## **Boundary Composition in Lead Registrant Dossier**

**Substance:** molybdenum disulfide - chemically produced (synthetic)

EC Number 235-721-1 Type of substance: mono-constituent

Name of boundary composition:

"Boundary composition: molybdenum disulfide - chemically produced (synthetic)"

State / form:

solid: particulate/powder

**Description of composition:** 

Production/use of MoS2 in refining & petrochemical catalysts:

In addition to natural ore molybdenite, the substance MoS2 is produced chemically during the activation or so called (pre-)sulfiding of refining & petrochemical catalysts.

The processes using these catalysts are hydrotreating or hydroprocessing in which heteroelements such as sulfur, nitrogen, oxygen or metals are removed from the feedstock. These processes increase the purity of the products and help to increase the efficiency of further processing steps.

The catalysts used in these hydrotreating processes are mixtures containing Molybdenum (typically between 2-30% mass) on a support material, which is usually alumina (Al2O3) In many cases additional metal containing compounds like cobalt or nickel are added as promoters. These solid shaped catalysts are typically in the form of spheres or cylinders of approx. 3-5 mm length. To become catalytically active, molybdenum oxide (MoO3) needs to be transformed by reaction with a sulfur compound (2R2S or RSSR or H2S) into its sulfidic form (MoS2). This process is called activation and it can take place in situ or ex situ. For in situ activation the catalyst is loaded into the hydrotreating reactor in the refinery/petrochemical plant and then activated. Ex situ pre-sulfiding is carried out by dedicated companies, who then deliver the pre-sulfided catalyst to the refineries/petrochemical plants.

This text has been prepared using the following references:

[1] Information provided by the four companies Tricat, Eurecat, Porocel and Grace (all members of the European Catalyst Manufacturers Association, ECMA)

[2] European Commission: Integrate Pollution Prevention and Control (IPPC): Reference Document on the Best Available Techniques for Mineral Oil and Gas Refineries, February 2003. Available for download from http://eippcb.jrc.es/reference/BREF/ref bref 0203.pdf (accessed 2012-01-30).

[3] Texier, S. et al. (2004): Activation of alumina-supported hydrotreating catalysts by organosulfides: comparison with H2S and effect of different solvents. Journal of Catalysis 223, 404-418.

Under the REACH Regulation the catalytic process whereby molybdenum trioxide in the catalysts is reduced down to chemically-produce molybdenum disulfide during the catalytic process means the plant is deemed to have manufactured chemically-produced molybdenum disulfide within the complex spent catalyst residue.

Degree of purity	100		%(w/w)			
	typical	min	max			
	% (w/w)	% (w/w)	% (w/w)			
					Impurities Relevant	
				<b>Selected Substance References</b>	for C&L	Remarks
Constituents				EC number CAS number		
molybdenum disulfide	100	100	100	235-721-1 12612-50-9		

## **Impurities**

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## **Additives**

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