Molybdenum Consortium

An initiative of the International Molybdenum Association

Substance Identification and Hazard Classification of "Molybdenum Sulfide (MoS_2), roasted"

1. Identification:

The MoCon Technical Working Group has worked extensively on the REACH issue of Substance Identity and Hazard Classification for "Molybdenum Sulfide (MoS_2), roasted".

The most appropriate Substance Identity category option for '**Molybdenum Sulfide (MoS_2), roasted'** is that of **UVCB** (Unknown or Variable Composition, Complex Reaction Products or Biological Materials) as defined below:

EC Name: Molybdenum Sulfide (MoS_2), roasted
Synonyms: Roasted Molybdenite Concentrates
Trade names: RMC, Technical Grade Molybdenum Oxide
EINECS No.: 289-178-0
CAS No.: 86089-09-0
- The product obtained from roasting molybdenum disulfide and gangue material at temperatures between 482°C to 677°C to remove sulfur. Composed primarily of a mixture of molybdenum oxides.

2. Composition:

Constituent composition of the above-indicated UVCB substance that will be REACH-registered by the Lead Registrant:

Constituent	Typical concentration	Concentration range	Remarks
MoO_3 EC no.: 215-204-7 CAS No: 1313-27-5	80 %(w/w)	≥ 50 — ≤ 96 % (w/w)	Constituent relevant for hazard classification
SiO_2 (quartz) EC no : 238-878-4 CAS No. 14808-60-7	3 %(w/w)	≥1% — ≤ 15 % (w/w)	Constituent relevant for hazard classification if > 1% present as respirable crystalline silica
Mo Suboxides	6 %(w/w)	≥ 2 — ≤ 30 % (w/w)	According to XRD-analysis, mainly MoO_2, Mo_4O_{11}, Mo_8O_{23}, Mo_9O_{26} (Mo_4O_{11} can individually be present in concentration ≥ 10%)

Table continuation: **Constituent**	**Typical Concentration**	**Concentration Range**	**Remarks**
Iron molybdates	4 %(w/w)	≥ 1 — ≤ 15 % (w/w)	Based on expert judgement and/or XRD-analysis, expected to be present as $FeMoO_4$, $Fe2(MoO_4)3$, $Fe_3Mo_3O_{12}$
Lead compounds	0.03% (w/w) Pb	≤ 0.25 % Pb (w/w)	Based on expert judgement, expected to be present as lead oxide (EINECS No. 215-267-0/CAS No 1317-36-8)
Arsenic compounds	0.012 % (w/w) As	≤ 0.075 % (w/w) As	Based on expert judgement, expected to be present as diarsenic trioxide (EINECS No. 215-481-4/CAS No. 1327-53-3)
Copper compounds	0.45 % (w/w) Cu	≤ 4 % (w/w) Cu	Based on XRD analysis and expert judgement, copper is present as CuO (EINECS No. 215-269-1/CAS No. 1317-38-0), copper molybdates and copper silicates; and is not present as Cu2O. The compounds in which copper is present have no impact on the classification.
Calcium molybdate EC no.: 232-192-9 CAS No: 7789-82-4	1 % (w/w)	≥0 — ≤ 5 % (w/w)	

Remark: Other constituents can be present in concentrations that do not change the GHS/CLP-classification below.

3. CLP-classification:

Classification under GHS/CLP - See also Annex 1 attached:

The UVCB substance as defined above has the following classification:

For Human Health: Carcinogenicity Category 2, H351: Suspected of causing cancer – see Note 1 below

IMPORTANT NOTE:

All intending registrants must inform the MoCon Secretariat prior to submission of the Lead Registrant dossier if either:

- the levels of lead or arsenic in the RMC UVCB substance they will register exceed those indicated in the 'concentration range' column of the table in point 2 of this document, and/or
- if the level of respirable crystalline silica is > 1%, and/or
- if other hazardous constituents are present in classifiable quantities.

This is necessary because a separate classification entry in IUCLID Section 2 of the Lead Registrant dossier will need to be made.

Note 1 on the rationale for Classification: This is a REACH 'Self-Classification'. The outcome of the Chemical Safety Assessment under REACH, as documented in the Chemical Safety Report, is that this substance meets the criteria for self-classification as a dangerous substance.

Background: REACH contains a requirement to hazard assess and self-classify if the (CLP) criteria for hazard classification are met. Phys-Chem, human health and environment parameters all need to be assessed. MoO_3 was classified in 2009 in the EU as a Category 2 Carcinogen in the 1st ATP to the EU Classification, Labelling & Packaging Regulation (CLP). In the case of RMC the relevant CLP rule is:

- Carcinogenicity category 2 if the concentration of a substance is =>1%

The MoO_3 content of RMC is substantially greater than 1% and therefore this existing EU classification MoO3 classification must be read-across and applied to the RMC.

Remark : The classifications Eye Irrit.2 and STOT SE 3 are not read-across from MoO3 (see Annex 1).

Annex 1

1. MoO_3, CAS No: 1313-27-5, EINECS No: 215-204-7, CLP Ist ATP Index No: 042-001-00-9

The existing EU harmonized hazard classification of the substance MoO_3, stipulated in the 2009 1st ATP to the EU CLP, is:

- *Carcinogenicity category 2*
  - H351: Suspected of causing cancer <state route of exposure if it is conclusively proven that no other routs of exposure cause the hazard>
- *Eye irritation category 2*
  - H319: Causes serious eye irritation.
- *STOT- SE category 3*
  - H335: May cause respiratory irritation.

Below are the rationale for not reading-across the Eye Irritation and STOT-SE classifications from MoO3 to 'molybdenum sulfide (MoS2) roasted'

Note on Assessment of Applicability of Existing MoO_3 EU-harmonized Classifications to 'molybdenum sulfide (MoS2) roasted' (RMC).

1. Eye Irritation

The conclusion of the recent assessment by MoCon TWG is that the basis for the classification of MoO_3 as 'Eye Irritant, Category 2' by the EU was unwarranted. This is because examination of the data from an OECD 405 guideline-conform study with MoO_3 (see page 5) reveals that the calculated mean scores are below the cut-off values for eye irritation classification. Furthermore, a similar study exists for RMC itself where the results are also below the cut-off values for classification (see page 6).

MoCon will therefore not read-across the MoO_3 eye irritation classification to RMC.

2. Respiratory Irritation

An OECD 403 guideline-conform study (Leuschner 2010) on acute inhalation toxicity with extended histopathology to investigate potential respiratory irritation has recently been conducted. Based on the results, molybdenum trioxide does not require classification for either acute inhalation toxicity or for respiratory irritation. The existing classification of MoO_3 as STOT SE Category 3 (H335: May cause respiratory irritation) appears unwarranted. MoCon will not read-across the MoO3 respiratory irritant classification to RMC.

Tables for MoO_3:

Irritant Effects on the Rabbit Eye of molybdenum trioxide
Calculations for C&L, according to Directive 67/548/EEC and Regulation (EC) 1272/2008
Attachment to study: Liggett and McRae (1990): Irritant effects on the rabbit eye of pure molybdic oxide. Huntingdon Research Centre Ltd., Huntingdon, UK. Report No. 90948D/IMA 4/SE

67/548/EEC - calculation of means over all six animals for 24/48/72 hours

Corneal Opacity							
Animal	1 h	24 h	48 h	72 h	4 d	7 d	21 d
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
mean	0,00	0,00	0,00	0,00	0,00	0,00	0,00
mean (24/48/72)			**0,00**				

Iris Lesion							
Animal	1 h	24 h	48 h	72 h	4 d	7 d	21 d
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
mean	0,00	0,00	0,00	0,00	0,00	0,00	0,00
mean (24/48/72)			**0,00**				

Conjunctivae Redness							
Animal	1 h	24 h	48 h	72 h	4 d	7 d	21 d
1	1	1	0	0	0	0	0
2	1	0	0	0	0	0	0
3	1	1	1	1	1	0	0
4	1	0	0	0	0	0	0
5	1	1	1	0	0	0	0
6	1	1	1	0	0	0	0
mean	1,00	0,67	0,50	0,17	0,17	0,00	0,00
mean (24/48/72)			**0,44**				

Conjunctivae Oedema (Chemosis)							
Animal	1 h	24 h	48 h	72 h	4 d	7 d	21 d
1	1	1	0	0	0	0	0
2	1	0	0	0	0	0	0
3	1	1	1	1	0	0	0
4	1	0	0	0	0	0	0
5	1	1	0	0	0	0	0
6	1	1	0	0	0	0	0
mean	1,00	0,67	0,17	0,17	0,00	0,00	0,00
mean (24/48/72)			**0,33**				

Conclusion: The calculated mean scores are below the respective cut-off values as per Directive 67/548/EEC.
No Classification for eye irritancy according to Directive 67/548/EEC.

Regulation (EC) 1272/2008 - calculation of means for individual animals for conjuntivae redness and oedema

Corneal Opacity					
Animal	1 h	24 h	48 h	72 h	mean 24/48/72
1	0	0	0	0	**0,00**
2	0	0	0	0	**0,00**
3	0	0	0	0	**0,00**
4	0	0	0	0	**0,00**
5	0	0	0	0	**0,00**
6	0	0	0	0	**0,00**

Iris Lesion					
Animal	1 h	24 h	48 h	72 h	mean 24/48/72
1	0	0	0	0	**0,00**
2	0	0	0	0	**0,00**
3	0	0	0	0	**0,00**
4	0	0	0	0	**0,00**
5	0	0	0	0	**0,00**
6	0	0	0	0	**0,00**

Conjunctivae Redness					
Animal	1 h	24 h	48 h	72 h	mean 24/48/72
1	1	1	0	0	**0,33**
2	1	0	0	0	**0,00**
3	1	1	1	1	**1,00**
4	1	0	0	0	**0,00**
5	1	1	1	0	**0,67**
6	1	1	1	0	**0,67**

Conjunctivae Oedema (Chemosis)					
Animal	1 h	24 h	48 h	72 h	mean 24/48/72
1	1	1	0	0	**0,33**
2	1	0	0	0	**0,00**
3	1	1	1	1	**1,00**
4	1	0	0	0	**0,00**
5	1	1	0	0	**0,33**
6	1	1	0	0	**0,33**

All effects fully reversed by 21 days.

Conclusion: The calculated mean scores per animal are below the respective cut-off values as per Regulation 1272/2008.
No Classification for eye irritancy according to Regulation 1272/2008.

Tables for RMC:

Irritant Effects on the Rabbit Eye of roasted molybdenite concentrate
Calculations for C&L, according to Directive 67/548/EEC and Regulation (EC) 1272/2008
Attachment to study: Liggett and McRae (1990): Irritant effects on the rabbit eye of technical molybdic oxide. Huntingdon Research Centre Ltd., Huntingdon, UK. Report No. 90946D/IMA 4/SE

67/548/EEC - calculation of means over all six animals for 24/48/72 hours

Corneal Opacity							
Animal	1 h	24 h	48 h	72 h	4 d	7 d	21 d
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
mean	0,00	0,00	0,00	0,00	0,00	0,00	0,00
mean (24/48/72)			0,00				

Iris Lesion							
Animal	1 h	24 h	48 h	72 h	4 d	7 d	21 d
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
mean	0,00	0,00	0,00	0,00	0,00	0,00	0,00
mean (24/48/72)			0,00				

Conjunctivae Redness							
Animal	1 h	24 h	48 h	72 h	4 d	7 d	21 d
1	1	2	1	1	0	0	0
2	1	1	1	0	0	0	0
3	1	1	1	1	1	1	0
4	1	1	1	1	2	2	0
5	1	2	1	1	1	0	0
6	1	2	1	1	1	1	0
mean	1,00	1,50	1,00	0,83	0,83	0,67	0,00
mean (24/48/72)			1,11				

Conjunctivae Oedema (Chemosis)							
Animal	1 h	24 h	48 h	72 h	4 d	7 d	21 d
1	1	1	1	0	0	0	0
2	1	2	1	0	0	0	0
3	1	1	1	1	1	1	0
4	1	1	1	1	2	2	0
5	1	2	1	1	1	0	0
6	1	2	1	1	1	1	0
mean	1,00	1,50	1,00	0,67	0,83	0,67	0,00
mean (24/48/72)			1,06				

Conclusion: The calculated mean scores are below the respective cut-off values as per Directive 67/548/EEC.
No Classification for eye irritancy according to Directive 67/548/EEC.

Regulation (EC) 1272/2008 - calculation of means for individual animals for conjuntivae redness and oedema

Corneal Opacity					
Animal	1 h	24 h	48 h	72 h	mean 24/48/72
1	0	0	0	0	0,00
2	0	0	0	0	0,00
3	0	0	0	0	0,00
4	0	0	0	0	0,00
5	0	0	0	0	0,00
6	0	0	0	0	0,00

Iris Lesion					
Animal	1 h	24 h	48 h	72 h	mean 24/48/72
1	0	0	0	0	0,00
2	0	0	0	0	0,00
3	0	0	0	0	0,00
4	0	0	0	0	0,00
5	0	0	0	0	0,00
6	0	0	0	0	0,00

Conjunctivae Redness					
Animal	1 h	24 h	48 h	72 h	mean 24/48/72
1	1	2	1	1	1,33
2	1	1	1	0	0,67
3	1	1	1	1	1,00
4	1	1	1	1	1,00
5	1	2	1	1	1,33
6	1	2	1	1	1,33

Conjunctivae Oedema (Chemosis)					
Animal	1 h	24 h	48 h	72 h	mean 24/48/72
1	1	1	1	0	0,67
2	1	2	1	0	1,00
3	1	1	1	1	1,00
4	1	1	1	1	1,00
5	1	2	1	1	1,33
6	1	2	1	1	1,33

All effects fully reversed by 21 days.

Conclusion: The calculated mean scores per animal are below the respective cut-off values as per Regulation 1272/2008.
No Classification for eye irritancy according to Regulation 1272/2008.