer of carbon black. Oxidization occurs in fluidized bed reactors, or stirred stationary bed reactors in which the carbon black is continuously kept in motion - the type of process/reaction: oxidization
- relevant ranges of process parameters such as reaction conditions (pH, temperature): room temperature
- any purification step: no
- Functionalities introduced by the treatment: Carboxylic, hydroxylic, lactonic, quinonic, basic oxides.

Following the oxidisation procedure, the carbon black particles are subjected to a treatment with hot air; hot air (@ ca. 300°C) is blown for several hours through the layer of carbon black. This step removes any remnants of treatment agent or free radicals that may have been trapped within the layers of carbon black during oxidation. Further, O_3 is very unstable and decomposes rapidly to O_2.

Coverage of particle surface in %: >75

#1 (surface treatment order), Surface treatment agent: Substance Name: ozone (EC no:

(range: >0.6 - <13 - Remarks:

Surface treatment: Oxidisation with Nitric acid;
External Layer: hydrophobic
- Main features of the surface treatment/functionalisation process: Nitric acid is added to pelletizing water. The carbon black is oxidized at elevated temperatures during drying. A second method is oxidization in a tubular kiln
- the type of process/reaction: oxidization - relevant ranges of process parameters such as reaction conditions (pH, temperature): elevated temperature
- any purification step: no
- Functionalities introduced by the treatment: Carboxylic, hydroxylic, lactonic, quinonic, basic oxides
Following the oxidisation procedure, the carbon black particles are subjected to a treatment with hot air; hot air (@ ca. 300°C) is blown for several hours through the layer of carbon black. This step removes any remnants of treatment agent that may have been trapped within the layers of carbon black during oxidation.

Coverage of particle surface in %: >75

#1 (surface treatment order), Surface treatment agent: Substance Name: Nitric acid (EC no:
(range: >0.6 - <13 - Remarks:

Surface treatment: Oxidisation with N_2O_4 (NOx);
External Layer: hydrophobic
- Main features of the surface treatment/functionalisation process: Carried out in fluidized bed reactors. This is a two-step process. Carbon black is oxidized with nitrogen oxide/air mixture. In the second step, NO_2 absorbed on the surface of the carbon black is desorbed by treatment with hot air.
- the type of process/reaction: oxidization
- relevant ranges of process parameters such as reaction conditions (pH, temperature): between 200 - 300°C
- any purification step: no
- Functionalities introduced by the treatment: Carboxylic, hydroxylic, lactonic, quinonic, basic oxides

Following the oxidisation procedure, the carbon black particles are subjected to a treatment with hot air; hot air (@ ca. 300°C) is blown for several hours through the layer of carbon black. This step removes any remnants of treatment agent that may have been trapped within the layers of carbon black during oxidation.)

Coverage of particle surface in %: >75

#1 (surface treatment order), Surface treatment agent: Substance Name: Dinitrogen Tetroxide (EC no:
(range: >0.6 - <13 - Remarks:

With kind regards

CB4REACH Consortium

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