SUBSTANCE EVALUATI ON CONCLUSION

as required by REACH Article 48

and

EVALUATION REPORT

for

Reaction product of ammonium molybdate and C12-C24-diethoxylated alkylamine (1:5-1:3)

EC No 412-780-3

CAS No -

Evaluating Member State(s): FRANCE

Dated: 19 Debember 2019

Evaluating Member State Competent Authority

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Year of evaluation in CoRAP: Transitional former notified substance under Dir. 67/548/EEC to REACH Art. 135

Before concluding the substance evaluation a Decision to request further information was issued on: 09 September 2016

Further information on registered substances here:

http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances

DISCLAIMER

Foreword

Substance evaluation is an evaluation process under REACH Regulation (EC) No. 1907/2006. Under this process the Member States perform the evaluation and ECHA secretariat coordinates the work. The Community rolling action plan (CoRAP) of substances subject to evaluation, is updated and published annually on the ECHA web site[1].

Substance evaluation is a concern driven process, which aims to clarify whether a substance constitutes a risk to human health or the environment. Member States evaluate assigned substances in the CoRAP with the objective to clarify the potential concern and, if necessary, to request further information from the registrant(s) concerning the substance. If the evaluating Member State concludes that no further information needs to be requested, the substance evaluation is completed. If additional information is required, this is sought by the evaluating Member State. The evaluating Member State then draws conclusions on how to use the existing and obtained information for the safe use of the substance.

This Conclusion document, as required by Article 48 of the REACH Regulation, provides the final outcome of the Substance Evaluation carried out by the evaluating Member State. The document consists of two parts i.e. A) the conclusion and B) the evaluation report. In the conclusion part A, the evaluating Member State considers how the information on the substance can be used for the purposes of regulatory risk management such as identification of substances of very high concern (SVHC), restriction and/or classification and labelling. In the evaluation report part B the document provides explanation how the evaluating Member State assessed and drew the conclusions from the information available.

With this Conclusion document the substance evaluation process is finished and the Commission, the Registrant(s) of the substance and the Competent Authorities of the other Member States are informed of the considerations of the evaluating Member State. In case the evaluating Member State proposes further regulatory risk management measures, this document shall not be considered initiating those other measures or processes. Further analyses may need to be performed which may change the proposed regulatory measures in this document. Since this document only reflects the views of the evaluating Member State, it does not preclude other Member States or the European Commission from initiating regulatory risk management measures which they deem appropriate.

[1] http://echa.europa.eu/regulations/reach/evaluation/substance-evaluation/community-rolling-action-plan

Contents

Part A. Conclusion

1. CONCERN(S) SUBJECT TO EVALUATION

Reaction product of ammonium molybdate and C12-C24-diethoxylated alkylamine (1:5-1:3) (hereafter named "Additiv 104") was originally selected for substance evaluation in order to clarify concerns about:

- Potential PBT/vPvB properties.

2. OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Additiv 104 is a substance notified according to Notification of New Substances (NONS) under Directive 67/548/EEC first in Germany (October 27th 1993) and then in France. For further details, please see part B, section 7.2.

3. CONCLUSION OF SUBSTANCE EVALUATION

The evaluation of the available information on the substance has led the evaluating Member State to the following conclusions, as summarised in the table below.

Table 1

CONCLUSION OF SUBSTANCE EVALUATION Conclusions	Tick box
Need for follow-up regulatory action at EU level	
Harmonised Classification and Labelling	
Identification as SVHC (authorisation)	
Restrictions	
Other EU-wide measures	
No need for regulatory follow-up action at EU level	X[2]

PBT assessment approach

During the Substance Evaluation process it was not possible to clarify the concern initially identified for PBT/vPvB properties. Indeed, after obtaining more insight on the composition

[2] There was an issue regarding a constituent that disappeared when the ECHA dissemination was updated (July 2019), without having established the importance (or not) of this information. Following this update, the content of this document has been simplified erasing important issues. In addition, this constituent is registered on its own and was manually screened by eMSCA. Following manual screening, it was concluded that a CCH should be performed on this constituent before being evaluated by PetCo group.

of the substance in 2014, the evaluating MSCA decided to use a "known constituents approach" to elucidate the properties of Additiv 104 and evaluate the P, B and T properties of the main constituents separately according to ECHA's guideline (Chapter R.11: PBT/vPvB assessment). Indeed, the registrant proposed different molecular structures to represent some constituents which are expected to be present in Additiv 104. Except for one consituent, no experimental information of the physico-chemical properties, environmental fate and toxicity is available for the constituents. Predictions from QSAR models (Epi Suite) for every structure proposed were generated to evaluate the P and B properties. Besides one additional UVCB constituents have been identified in the scope of activities of the PetCo program. The substance was not considered in these assessment, despite its significant concentration.

Regarding readily biodegradation properties, only two proposed structures are inside the applicability domain of the QSAR model, one of them screens as potential P/vP. Concerning experimental data, three screening tests are available for Additiv 104. Only one reliable (study (OECD 301B) allowed to conclude that Additiv 104 is not readily biodegradable. Because no further information is available, Additiv 104 is concluded to be potentially P/vP.

Based on literature data, some structure were supposed to hydrolyse, in September 2016, a decision was addressed to the registrant in order to require a new hydrolysis study (OECD 111. The registrant conducted a preliminary hydrolysis study, in which additional information regarding the identity of the test material were provided. These information allowed to refine the knowledge on the composition of the Additiv 104. Indeed, tentative of molecular structures for some type of constituents were proposed by the registrant but on the other hand it was noted that it appears analytically difficult to define clearly the structure for other constituents.

Low hydrolysis rate were reported at environmental pH and temperature. The attempt of analysis of constituents and degradation products required a filtration step leading to the formation of additional chemicals which make difficult the analysis and the interpretation of the results. At last, the complex composition and insolubility of the constituents of Additiv 104 led to complex analytical issues to determine possible hydrolysis products. In the hydrolysis report, results description mainly consist of observations which were not interpretable because of analytical difficulties. Only molybdenum could be monitored by IC (ionic chromatography) and recovery of all constituents were determined gravimetrically.

Regarding the bioaccumulation properties, the assessment was based on QSAR predictions of each molecular structure proposed by registrant. This assessment indicates that the B criterion would not be fulfilled for any of the molecular structures. However, a detailed analysis of the applicability domain of these QSARs indicates that predictions are relevant for only one constituent. Indeed, the physico-chemical properties of the identified constituents make the assessment difficult, because of analytical and experimental limitations (for instance low solubility) and because constituents are often outside the domain of applicability of the available models.

Regarding the toxicity properties, no chronic aquatic toxicity tests are available. Low or no adverse effects in fish and invertebrates are observed in acute toxicity tests, whereas toxic effects were reported in an algae test. However, the reliability of the studies is questionable because they were carried out at concentrations exceeding the water solubility of Additiv 104 or with a water accommodated fraction (WAF) approach but without analysis of the tested substance. Chronic terrestrial toxicity tests were provided in the registration dossier, that are used by the registrant to claim that the T criterion is not fulfilled. However, according to ECHA guidance R.11(item 4.1.3), the assessment of T criterion should be based on aquatic toxicity test. Therefore, no conclusion can be drawn for the T criterion because the data provided are incomplete. In particular, chronic aquatic toxicity data are lacking. Because of technical difficulties encountered to conduct the hydrolysis study, no further testing on aquatic toxicity is requested under this substance evaluation.

Therefore, based on available information, Additiv 104 can be concluded to be potentially P/vP based on screening data and no conclusion can be drawn on the B and T criteria.

A constituent of Additiv 104 has been identified in the scope of activities of the Petroleum and Coal stream Substances (PetCo) Working Group. The methodology to assess the PBT/vPvB properties of such substances is still under discussion by registrants and member states. Thus, no conclusion can currently be made regarding potential PBT/vPvB properties of this constituent.

Conclusion

More investigations are needed to conclude on the PBT properties of Additiv 104. However, due to the analytical difficulties to clearly identify the structures of some constituents, the physico-chemical properties of the identified constituents (low water solubility, high adsorption), the incapacity to determine which constituents or potential transformation/degradation products could be relevant for further testing (because constituents are often outside the domain of applicability of the available models) and because of analytical and experimental limitations as it was raised in the recently provided hydrolysis study, further testing is not technically feasible.

The REACH Annex XIII Section 2.1 gives the Registrant the option to treat the substance "as if it is PBT/vPvB" when:

- screening information indicates that a substance may have PBT/vPvB properties
AND
  - when emissions can be strictly controlled, to avoid further testing.

In ECHA's guideline (Chapter R.11: PBT/vPvB assessment p 100), it is indicated that "there may be cases where it is simply technically not possible to conduct testing, either at screening or at confirmatory level and therefore not possible to derive conclusion (i) or (ii). If there are no indications or justification which would exclude the possibility that the substance could potentially fulfil the criteria, conclusion (iii) should be drawn."

Conclusions (i), (ii) and (iii) are described in the same guidance on p 21:

- "Conclusion (i): The substance does not fulfil the PBT and vPvB criteria. For screening assessment: there is no indication of P or B properties.

- Conclusion (ii): The substance fulfils the PBT or vPvB criteria.

- Conclusion (iii): The available information does not allow to conclude (i) or (ii). The substance may have PBT or vPvB properties. Further information for the PBT/vPvB assessment is needed."

For the Conclusion (iii) two options are proposed:

"-The registrant must generate relevant additional information (including, where necessary, submission of a testing proposal) and carry out Step 1 again,
OR
- The registrant must treat the substance "as if it is a PBT or vPvB".

Therefore, if dispersive uses occur more investigations should be required to state on the PBT properties of Additiv 104. However, because of technical issues mentioned above, additional testing is not technically feasible for the time being.

In order to apply the "known constituent approach" to elucidate the PBT properties of Additiv 104, it should be identified which constituents could be a worst case for persistency and bioaccumulation and focus on them. However, according to the registrant, it is not possible to synthetize individual constituents in sufficient amounts which would allow carrying out the different relevant tests. Moreover, if it turns out that some constituents are not PBT, it will not allow to conclude on Additiv 104 which contains several other constituents in significant amounts (>0.1%). In particular, the evaluating MSCA has no

information to decide which constituent(s) could be considered as worst case regarding PBT properties.

Besides, investigating substances with structures close to the proposed structures of Additiv 104 still remains very challenging. Indeed, Additiv 104 is an UVCB, for which only proposal of representative constituents are available. Moreover, relevant analytical methods for the quantification of proposed representative structures are not available at the being time, therefore it is not expected that experimental data could be found in the literature.

Nevertheless, the evaluating MSCA agrees that read across with substances with similar structures would allow gathering additional data regarding the different constituents of Additiv 104 on their PBT properties. However, such investigations should be carried out through a grouping approach in order to strengthen the findings. It would also legitimate the work to be performed by increasing the tonnages involved when considering several substances through the grouping approach. This alternative should also be considered by industry as a way forward to dig into the question if some constituents exhibit PBT/vPvB properties or alternatively to consider Additiv 104 as a PBT.

In view of these considerations, the evaluating MSCA concludes that no further testing is technically feasible nowadays to clarify the PBT/vPvB properties of Additiv 104. Therefore, the evaluating MSCA recommends to Registrants either to treat the substance as PBT/vPvB based on the precautionary principle or to build a strategy for concluding on its PBT/vPvB properties from information of similar substances.

So far, the concern PBT/ vPvB remains unsolved.

4. FOLLOW-UP AT EU LEVEL

4.1. Need for follow-up regulatory action at EU level

4.1.1. Harmonised Classification and Labelling

Not applicable.

4.1.2. Identification as a substance of very high concern, SVHC (first step towards authorisation)

Not applicable.

4.1.3. Restriction

Not applicable.

4.1.4. Other EU-wide regulatory risk management measures

Not applicable.

5. CURRENTLY NO FOLLOW-UP FORESEEN AT EU LEVEL

5.1. No need for regulatory follow-up at EU level

The PBT/vPvB concern could not be removed because nowadays it is not technically feasible to perform testing to clarify the PBT/vPvB properties of Additiv 104. However, the evaluating MSCA recommends to Registrants either to treat the substance as PBT/vPvB based on the precautionary principle or to build a strategy for concluding on its PBT/vPvB properties based on information from similar substances.

5.2. Other actions

Not applicable.

6. TENTATIVE PLAN FOR FOLLOW-UP ACTIONS (IF NECESSARY)

Not applicable.

Part B. Substance evaluation

7. EVALUATION REPORT

7.1. Overview of the substance evaluation performed

Additiv 104 was originally selected for substance evaluation in order to clarify concerns about:

- PBT/vPvB properties

Table 2

EVALUATED ENDPOINTS	
Endpoint evaluated	**Outcome/conclusion**
PBT properties	Additiv 104 is potentially P/vP based on screening data and no conclusion can be drawn on the B and T criteria. Not further testing is technically feasible nowadays.

7.2. Procedure

Additiv 104 is a NONs substance which was first notified in Germany in 1993 before being notified in France. In July 2008, further information was requested from the registrant by the French Competent Authority (CA) under Directive 67/548/EEC.

- For the purpose of risk assessment: It was requested an in vitro Mammalian Cell Gene Mutation Test- OECD TG 476, and an adsorption/desorption test – OECD TG 106. The registrant provided a summary of the OECD TG 476 test conducted and a waiving justification for the test OECD 106
- For PBT assessment, bioconcentration and water sediment studies (OECD tests 305 and 308) were requested given the potential PBT/vPvB concern of the substance according to screening criteria. However, the studies were not provided. The registrant challenged the expected low biodegradability of the substance and proposed to defer OECD tests 305 and 308 until further clarity on the biodegradation properties is obtained. Besides, additional analytical investigations of Additiv 104 had brought new insights dealing with the identity of the substance. The PBT assessment was therefore completely revised based on these new data.

Additiv 104 was subject to the transitional arrangements in Article 135(2) of REACH. Therefore, information requested under Directive 67/548/EEC was considered as a decision adopted in accordance with Article 52 of the REACH Regulation. The substance was regarded as being included in the CoRAP. In accordance with Article 52 of REACH, the evaluating MSCA was requested to conduct an evaluation of the updated IUCLID 5 dossier of the substance (last update in May 2013).

During the phase of evaluation by the evaluating MSCA, the substance was discussed in the PBT EG meeting (May 2014). The PBT EG brought advices to further investigate the PBT properties of Additiv 104.

A draft decision was prepared requesting further information to clarify the PBT properties of the substance. Among the requests, it was proposed to first solve the stability issue of Additiv 104 in the environment, in order to determine which constituents and/or degradation products are expected to enter in the environment. Indeed, bibliographical information indicates that the stability of Additiv 104 in the environment could be questionable. It was judged efficient and proportionate to focus the assessment on relevant constituents of Additiv 104 which will enter in the environment and/or relevant degradation products

In September 2016, a substance evaluation decision was addressed to the registrant in order to require a new hydrolysis study. The hydrolysis study was provided in May 2018.

7.3. Identity of the substance

Table 3

SUBSTANCE IDENTITY	
Public name:	Reaction product of ammonium molybdate and C12-C24 diethoxylated alkylamine (1:5-1:3)
EC number:	412-780-3
CAS number:	No CAS is assigned for this substance
Index number in Annex VI of the CLP Regulation:	042-004-00-5
Molecular formula:	A complex mixture of species so no unique molecular formula can be given
Molecular weight range:	>473.0 - <1782.0 g/mol
Synonyms:	Additiv 104

Type of substance ☐ Mono-constituent ☐ Multi-constituent x UVCB

Structural formula:

C22H53Mo2N3O9

The analysis of the composition of this complex mixture was performed with adequant and relevant analytical technics. However, the separation of each constituent of the mixture is very hard which increases the difficulties to identify accurately the chemical structure of each constituent. The constituents reported in the registration dossier are considered as potential composition of the Additive 104 derived from analytical observations.

7.4. Physico-chemical properties

Table 4

OVERVIEW OF PHYSICOCHEMICAL PROPERTIES	
Property	**Value**
Physical state at 20°C and 101.3 kPa	Liquid viscous dark red
Vapour pressure	**Value used for CSA:** **Experimental data :** At 20°C : 0.4 Pa At 25°C : 0.72 Pa At 50°c : 10.64 Pa Method OECD 104
Water solubility	**Value used for CSA:** **Experimental data :**<0.85 mg/L at 20°C, pH is not indicated Method EC A6.
Partition coefficient n-octanol/water (Log Kow)	**Value used for CSA:** **Experimental data :** Log Kow > 6.1 at 20°C Method OECD 117 The partition coefficient is estimated as the quotient of the n-octanol and water solubility
Flammability	**Value used for CSA:** Not flammable **Experimental data :** Flash point > 200°C Method EC A.9 The vapour of the substance was not flammable. At room temperature, the substance is stable and does not evolve flammable gases in contact with water or humid air.
Explosive properties	**Value used for CSA:** Not explosive Explosive under influence of flame : No More sensitive to shock than m-dinitrobenzen : No More sensitive to friction than m-dinitrobenzen : not determinated Method EC A.14
Oxidising properties	**Value used for CSA:** Not oxidising Based on the chemical structure of the component of the substance (absence of oxidizing group), no test was conducted.
Granulometry	Not relevant
Stability in organic solvents and identity of relevant degradation products	Based on the composition of the substance, it can be considered as stable in organic solvent
Dissociation constant	Not relevant

7.5. Manufacture and uses

7.5.1. Quantities

Table 5

AGGREGATED TONNAGE (PER YEAR)				
☐ 1 – 10 t	☐ 10 – 100 t	☐ 100 – 1000 t	☐ 1000- 10,000 t	☐ 10,000-50,000 t
☐ 50,000 – 100,000 t	☐ 100,000 – 500,000 t	☐ 500,000 – 1000,000 t	☐ > 1000,000 t	☒ Confidential

7.5.2. Overview of uses

Not public information available.

7.6. Classification and Labelling

7.6.1. Harmonised Classification (Annex VI of CLP)

Additiv 104 is listed on Annex VI of CLP (Index Number: 042-004-00-5)

- Skin Irrit.2, H315
- Skin Sens.1, H317
- Aquatic Chronic 2, H411

7.6.2. Self-classification

Notified classification and labelling according to CLP criteria

- Skin Irrit.2, H315
- Skin Sens.1, H317
- Eye Irrit. 2, H319
- Aquatic Chronic 2, H411

7.7. Environmental fate properties

7.7.1. Degradation

Hydrolysis

No hydrolysis study was initially provided. However, based on the literature, it was assumed that water could induce decomposition of Additiv 104, especially when Mo constituents are separated from the oil constituent in the environment. Indeed, the oil constituent of Additiv 104 was known to act as a moisture protectant and a stabilizer.

However, the characterization of the reaction (kinetic, potential request of catalyst) is not completely elucidated and it was considered relevant to investigate if hydrolysis could occur in environmental conditions, and which constituents and/or degradation products have to be assessed.

A preliminary study showed that hydrolysis of whole Additiv 104 can be carried out. It was argued that the moisture protectant allows a better dispersion of the substance through micelle formations. But on the other hand, more hydrophobic constituents could be retained in the micelle adding a step of separation/diffusion in the experiment which could interfere with the hydrolysis reaction. High hydrolysis rate was reported at pH 9 at 50°C (96% after 5 days), whereas low hydrolysis was observed at pH 4 and 7 at 50°C (8 and 16%, respectively after 5 days). The definitive test showed a very small rate of hydrolysis at environmental pH. A test carried out at 3 different temperatures at pH 7 allows to extrapolate the hydrolysis rate at 20°C and 12°C, leading to half-lifes of 93.2 d and 302 d, respectively.

In the hydrolysis study, the analysis conducted needed a filtration step which leads to the formation of additional chemicals which make difficult the analysis and the interpretation of the results. At last, the complex composition and insolubility of the constituents of Additiv 104 lead to strong analytical issues to determine possible analysis products. In the hydrolysis report, results description mainly consists of observations which could not have been interpreted because of these analytical difficulties. Only molybdenum could be monitored by IC (ionic chromatography) and recovery of all constituents were determined gravimetrically.

Biodegradation

Three ready biodegradation tests were provided for Additiv 104. Only one reliable (RI=2 reliable with restrictions) study (OECD TG 301B) allowed to conclude that the substance is not ready biodegradable. In all three ready biodegradation studies, biodegradation of Additiv 104 remained low. However as some biodegradation occurred, an assessment of the potential relevant metabolites should be required through simulation studies to conclude on the P criterion. Nevertheless, the last provided hydrolysis study shows that testing Additiv 104 raises several technical issues, which support that at present no further testing on Additiv 104 is technically feasible.

Table 6. Screening tests for biodegradation in water

Method	Results	Remarks	Reference
Test type: ready biodegradability OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) sewage, domestic, non-adapted The substance has first been dissolved in tetrahydrofuran and mixed with a filter paper. After evaporation of the solvent, the filter paper was added to the test and toxicity item. Filter paper without tested substance was added to each control and reference item	no biodegradation observed, however test material seen to inhibit micro-organisms % Degradation of test substance (tested at 10 mg C/L), (CO_2 evolution) : 12 after 14d 8 after 21d 0 after 28 d 0 after 60 d Some inhibition of the activated sewage sludge micro-organisms occurred. % Degradation of reference substance (sodium benzoate) 80 after 14 d % Degradation of reference substance in the toxicity control (20 mg C/L of tested substance) 38 after 14d	3 (not reliable)	registration dossier, study report, 2012)
Test type: ready biodegradability OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) activated sludge, domestic, non-adapted Concentration of sludge 30 and 300 mg/L Substance was preliminary dissolved in hexane which has evaporated before the test	inconclusive, but indicating that when bioavailable, test material is biodegradable % Degradation of test substance (10 and 100 µg/L) : 10% after 28 d (Radiochem. meas.) 12-13% after 61 d (Radiochem. meas.) (It is not possible to put the $^{14}CO_2$ concentration into a quantifiable mass balance context to bioavailable [14C]test material due to the radioactivity strongly adhering to the glassware and not being removable during the course of the study.) % Degradation of reference substance (benzoic acid 100 µg/L) without solvent 72-78 after 14 days % Degradation of reference substance (benzoic acid 100 µg/L) with solvent 75-78 after 14 days % Degradation of reference substance in the toxicity control (10 or 100 µg C/L of tested substance + 1.0 mg/L benzoic acid) 76-83 after 14 days	2 (reliable with restrictions) Inorganic carbon content is not provided in the IUCLID file. The validity criterion associated with this parameter has therefore not been checked	registration dossier, study report, 2012

Method	Results	Remarks	Reference
Test type: ready biodegradability EC C.5	not readily biodegradable % Degradation of test substance: ca. 9 after 28 d % Degradation of reference substance (sodium acetate): Ca. 88% after 28d	3 (not reliable) supporting study Test material not provided in IUCLID	registration dossier, study report, 2012

Predictions from QSAR models (Epi Suite) for every representative structure proposed in 2013 (see 7.16) were generated to evaluate the readily biodegradability of each structure supposed to be in Additiv 104 as proposed by the applicant before the recent hydrolysis study (which showed additional constituents).

Constituent and Relevant Property	Mo-containing Structure					Structure without Mo		
	1	2	3	4	5	1	2	3
Ready biodeg. overall BIOWIN	No	No	No	No	No	Yes	No	No
Biowin 2	0.01	0.0001	0.0000	0.0000	0.0000	0.45	0.0002	0.0000
Biowin 3	2.18	1.47	0.46	-0.57	0.84	2.77	2.06	1.35
Biowin 6	0.01	0.0004	0.0000	0.0000	0.0000	0.85	0.31	0.03
Ready biodeg. overall (exp.)	n/a	n/a	n/a	n/a	n/a	inherently biodeg (44% in a 301D test)	n/a	n/a

*. Silica gel has been added to decrease the concentration in the water phase to reduce the toxicity of the tested substance on microorganism. Concentrations of O2 during the test are not provided in the IUCLID file and validity criteria related to this parameter have therefore not been assessed.

According to ECHA Guidance R11, 2017, a substance can be considered as potentially persistent if Biowin 2 probability <0.5 and Biowin 3 probability <2.2 or if Biowin 6 probability <0.5 and Biowin 3 probability <2.2. According to the Biowin predictions, the proposed representative structures of Additiv 104 can be considered as potentially persistent, except one constituent, which has additionally been shown biodegradable even if not readily.

According to the results of QSAR for readily biodegradability, the proposed Mo-containing structures and two others proposed representative structures without Mo were screened as potential P/vP. Nevertheless, only two proposed structures (structure without Mo 1 and 2) are inside the applicability domain of the QSAR. Indeed, software in EPI Suite is commonly applied to assess organic substances and organometallic chemicals generally can be considered outside the domain. Additionally, chemicals with a molecular weight over 698 g/mol are also outside the domain, which is the case for proposed representative structures of Additiv 104, except for the Mo-containing structure 1 and the structure without Mo 1 and 2.

In all three biodegradation tests, biodegradation of Additiv 104 remained low. However as some biodegradation occurred, an assessment of the potential relevant metabolites would be required through simulation studies to conclude on the P criterion. Nevertheless, the last provided hydrolysis study shows that testing Additiv 104 raises several technical

issues, which support that at present no further testing on Additiv 104 is technically feasible. Based on available data, one structure without Mo is expected to be "not persistent". According to their linear structures, the two other structures without Mo are likely to undergo primary degradation, but due to their high molecular size and their high adsorptive capacity, they may have a very limited bioavailability, and hence, a slow degradation. Due to lack of additional information, Additiv 104 should be considered as potentially P/vP based on screening data. Based on linear chain structure considerations, degradation products of one constituent are expected to be "not persistent".

7.7.2. Environmental distribution

Not assessed during the evaluation of the substance.

7.7.3. Bioaccumulation

Regarding to bioaccumulation properties, the assessment was based on QSAR estimations of both Log Kow and BCF values (BCFBAF V3.01) of each representative structure which were proposed in 2013 (see 7.16). These values and the bioaccumulation estimations are reported in the table below.

Constituent and Relevant Property	A104	Mo-containing Structure					Structure without Mo		
		1	2	3	4	5	1	2	3
pKa ACD labs (major base)	n/a	6.16[1]	5.7[1]	6[1]	6[1]	6.4[1]	8.84	8.01	8.01
Log Kow ACD labs	n/a	n/a	n/a	n/a	n/a	n/a	7.63	15.4	23.16
Log Kow KOWWIN	n/a	8.53	12.83	23.13	31.43	11.80	6.63	14.19	21.74
Log Kow SPARC	n/a	n/a	n/a	n/a	n/a	n/a	7.08	13.64	20.1
Log Kow exp.	> 6.1	n/a	n/a	n/a	n/a	n/a	3.4	n/a	n/a
BCF (L/kg) regression base method	n/a	600	19	3.2	3.2	15	466 (81 using exp Log K_{ow})	4	3.2
Biotransformation half-life (days)	n/a	1.96	68.63	16190	92690	10	0.42 (0.04 using exp Log K_{ow})	16.1	622
BCF upper trophic, Arnot-Gobas method	n/a	12	0.92	0.89	0.89	0.92	93.2 (17.2 using exp Log K_{ow})	0.89	0.89
BAF upper trophic, Arnot-Gobas method	n/a	92	32	0.89	0.89	5.50	96.6 (17.2 using exp Log K_{ow})	0.96	0.89

[1]pKas for the organometallics were obtained using structural analogues, replacing Mo with S

Several proposed representative structures fulfil the screening criteria for bioaccumulation (log Kow>4.5). Besides, according to the BCF model predictions, none of the proposed representative constituents should fulfil the B or vB criterion. Nevertheless, most of these constituents are outside the applicability domain of the QSAR.

Indeed, 5 representative constituents are organometallic compounds and SPARC and ACD Labs do not provide predictions for these chemicals. Episuite provided calculations for such chemicals, but results remain uncertain and warning /disclaimer are associated with these predictions. For the proposed representative structures without Mo, the log Kow predictions are relatively consistent between the three models. However, the predictions for one of these constituents are >20, which is considered as implausible and uncertain. Even if Log Kow predictions were relevant, it should be reminded that measured BCF data for chemicals with measures log Kow > ~9 is questionable and only the Mo-containing structure 1 and one structure without Mo have predicted log Kow <9. At last, half of the proposed representative constituents have molecular mass over 1000 g/mol. Nevertheless, because of these high molecular weight, these structure are not expected to be bioaccumulative.

Some constituents are cationic surfactants, and are in the ionic form at environmental pH. The log Kow values are calculated by the software for the neutral forms of the chemicals. Recent evaluations of BCF model indicate that predictions based on the neutral species are assumed to provide conservative BCF estimates for ionic organic carbon (IOCs), based on the dissolved water concentrations, i.e., may be suitable for screening-level predictions (Armitage *et al.*, 2013). However, measured BCF data for cationic surfactants are very limited. In Armitage *et al.* (2013), only data for one of such chemicals is available. This chemical, 1-octanamine, N,N-dioctyl-, (CAS 1116-76-3), is a tertiary amine (C24 H51 N1) with some structural similarity to the organic constituents in Additiv 104. The predicted neutral log Kow for 1-octanamine, N,N-dioctyl- is 10. The measured BCF based on total water concentration is 85 L/kg. The regression BCF in EPI Suite predicts a BCF of 77 L/kg for this chemical. It is noted that there is uncertainty in the Kow of the chemical, as this value does not take into account dissociation. Importantly, the measured BCF value for a structural analogue of some of the Additiv 104 organic molecule constituents is in the range of the predictions for the proposed representative structures without Mo, providing some supportive evidence for the model results.

The log D of structure without Mo has been determined using ADME Boxes version 4.9. The Log D of this constituent is predicted to be 12.6 at pH 9, 9.5 at pH 7 and 8.3 at pH 4 and BCF, BAF and biotransformation half-life have been calculated (see Table below). Taking into account of Log D do not support the assumption that the QSAR based on Kow of neutral form are worst case. However, even with the lowest Log D, derived BCF are below the threshold for the B criterion.

Constituent and Relevant Property	Structure without Mo - 2		
	pH 4	pH 7	pH9
Log D	8.3	9.5	12.6
BCF (L/kg) regression base method	777.1	200.7	23.4
Biotransformation half-life (days)	0.25	0.58	5.23
BCF upper trophic, Arnot-Gobas method	3.3	1.26	0.89
BAF upper trophic, Arnot-Gobas method	3.6	1.53	1.02

The assessment of the biotransformation and resulting predicted BCF values has also been carried out by Arnot Research & Consulting. Indeed, proposed representative structures without Mo of Additiv 104 include alkyl chains and hydroxyl groups which are known to be subject to biotransformation. Two QSAR models were used to assess this parameter to estimate the biotransformation parameter (k_M): QSAR model is the Episuite and the Iterative Fragment Selection k_M-QSAR, which is more related to structural similarity. The two k_M-QSARs used the same database with however some differences in the training and testing set splitting. The combined analysis of the domain of application suggests that the QSARs give "reliable confidence" predictions for only one chemical. The other predictions could potentially be considered but the values should be interpreted carefully.

In a 28 days study conducted with Addtiv 104 in rats, a poor absorption is reported, but with a low metabolism which could indicate a bioaccumulation potential in mammals. Moreover, a log Koa > 5 support a potential bioaccumulation in air-breathing organisms.

Estimated BCF values are below the threshold for B criteria without taking into account biotransformation. However, because of Mo content or physico-chemical properties, the relevance of these estimations are questionable, except for the structure without Mo - 1. For further investigations, it should be kept in mind that biotransformation could be an important parameter for the assessment of the bioaccumulation of Additiv 104 constituents.

Finally, considering the applicability domain based on molecular weight, metal content and predicted log Kow values, only structure without Mo - 1appears as belonging to the application range of the QSAR developed in Episuite for the bioaccumulation. Nevertheless, because of their high molecular weight, several structures are not expected to be bioaccumulative.

7.8. Environmental hazard assessment

7.8.1. Aquatic compartment (including sediment)

7.8.1.1. Fish

Two studies were carried out on *Cyprinus carpio* according to EC C1 in a semi-static design. In the first study, no significant effect was observed at 10 mg/L of Additiv 104 at 96h. A second study was performed in a WAF approach (solutions stirred for circa 67h). As no analytical method was sensitive enough to measure Additiv 104 concentration, EC50 and NOEC were considered to be over the limit of solubility. Despite the low solubility of Additiv 104, no chronic data were provided.

7.8.1.2. Aquatic invertebrates

Two studies were carried out on undetermined aquatic crustacean according to EC C2. In the first study, at 48h the EC50 was 6.8 mg/L and the NOEC was 3.6 mg/L. The second study was performed in a WAF approach (solutions stirred for circa 67h). As no analytical method was sensitive enough to measure Additiv 104 concentration, EC50 and NOEC were considered to be over the limit of solubility. Despite the low solubility of Additiv 104, no chronic data were provided. Chronic data are available for the representative structure without Mo n°1 in ECHA dissemination web site and indicate a high chronic toxicity

especially for *Daphnia magna* (EC10=10.7 µg/L for reproduction), the EC10 however is slightly over the threshold of the T criterion.

7.8.1.3. Algae and aquatic plants

A test according to EC C3 was carried out. The species of tested algae is not reported. Several concentrations (12.5 - 200 mg/L) were tested in a water accommodated fraction (WAF) approach (solutions stirred for 23h).The actual concentration of the test substance in the WAF's could not be determined, since the available analytical method was not sensitive enough. At the two highest loading rates, 100% of inhibition of growth and biomass were reported. Therefore, EC50 was considered to be below the limit of solubility of the substance (0.85 mg/L).

7.8.1.4. Sediment organisms

No data.

7.8.1.5. Other aquatic organisms

No data.

7.8.2. Terrestrial compartment

The terrestrial toxicity tests were provided to show that even if Additiv 104 can strongly be adsorbed onto soil, there would be few adverse effects on organisms. For the registrant, the lack of chronic toxicity effect on terrestrial organisms (earthworm and plants) support that the T criterion is not fulfilled. The evaluating MSCA considers that no conclusion can be drawn on this criterion based on the provided data and due to the lack of chronic aquatic toxicity data. Indeed, the threshold for the T criterion in environment is based on chronic aquatic toxicity data.

A limit test according to OECD TG guideline 222 was carried out on *Eisenia fetida.* The coefficient of variation for reproduction were slightly higher (34% for water control and 40% for solvent control) than recommended in the OECD TG 222 guideline (30%). No statistically significant differences were observed between the Additiv 104 treatment group at 1000 mg/kg dry soil and the solvent control group for production of juveniles.

The long-term effects of Additiv 104 on the emergence, early growth and reproduction of a turnip rape (Brassica rapa) and oat (Avena sativa) were assessed for a period of 45 and 48 days after emergence (DAE), respectively. For turnip, the EC50s for seed pod production and seed pod dry weight were determined as 783.95 and 744.16 mg/kg dry soil, respectively. These were the lowest short-term endpoint values observed, while all other EC50s (including emergence) were in excess of the highest concentration tested (1000 mg/kg dry soil). The lowest No Observed Effect Concentration or NOECs were 62.5 mg/kg dry soil at 14 DAE for turnip rape fresh plant weight, and at 45 DAE for the turnip. For oat, the EC50 for flower production was determined as 863.64 mg/kg dry soil, while the EC50s for flower fresh and dry weight at 810.79 and 494.16 mg/kg dry soil, respectively. The NOECs were either 500 mg/kg for flower production and inflorescences fresh & dry weight, or 1000 mg/kg for shoot fresh and dry weight.

7.8.3. Microbiological activity in sewage treatment systems

No data.

7.8.4. PNEC derivation and other hazard conclusions

Not assessed.

7.8.5. Conclusions for classification and labelling

Substance already classified for environment (Aquatic Chronic 2, H411). Based on data of the proposed structure without Mo n°1, the chronic 2 classification is justified.

7.9. Human Health hazard assessment

Not assessed.

7.10. Assessment of endocrine disrupting (ED) properties

Not assessed.

7.11. PBT and VPVB assessment

1) Persistence,

Experimental studies indicate that Additiv 104 is not readily biodegradable. However, some biodegradation still occurs and it should be investigated if relevant metabolites could result from such degradation. Estimations by QSAR lead to the same conclusion, except for one constituent without Mo which could be considered as "not persistent". However, most of the proposed representative constituents of Additiv 104 are outside of the applicability domain of the QSAR. Based on available experimental data, one constituent without Mo is expected to be "not persistent". According to their linear structure, the two other constituents without Mo which are supposed to be constituents of Additiv 104 are likely to undergo primary degradation, but due to their high molecular size and their high adsorptive capacity, they may have a very limited bioavailability, and hence, a slow degradation. Due to lack of additional information, Additiv 104 should be considered as "potentially P/vP" based on screening data. Based on linear chain considerations, degradation products of supposed constituents of Additiv 104 are unlikely to be persistent. The CATALOGIC model was run with proposed representative constituents of Additiv 104. Most of them were outside the applicability domain of the models, but for those within domain, the BCF were determined using BCFBAF and CATALOGIC. The results did not indicate that any potential metabolite would have a BCF >= 2000 L/kg. Structures with molybdenum are supposed to hydrolyse in the environment leading to molybdenum and the supposed structures without Mo, however the hydrolysis study provided does not support a fast hydrolysis of Additiv 104 in the environment. Moreover, once released in the environment, constituents of Additiv 104 could be still associated with oil which will to some extent protect them from moisture and then from any hydrolysis.

Furthermore, the provided hydrolysis test also indicated that, despite a lot of attempts of technical adaptation and analysis investigations, several technical issues cannot be solved. Indeed, identification of initial constituents remain difficult and speculative considering the used methods. Moreover the formation of potential degradation products and the formation of additional chemicals through the necessary filtration step increase the complexity of the analyses and make the results not possible to interpret. These observations support the conclusion that at present no further testing on Additiv 104 is technically feasible.

The attempt of analysis of constituents and degradation products required a filtration step leading to the formation of additional chemicals which make difficult the analysis and the interpretation of the results. At last, the complex composition and insolubility of the constituents of Additiv 104 led to complex analytical issues to determine possible hydrolysis products. In the hydrolysis report, results description mainly consists of observations which were not interpretable because of analytical difficulties. Only molybdenum could be monitored by IC (ionic chromatography) and recovery of all constituents was determined gravimetrically.

Therefore, due to lack of further data, Additiv 104 is considered as "potentially persistent / very persistent".

2) Bioaccumulation

The assessment of bioaccumulation criterion has been based on QSAR estimations of both Log Kow and BCF values (BCFBAF V3.01) of each representative structure which were proposed in 2013. For each representative constituent considered, QSAR results indicated that B criterion is not fulfilled. However, proposed representative constituents (Mo containing structures, molecular weight over 1000 g/mol for some of the identified constituents, cationic surfactants) are outside the applicability domain of the used QSAR. Because of molecular weight over 1000 g/mol, several structures are not expected to be bioaccumulative. However, this cannot be stated for the other structures.

It is therefore difficult to conclude on the B criterion of the Additiv 104. According to Arnot Research & Consulting, other QSAR models, which could be more suitable for such chemicals could be applied. However, if these QSARs, when they will be available, do not allow to conclude on the B criterion, experimental studies should be carried out. In this case the dietary fish bioaccumulation test should be carried out because of the physico-chemical properties of the substances (low solubility, high Kow). Nevertheless, a recently provided hydrolysis test indicated, despite a lot of attempts of technical adaptation and analysis investigations that several technical issues cannot be solved, which support the conclusion that at present no further testing on Additiv 104 is technically feasible.

In a 28 days study conducted with Additiv 104 in rats, a poor absorption is reported, but with a low metabolism which could indicate a bioaccumulation potential in mammals. Moreover, a log Koa > 5 supports a potential bioaccumulation in air-breathing organisms.

Due to technical difficulties, it is not possible to perform testing to conclude the bioaccumulation assessment for Additiv 104.

3) Toxicity

Despite the low solubility of Additiv 104, only acute aquatic tests have been provided. No adverse effect are observed in the tests on fish. As the tests were carried out at concentrations over the solubility and or with a WAF system (with no analysis of the tested substance), it was considered that EC50 are over the limit of the solubility of Additiv 104.

Two studies were carried out on undetermined aquatic crustacean. In the first study, at 48h, the EC50 was over the limit of solubility and no adverse effect are observed in the second test which was performed in a WAF approach (with no analysis of the tested substance). In a test on a unidentified algae, 100% of inhibition of growth and biomass were reported at several tested load (WAF approach no analysis of the tested substance). Therefore, EC50 was considered to be below the limit of solubility of the substance (0.85 mg/L). Chronic data are available for one proposed representative structure in ECHA

dissemination web site and indicate a high chronic toxicity especially for *Daphnia magna* (EC10=10.7 µg/L for reproduction), the EC10 however is slightly over the threshold of the T criterion.

Chronic terrestrial toxicity tests were provided in the registration dossier to support that the T criterion is not fulfilled. Nevertheless, the evaluating MSCA considers that no conclusion on this criterion can be drawn based on the provided data and due to the lack of chronic aquatic data.

4) Overall conclusion

Experimental studies indicate that Additiv 104 is not readily biodegradable but some biodegradation cannot be completely excluded. However, degradation models are not applicable to organometallics compounds and experimental identification of the potential degradation products will raise technical issues which can at present not be solved.

Due to linear chain considerations, degradation products of proposed representative structures without Mo are unlikely to be persistent. According to their linear structure, structures without Mo are likely to undergo primary degradation but due to their high molecular size, they may have limited bioavailability, and hence, a slow degradation potential. Structures with molybdenum are supposed to hydrolyse in the environment, leading to molybdenum and constituents without Mo. However the hydrolysis study which has been submitted following the substance evaluation decision does not support a fast hydrolysis of Additiv 104 in the environment. Moreover, once released in the environment, constituents of Additiv 104 could be still associated with oil, which will to some extent protect them from moisture and subsequently from any hydrolysis. QSAR results indicate that the proposed representative constituents of Additiv 104, except one, have to be potentially "P or vP" but not "B". However, constituents are outside the applicability domain of the used QSAR. Due to molecular weight over 1000 g/mol, several structures are not expected to be bioaccumulative. However this can not be stated for the other structures.

No chronic aquatic toxicity tests were provided. Low or no adverse effects were observed in the fish and invertebrate studies which where carried out at concentrations over the water solubility of Additiv 104 or with a WAF approach, but without analysis of the tested substance. Strong growth inhibition were reported in a algae study, however, as this study was performed with a WAF approach with no analysis of the tested substance, no conclusion on the T criteria can be drawn from this study. Chronic terrestrial toxicity tests were provided in order to support that the T criterion should not be fulfilled. Nevertheless, the evaluating MSCA prefers not to conclude on this criterion, based on the provided data and due to the lack of chronic aquatic toxicity data.

Therefore, based on available information, Additiv 104 can be concluded to be potentially "P/vP" based on screening data and no conclusion can be drawn on the B and T criteria.

The REACH Annex XIII Section 2.1 gives the Registrant the option to treat the substance "as if it is PBT/vPvB" when:

- screening information indicates that a substance may have PBT/vPvB properties
  AND
  - when emissions can be strictly controlled, to avoid further testing.

In ECHA's guideline (Chapter R.11: PBT/vPvB assessment p 100), it is indicated that "there may be cases where it is simply technically not possible to conduct testing, either at screening or at confirmatory level and therefore not possible to derive conclusion (i) or (ii). If there are no indications or justification which would exclude the possibility that the substance could potentially fulfil the criteria, conclusion (iii) should be drawn."

Conclusions (i), (ii) and (iii) are described in the same guidance on p 21:

- "Conclusion (i): The substance does not fulfil the PBT and vPvB criteria. For screening assessment: there is no indication of P or B properties.
- Conclusion (ii): The substance fulfils the PBT or vPvB criteria.

- Conclusion (iii): The available information does not allow to conclude (i) or (ii). The substance may have PBT or vPvB properties. Further information for the PBT/vPvB assessment is needed."

For the Conclusion (iii) two options are proposed:

"-The registrant must generate relevant additional information (including, where necessary, submission of a testing proposal) and carry out Step 1 again,
OR
- The registrant must treat the substance "as if it is a PBT or vPvB".

Therefore, if dispersive uses occur, more investigations should be required to state on the PBT properties of Additiv 104. However, because of technical issues mentioned above, additional test is not technical feasible at the time being.

The hydrolysis test provided by the registrant shows several technical and analytical issues which could limit the proportionality for requesting further tests. This study particularly shows that despite a lot of attempts of technical adaptation and analysis investigations, strong technical issues were raised, which could not be solved.

One possibility would be to focus on selected constituents, which seems to be easier constituent to analyse or the heaviest Mo containing structure, as a worst case for persistency. However, according to the registrant, it is not possible to synthesize individual constituents in sufficient amounts which would allow carrying out the different relevant tests. Moreover, if it turns out that the selected constituent is not PBT it will not allow to conclude on Additiv 104 which contains several constituents in significant amounts (>0.1%). In particular, we have no information to decide which constituent(s) could be considered as worst case regarding PBT properties.

Besides, investigating substances with structures close to the proposed structures of Additiv 104 still remains very challenging. Indeed, Additiv 104 is an UVCB, for which only a proposal of representative constituents is available. Moreover, relevant analytical methods for the quantification of proposed representative structures are not available for the time being, therefore it is not expected that experimental data could be found in the literature.

Another option could be to investigate substances with structures close to the proposed structures of Additiv 104. This approach would allow gathering additional data regarding the different constituents of Additiv 104 on their PBT properties. Such investigations should be carried out through a grouping approach in order to strengthen the findings. It would also legitimate the work to be performed by increasing the tonnages involved when considering several substances through the grouping approach. This alternative should also be considered by industry as a way forward to dig into the question if some constituents exhibit PBT/vPvB properties or alternatively to consider Additiv 104 as a PBT.

Another constituent of the substance has been identified in the scope of activities of the the Petroleum and Coal stream Substances (PetCo) Working Group. Thus, any conclusion regarding its potential PBT/vPvB properties cannot be made at this point in time.

In view of these considerations, the evaluating MSCA concludes that no further testing is technically feasible nowadays to clarify the PBT/vPvB properties of Additiv 104. The

evaluating MSCA recommends to Registrants either to treat the substance as PBT/vPvB based on the precautionary principle or to build a strategy for concluding on its PBT/vPvB properties from information of similar substances.

So far, the concern PBT/ vPvB remains unsolved.

7.12. Exposure assessment

Not assessed during the evaluation of the substance (not targeted in Substance Evaluation – no initial concern).

7.13. Risk characterisation

Not assessed during the evaluation of the substance (not targeted in Substance Evaluation – no initial concern).

7.14. References

Armitage, J. M.; Arnot, J. A.; Wania, F.; Mackay, D., Development and evaluation of a mechanistic bioconcentration model for ionogenic organic chemicals in fish. *Environ. Toxicol. Chem.* **2013,** *32,* 115–128.

7.15. Abbreviations

BAF: bioaccumulation factor

BCF: bioconcentration factor

CA: competent authority

CoRAP: Community rolling action plant

DAE : day after emergence

EC50: concentration with 50% adverse effect

IC : ionic chromatography

Kow: octanol water partition coefficient

k_M: metabolic rate constant

NOEC: No Observed Effect Concentration

NONS : Notification of New Substances

PetCo: Petroleum and Coal stream Substances

PBT: persistent, bioaccumulative and toxic

PBT EG: PBT expert group

QSAR: Quantitative structure activity relationship

UVCB: substances of Unknown or Variable composition, Complex reaction products or Biological materials

vPvB: very persistent and very bioaccumulative

WAF : water accommodate fraction

7.16. Annex I: Composition of additive 104 (confidential information)

This annex is removed from the public version of this document.