CHEMICAL SAFETY REPORT

Update 3: Submitted October 2021

Replaces Update 2 (June 2016), Update 1 (November 2013) and original Version (2012)

Substance Name: molybdenum sulfide (*chemically-produced*)
EC Number: 235-721-1
CAS Number: 12612-50-9
Registrant's Identity: Joint CSR submitted by the Lead Registrant (GRACE GmbH & Co. KG) on behalf of all members of the joint submission MOCONJS- CPMOS2. Document prepared by the IMOA REACH Molybdenum Consortium (MoCon).

Important Introductory Remarks:

The substance addressed in this Chemical Safety Report is chemically-produced molybdenum disulfide, MoS_2 . Because this substance is not produced in isolation, with the exception of the datapoint about self-heating the data within this CSR is derived from naturally-occurring MoS_2 and read-across to chemically-manufactured molybdenum disulfide. Molybdenum disulfide is the chemical substance, as which the element molybdenum is deposited in ore bodies. This natural, mineral form of MoS_2 is also called molybdenite. After mining, molybdenite is purified by physical means and used for further processing to molybdenum compounds. This natural ore form of MoS_2 (CAS 1309-56-4 & 1317-33-5/EC 215-172-4 & 215-263-9) is formally exempt from REACH registration obligation according to Article 2(7)(b) and Annex V(7) of Regulation EC 1907/2006.

In addition to this natural MoS_2 (the ore molybdenite), the substance MoS_2 is also produced chemically during the production and recycling of molybdenum containing catalysts. This chemically-produced MoS_2 is subject to REACH registration, and is the subject of this dossier.

However, during these technical processes and also in the finished catalysts, chemically-produced MoS_2 never occurs in isolation as the substance as such. It is always included in or adsorbed onto a matrix. Therefore, the physico-chemical, toxicological and ecotoxicological properties of MoS_2 cannot be determined with a sample of such chemically produced MoS_2. In consequence, the studies where MoS_2 is the test substance reported in this CSR have been conducted with the natural form of MoS_2, i.e. molybdenite, which is readily available as a sample.

Only for analytical verification of the substance identity a small quantity of MoS_2 has been prepared artificially in the laboratory. Both this artificial sample and a sample of naturally occuring MoS_2, i.e. molybdenite, have been analysed by x-ray diffraction analysis. These analyses show that the two products are structurally and chemically identical, thus allowing unrestricted read-across from studies conducted with natural MoS_2 to chemically produced/artificial MoS_2.

It is important to note that MoS_2 is practically insoluble and chemically inert, including under normal environmental or physiological conditions. In an experimental water solubility study (acc. to OECD 105 method, Rüdel (2009)) MoS_2 was agitated in pure water for 8 days at a loading of 1 g / 500 mL.

The resulting dissolved molybdenum concentrations were below 100 µg/L, confirming that MoS_2 is practically insoluble (solubility of MoS_2 well below 200 µg/L). Furthermore, in-vitro bioaccessibility studies have been conducted with a number of molybdenum substances, including MoS_2 . In these tests, the solubility of molybdenum substances in various artificial physiological fluids, i.e. phosphate buffered saline, artificial lysosomal fluid, Gamble's solution, artificial gastric fluid and artificial sweat was studied (Ullmann, Y. and Odnevall Wallinder, I., 2009). The loading in these tests was 0.1 g/L. In these tests, MoS_2 was by far the most inert / insoluble molybdenum substance, with only up to 0.04 % (mass) of the solid material dissolving in 24 h, independent of the nature of the physiological solution, including under the acidic conditions in artificial gastric juice (represented by diluted hydrochloric acid at pH=1.7). The maximum measured concentration of dissolved molybdenum was 20 µg Mo/L after 24 h in the artificial gastric fluid, with concentrations in other media being even lower. The minimal amount of MoS_2 that eventually dissolves in aqueous media is present predominantly in form of the molybdate ion MoO_4^{2-}. This has been verified by UV-spectroscopic analysis of aqueous solutions of MoS_2 (see attached report by Mitchell, P.C.H., 2010).

In consequence, MoS_2 may reasonably be considered as basically insoluble in aqueous solutions and under physiological or environmental conditions. Since solubility is a prerequisite for any kind of systemic toxicological effect in humans or for any effects on environmental organisms, MoS_2 is generally not considered to be of any concern in this regard. This is also supported by the available toxicological and ecotoxicological studies, in which no relevant, substance specific effects were observed.

See also the ***2014 OECD Highly Soluble Molybdenum Salts Mutual Acceptance of Data (MAD) dataset (containing primarily sodium molybdate data used for read-across in many instances in this CSR),*** which is attached to IUCLID section 13. The afore-mentioned MAD status data is:

1) likewise contained in the relevant individual sections within this CSR.
2) also downloadable from the OECD website at:

https://hpvchemicals.oecd.org/UI/SIDS_Details.aspx?id=5c88d62f-4401-4cad-b521-521a4bd710f3

Several supporting documents/reports are to be considered together with the CSR. They are referenced in the CSR, and are attached in the technical registration dossier in IUCLID section 13.2:

- MoCon read-across concept/justification for human health hazards
- MoCon read-across concept/justification for environmental hazards
- Speciation of molybdenum compounds in water: UV spectra (in support of the above)
- DNEL derivation report
- Background document – Environmental Effects Assessments *(updated July 2021)*
- Background document – Environmental Fate properties *(updated May 2021)*
- Background document – Regional / ambient monitoring data (water, soil, sediment)
- OECD SIDS Initial Assessment Profile (SIAP), containing the dataset with MAD status
- List of assessors (list of professionals that contributed to the registration dossier).

2. MANUFACTURE AND USES

Table 4. Quantities (in tonnes/year)

Year	Tonnages (tonnes per year)
-	For confidentiality reasons the data on manufactured or imported **quantities per registrant are not provided in this joint CSR**, but are instead provided by each individual registrant of this substance in their technical registration dossier (section 3.2 in IUCLID).

2.1. Manufacture

Table 5. Manufacture

	Manufacture
M-1	**Manufacture of molybdenum disulfide-chemically produced(synthetic) within catalyst manufacture** Further description of manufacturing process: 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. Contributing activity/technique for the environment : **- ERC1: Manufacture of the substance** Contributing activity/technique for the workers : **- PROC 1: Chemical production or refinery in closed process without likelihood of**

	exposure or processes with equivalent containment conditions **- PROC 2: Chemical production or refinery in closed continuous process with occasional controlled exposure or processes with equivalent containment conditions** **- PROC 3: Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions** **- PROC 4: Chemical production where opportunity for exposure arises** **- PROC 8b: Transfer of substance or mixture (charging and discharging) at dedicated facilities [EU REACH]** **- PROC 9: Transfer of substance or mixture into small containers (dedicated filling line, including weighing)** **- PROC 14: Tabletting, compression, extrusion, pelletisation, granulation** **- PROC 26: Handling of solid inorganic substances at ambient temperature** **- PROC28: Manual maintenance (cleaning and repair) of machinery** Tonnage of substance for that use: tonnes/year Related assessment: use assessed in a joint CSR but not a lead's own use

2.2. Identified uses

Table 6. Formulation

	Formulation
F-1	**Formulation of molybdenum disulfide-chemically produced(synthetic)** Further description of the use: Contributing activity/technique for the environment : **- ERC2: Formulation into mixture** **- ERC3: Formulation into solid matrix** Contributing activity/technique for the workers : **- PROC 3: Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions** **- PROC 4: Chemical production where opportunity for exposure arises** **- PROC 5: Mixing or blending in batch processes** **- PROC 8b: Transfer of substance or mixture (charging and discharging) at dedicated facilities [EU REACH]** **- PROC 9: Transfer of substance or mixture into small containers (dedicated filling line, including weighing)** **- PROC 14: Tabletting, compression, extrusion, pelletisation, granulation** **- PROC 26: Handling of solid inorganic substances at ambient temperature** **- PROC28: Manual maintenance (cleaning and repair) of machinery** **Technical function of the substance:** no technical function Tonnage of substance for that use: tonnes/year Substance supplied to that use: as such Related assessment: use not assessed

Table 7. Uses at industrial sites

	Uses at industrial sites
IW-1	**Industrial use of molybdenum disulfide-chemically produced(synthetic) as catalyst** Further description of the use: Use of molybdenum disulfide-chemically produced(synthetic) as catalytic substance, e.g. in catalysing reactions of desulfurisation or denitrogenation of petroleum cuts. Contributing activity/technique for the environment : **- ERC4: Use of non-reactive processing aid at industrial site (no inclusion into or onto article)** **- ERC6b: Use of reactive processing aid at industrial site (no inclusion into or onto article)**

	Contributing activity/technique for the workers : **- PROC 1: Chemical production or refinery in closed process without likelihood of exposure or processes with equivalent containment conditions** **- PROC 2: Chemical production or refinery in closed continuous process with occasional controlled exposure or processes with equivalent containment conditions** **- PROC 3: Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions** **- PROC 4: Chemical production where opportunity for exposure arises** **- PROC 8b: Transfer of substance or mixture (charging and discharging) at dedicated facilities [EU REACH]** **- PROC 9: Transfer of substance or mixture into small containers (dedicated filling line, including weighing)** **- PROC 14: Tabletting, compression, extrusion, pelletisation, granulation** **- PROC 26: Handling of solid inorganic substances at ambient temperature** **- PROC28: Manufacture of machinery** **Product Category used:** PC 20: Products such as ph-regulators, flocculants, precipitants, neutralisation agents **Sector of end use:** SU 8: Manufacture of bulk, large scale chemicals (including petroleum products) ; SU 9: Manufacture of fine chemicals **Technical function of the substance:** catalyst Tonnage of substance for that use: tonnes/year Substance supplied to that use: in a mixture Subsequent service life relevant for that use: no Related assessment: use not assessed
IW-2	**Industrial use of molybdenum disulfide-chemically produced(synthetic) in catalyst regeneration and recycling** Further description of the use: Contributing activity/technique for the environment : **- ERC4: Use of non-reactive processing aid at industrial site (no inclusion into or onto article)** **- ERC6b: Use of reactive processing aid at industrial site (no inclusion into or onto article)** Contributing activity/technique for the workers : **- PROC 1: Chemical production or refinery in closed process without likelihood of exposure or processes with equivalent containment conditions** **- PROC 2: Chemical production or refinery in closed continuous process with occasional controlled exposure or processes with equivalent containment conditions** **- PROC 3: Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions** **- PROC 4: Chemical production where opportunity for exposure arises** **- PROC 8b: Transfer of substance or mixture (charging and discharging) at dedicated facilities [EU REACH]** **- PROC 9: Transfer of substance or mixture into small containers (dedicated filling line, including weighing)** **- PROC 14: Tabletting, compression, extrusion, pelletisation, granulation** **- PROC 22: Potentially closed processing operations with minerals/metals at elevated temperature. Industrial setting** **- PROC 26: Handling of solid inorganic substances at ambient temperature** **- PROC28: Manufacture of machinery** **Sector of end use:** SU 8: Manufacture of bulk, large scale chemicals (including petroleum products) ; SU 9: Manufacture of fine chemicals **Technical function of the substance:** catalyst ; stabilising agent Tonnage of substance for that use: tonnes/year Substance supplied to that use: in a mixture Subsequent service life relevant for that use: no Related assessment: use not assessed
IW-3	**Intermediate use of molybdenum disulfide-chemically produced(synthetic) as catalyst precursor**

	Further description of the use: Contributing activity/technique for the environment : **- ERC6a: Use of intermediate** Contributing activity/technique for the workers : **- PROC 1: Chemical production or refinery in closed process without likelihood of exposure or processes with equivalent containment conditions** **- PROC 2: Chemical production or refinery in closed continuous process with occasional controlled exposure or processes with equivalent containment conditions** **- PROC 3: Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions** **- PROC 4: Chemical production where opportunity for exposure arises** **- PROC 8b: Transfer of substance or mixture (charging and discharging) at dedicated facilities [EU REACH]** **- PROC 9: Transfer of substance or mixture into small containers (dedicated filling line, including weighing)** **- PROC 14: Tabletting, compression, extrusion, pelletisation, granulation** **- PROC 22: Potentially closed processing operations with minerals/metals at elevated temperature. Industrial setting** **- PROC 26: Handling of solid inorganic substances at ambient temperature** **- PROC28: Manual maintenance (cleaning and repair) of machinery** **Sector of end use:** SU 8: Manufacture of bulk, large scale chemicals (including petroleum products) ; SU 9: Manufacture of fine chemicals **Technical function of the substance:** intermediate (precursor) Tonnage of substance for that use: tonnes/year Substance supplied to that use: in a mixture Subsequent service life relevant for that use: no Related assessment: use not assessed