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Protecting the sources of our drinking water

A revised proposal for implementing criteria and an assessment procedure to identify Persistent, Mobile and Toxic (PMT) and very Persistent, very Mobile (vPvM) substances registered under REACH

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Acknowledgments

The German Environment Agency (UBA) submitted this proposal first to the Risk Management Expert Meeting (RiME-2/2017) on the 17th–18th of May 2017 in Łódź, Poland and to the 15th meeting of ECHAs PBT expert group (PBT EG) on the 23rd–24th of May 2017 for comments and suggested revisions. The authors would like to express their gratitude for the very thorough and descriptive comments received from members of both groups, which were mostly positive and supportive towards the need to address the hazards posed by PMT/vPvM substances to the sources of our drinking water. The comments were further discussed during a WEBEX-Meeting on the 16th of August 2017 with the members of the PBT EG and are summarised in the co-submitted documents. This rigorous and insightful feedback has helped progress this paper and our initiative. The feedback and suggestions have been, as far as possible, accommodated in this revised version. The list below provides details of the main changes that have been implemented from the previous version:

- ▶ The goal and scope of this initiative have been clarified in a new section entitled “Aims”.
- ▶ The term irreversible threat was removed and replaced with hazard.
- ▶ The type of water bodies the PMT concept seeks to protect, i.e. the “sources of our drinking water” is now defined as “pristine and sometimes remote freshwater ecosystems, surface water reservoirs, river water that undergoes bank filtration, groundwater aquifers or other aquatic environments that could potentially be used as a drinking water source”
- ▶ More clarity is given to the water treatment and analytical challenges for PMT/vPvM substances.
- ▶ The pH range used in the P and M criteria was extended to 4–9 to better reflect the standard hydrolyses test (OECD TG 111) and a more representative range of environmental pH values.
- ▶ The P criterion has been updated to specify the same temperature and pH range set in the updated PBT guidance document.
- ▶ The criteria and assessment procedure for mobility (M) was considered by most comments to be too conservative and further justification was requested by several comments. Therefore, the mobility criteria itself was adjusted to a less conservative value. A reference to the QSAR screening and impact assessment performed by colleagues from DK and an assessment of monitoring findings as reasoning was added. Additionally the octanol-water distribution coefficient, log D_{ow} , has now been included as a mobility criterion, to address situations in which K_{oc} data is lacking and to reduce workload for registrants.
- ▶ The majority of feedback was in favour of a criterion and assessment procedure for very persistent and very mobile (vPvM) substances. Such a concept has now been added, along with suggested criteria.
- ▶ In relation to the toxicity criterion (T), a clearer rationale on the inclusion of the protection of ecosystem health, as well as human health is now given. Based on the immeasurable value of clean drinking water for European society as a whole, the criteria has been widened compared to the existing Annex XIII for toxicity criteria. The WHO/IPCS definition of an endocrine disruptor, with the criteria laid down in the draft for the COMMISSION REGULATION (EU) .../... of XXX for setting out scientific criteria for the determination of endocrine disrupting properties and amending Annex II to Regulation (EC) 1107/2009 was added.

1 Preamble

Ensuring that the sources of our drinking water are secure from any threats caused by chemicals is of the utmost importance. The United Nations (UN, Resolution 64/292) and the World Health Organization (WHO Guidelines for drinking-water quality) consider access to clean drinking water essential to the realisation of human rights and the protection of human health. Similarly, the European Union's (EU) drinking water directive (98/83/EC, amended 2015/1787) has the objective *“to protect human health from the adverse effects of any contamination of water [...] by ensuring that it is wholesome and clean.”* In addition, the EU's groundwater directive (2006/118/EC) states, *“groundwater is a valuable natural resource and as such should be protected from [...] chemical pollution.”* Further, the EU's water framework directive (2000/60/EC) states that Member States should ensure *“for surface water, the highest ecological and chemical status possible is achieved, given impacts that could not reasonably have been avoided due to the nature of the human activity or pollution.”*

Two of the UN's Sustainable Development Goals (2015) for the next 15 years specifically address the need to protect water resources from chemicals: Goal No 6 *“Ensure availability and sustainable management of water and sanitation for all”* and Goal No 12 *“Ensure sustainable consumption and production patterns”*. Targets within these goals include *“by 2030 to improve water quality by reducing pollution, eliminating dumping and minimizing release of hazardous chemicals and materials...”* (Target 6.3), and *“by 2020 to achieve the environmentally sound management of chemicals and all wastes throughout their life cycle, in accordance with agreed international frameworks, and significantly reduce their release to air, water and soil in order to minimize their adverse impacts on human health and the environment”* (Target 12.4).

A desire to enact these goals is seen on a local scale in Europe. The ‘Memorandum regarding the protection of European rivers and watercourses in order to protect the provision of drinking water’ (IAWR, RIWA, AWE, IAWD, AWWR, 2013) prepared by 170 European water companies across 17 countries, expresses the vision that *“[w]ater must be protected for its own sake. Nobody has a right to pollute water bodies.”* One of the demands of this memorandum is to *“take negative effects on the quality of drinking water due to anthropogenic substances and their degradation and transformation products into account as a criterion in the tests carried out for the approval and registration of chemical substances.”*

These directives, goals and vision statements collectively address a growing threat to the sources of Europe's drinking water and aquatic environments: the increasing number and volume of chemical substances that are being produced every day as Europe's chemical industry continues to innovate and develop new products and technologies. A strategy is needed in order to allow Europe's chemical industry to continue to innovate competitively in the global market, but in a manner that ensures the protection of our drinking water and freshwater environments.

2 Aims of this initiative

With this initiative, the German Environment Agency (UBA) has set out to achieve three major aims: The first aim is to seek consensus on the *need to prevent undue emissions into the environment* by substances, registered under the EU's chemical regulation "REACH" (Regulation EC No 1907/2006), which have the intrinsic substance properties that indicate *a hazard to the sources of our drinking water*. Herein the phrase "sources of drinking water" refers to pristine and sometimes remote freshwater ecosystems, surface water reservoirs, water that undergoes bank filtration, groundwater aquifers or other aquatic environments that could potentially be used as a drinking water source.

The second aim is to establish persistency, mobility and toxicity (PMT) as well as very persistent and very mobile (vPvM) criteria and an assessment procedure that can be used to identify the substances that pose a hazard to the sources of our drinking water.

The third aim is to minimise environmental emissions of PMT/vPvM substances by encouraging registrants to implement risk reduction measures, similar to existing obligations in REACH for Persistent, Bioaccumulative and Toxic / very Persistent and very Bioaccumulative (PBT/vPvB) substances. This will avoid undue contamination to the sources of our drinking water and will protect this valuable resource for future generations.

The implementation of these aims will be beneficial to industry and society alike. It will assist registrants in fulfilling their responsibility of guaranteeing the safe use of registered substances, directly address the Sustainable Development Goals and European directives mentioned in the preamble, and reduce the need for unintended and costly drinking water remediation actions for European society as a whole.

3 What makes a substance a hazard to the sources of drinking water?

In order for a chemical substance emitted into the environment to threaten the sources of drinking water, it must be transported from the point of emission through soil layers, along water courses, through riverbanks, aquifers and other natural or even artificial barriers, over time scales of weeks or more. Only those substance that are both persistent in the environment and mobile in the aquatic environment will survive such a journey and enrich in the water cycle. Accumulating presence of such persistent and mobile substances in the sources of drinking water could reach levels that threaten both ecosystem and human health, particularly if they are toxic at low concentrations or are present at concentrations that exceed ecological thresholds (Liu et al., 2015).

Therefore, those substances that have the *intrinsic substance properties* of being persistent (P) in the environment, mobile (M) in the aquatic environment, and toxic (T) are the ones we must focus on. Analogously, substances that are considered very persis-

tent in the environment (vP) and very mobile in the aquatic environment (vM), regardless of their toxicity, must also be considered, due to their increased probability of reaching and accumulating in the sources of drinking water. We propose to call these substances of concern PMT substances (Neumann, 2017) and vPvM substances.

3.1 Challenges related to water treatment

Once raw water used for drinking water production is contaminated with PMT/vPvM substances, this may lead to an exposure risk for the general population served: A survey in 2014 found that 59 % of Europe used either non-treated drinking water or drinking water treated with only conventional technologies (van der Hoek et al., 2014). Only 41 % used more advanced technologies, such as advanced oxidation processes (like ozonation), granular-activated-carbon (GAC) filtration, ultra-filtration and reverse osmosis. However, even more elaborate treatment processes are not completely effective for all substances. A study of

113 organic compounds with diverse persistency and mobility found that even after clarification, disinfection (chlorination) and GAC filtration, some mobile substances were not effectively removed – e.g. DEET (26 % removal), nonylphenol (73 % removal), camphor (25 % removal) and bisphenol A (76 % removal) through this treatment train (Stackelberg et al., 2007).

The same intrinsic substance properties that lead to persistence in the environment and mobility in the aquatic environment can influence their breakthrough behaviour into raw water, drinking water, wastewater and sewage water treatment, as such substances can be both persistent and mobile through the different treatment steps. For situations in which emissions of PMT/vPvM substances are ongoing and removal during water treatment is poor, their environmental concentrations will increase over time as these substances circulate and enrich in the water cycle. When this occurs, contamination of the water cycle with PMT/vPvM substances can be irreparable (Steinhäuser and Richter, 2006). Relying on retrospective, potentially costly and elaborate water treatment in order to protect or remediate our drinking water is not enough, a pre-emptive and precautionary approach is needed to prevent and minimize emissions into the environment in the first place.

3.2 Challenges related to the analysis of water samples

A substantial analytical challenge exists related to detection and quantification of mobile (polar) substance in water samples. Conventional methods using gas-chromatography (GC) and reverse-phase liquid chromatography (RPLC) are able to detect and quantify a large number of compounds; however, they are not able to detect and quantify the most mobile (polar) substance, such as those with very low octanol-water partition coefficients ($\log K_{ow}$), or very low pH dependent octanol-water partition coefficients ($\log D_{ow}$). This has recently been described as the analytical and monitoring data gap (Reemtsma et al., 2016). There is good indication that there are several mobile (polar) substances in the aquatic environment that remain undetected, unmonitored and consequently unregulated due to the lack of existing analytical techniques. Specialised and often costly analytical techniques to detect mobile substances are currently being developed and may in the future help to ascertain the real dimension of these “undiscovered” contaminants. However, waiting for not-yet available analytical techniques to describe the extent of an already existing contamination by PMT and vPvM substances in Europe’s aquatic environment is irresponsible, if pre-emptive and preventative action can be taken to avoid such contamination in the first place.

4 Protection of the sources of our drinking water through REACH

Safe use of chemicals is a key component of REACH. It serves the purpose to “*ensure a high level of protection of human health and the environment*” (Article 1,1), and is “*underpinned by the precautionary principle*” (Article 1,3). REACH, in its aim and scope, states, that “*it is for manufacturers, importers and downstream users to ensure that they manufacture, place on the market or use such substances that do not adversely affect human health or the environment*” (Article 1,3). Through REACH, it becomes the responsibility of the registrants to characterize the intrinsic hazard of the substances and the risk of each of their uses over their complete life cycle. This inherently includes ensuring that their registered substances do not contaminate the sources of our drinking water. However, currently there is no guidance under REACH to iden-

tify, assess and manage the hazards posed by PMT/vPvM substances.

Registrants, Member States Competent Authorities and ECHA assess substances to see if they fulfil the criteria referred to in Article 57 of REACH and consequently need to be identified as substances of very high concern (SVHC). Persistent, bioaccumulative and toxic (PBT), and very persistent and very bioaccumulative (vPvB) substances are identified as SVHC according to the criteria set out in Annex XIII of REACH. The rationales given in ECHA’s PBT guidance document for this identification are: “*PBT or vPvB substances may have the potential to contaminate remote areas that should be protected from further contamination by hazardous substances resulting from*

human activity because the intrinsic value of pristine environments should be protected"; *"the effects of such accumulation are unpredictable in the long-term"*; and *"such accumulation is in practice difficult to reverse as cessation of emission will not necessarily result in a reduction in substance concentration"*(ECHA, 2017). Based upon these rationales it becomes apparent that PMT/vPvM substances should also be considered, as the concerns presented by their intrinsic substance properties are similar to PBT/vPvB substances: contamination of pristine environments, unpredictable effects, and a potential for long-term contamination even after cessation of emissions.

Currently, there are no criteria agreed on for identifying PMT/vPvM substances as SVHC. Such criteria must currently be applied under Article 57f and would be based on the presence of *"scientific evidence of probable serious effects to human health or the environment which give rise to an equivalent level of concern"*. The case for PMT/vPvM substances to exhibit this equivalent level of concern is that both PBT/vPvB and PMT/vPvM substances persist in the environment and survive the route of transport and of exposure to humans, to remote areas and to pristine environments, with the main difference being their pathways of exposure and transport. For PBT/vPvB substances, human and animal exposure is primarily via the diet, as these substances transport and accumulate via the food chain and biota. For PMT/vPvM substances, exposure is primarily through water sources, as these substances transport with and circulate and enrich within the water cycle, accumulate in remote water sources, and thereby could contaminate the sources of drinking water. Further, the ECHA guidance for PBT/vPvB assessment states the concern that *"a "safe" concentration in the environment cannot be established using the methods currently available with sufficient reliability for an acceptable risk to be determined in a quantitative way"* (ECHA, 2017). This also applies to PMT/vPvM substances, particularly when taking into account the analytical challenges presented in Section 3.2.

We put forth that a similar assessment procedure for PMT/vPvM substances, as currently exists for PBT/vPvB assessments, is warranted. This assessment is comprised of the following steps as outlined in Annex I (4.0.2):

Step 1: Comparison with the Criteria

Step 2: Emission Characterization

For PMT/vPvM substances, "Step 1: Comparison with the Criteria" must be developed, as there is currently no agreement of criteria to be used to identify PMT and vPvM substances. Therefore, it is the aforementioned second aim of this initiative to agree to such a criteria. In essence, "Step 2: Emission Characterization" for PMT/vPvM can follow a similar procedure as already in place for PBT/vPvB substances. Details of how this characterization can be carried out are given in sections R.11.3.4 and R.11.4.1.4 of the REACH PBT guidance document (ECHA, 2017).

Proposed criteria for "Step 1" are presented in the next section of this document. It is emphasized that in relation to Article 57f, substances that are identified as PMT/vPvM would not automatically lead to an initiation of the REACH Article 59 process by the Member State Committee (MSC) for inclusion on the Candidate List of SVHC. The third aim of this initiative is to provide registrants with a means to treat PMT/vPvM substances as they do PBT/vPvB substances (and for other substances meeting the criteria for hazard classes in Article 14(4) of REACH). That is, upon identification of such substances, exposure assessments including the generation of Exposure Scenario(s) for manufacturing and all identified uses over the chemical life cycle are conducted, following Annex I, Section 5. As part of this, recommendations for risk management measures (RMM) for downstream users are provided and enforced. In this way, and analogously to other hazardous substances, PMT/vPvM may only need to be considered for the authorisation regime under REACH, using a case-by-case approach, if registrants do not put the necessary RMM into place.

5 Proposal for the identification of PMT/vPvM substances

The proposed criteria and assessment procedure for identifying PMT/vPvM substances are presented in Figure 1 and discussed below. They were initiated by a research project (Kalberlah et al., 2014) and are based on data, information and procedure steps that are already required within the REACH registration process. Consequently, implementing this proposal for a PMT/vPvM assessment would not necessarily require additional workload for registrants.

Although conducting a PMT/vPvM assessment is the most straightforward for substances with single constituents, the intention is that it can also be used to assess relevant organic constituents, impurities, additives and transformation/degradation products or metabolites of each registered substance. It is not always possible to identify such constituents, for instance for substances of “unknown or variable composition, complex reaction products or biological material” (so called UVCB substances). For these substances, an identification of all substances that may be present over 0.1 % is recommended, as is done as part of the PBT/vPvB assessment (see REACH Article 14,2(b)).

Pure inorganic substances are exempted from this assessment. A formalized definition of organic and inorganic constituents was recently suggested in a screening exercise for persistency and mobility (Arp et al., 2017).

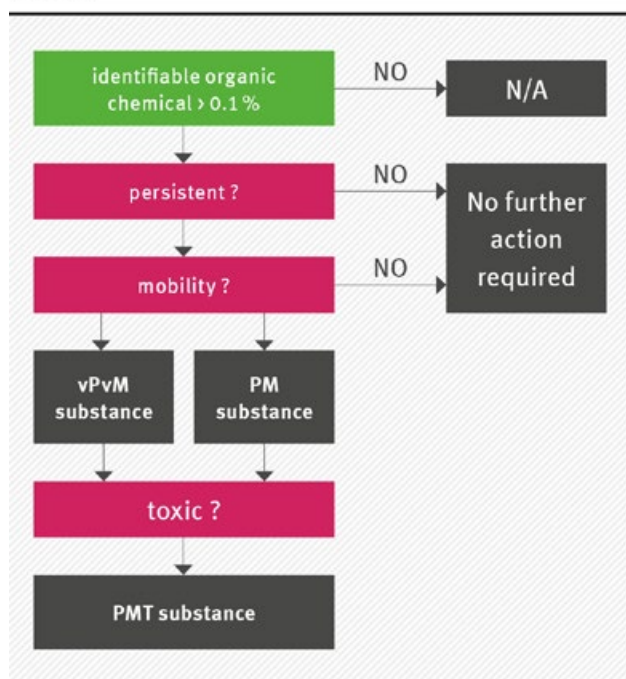
The first step of Figure 1 is to identify if organic and organometallic chemical constituents (including relevant impurities, additives, transformation products or metabolites) of a substance can be identified at greater than 0.1 % abundance. Each such constituent is then assessed for P/vP and M/vM properties. If the substance fails to fulfil the criteria for P/vP or M/vM, no further action is required within this PMT assessment concept. If it fulfils both sets of criteria for vP and vM, it is considered a vPvM substance, otherwise it is considered a PM substance. Following this, toxicity is assessed to see if the substance is considered a PMT substance. Note that some substances may meet the criteria for both vPvM and PMT. The criteria for P/vP, M/vM, and T are proposed below.

5.1 Persistence (P) and very persistent (vP)

For the PMT/vPvM assessment, the proposed persistence criterion (P) and “very persistent” criterion (vP) are the same as Annex XIII of REACH as part of the PBT/vPvB assessment. According to the most recent PBT guidance (ECHA, 2017), for marine environments the reference temperature for persistency data is 9 °C; whereas, for terrestrial and freshwater environments the reference temperature is 12 °C, the pH range to be considered is 4–9 (via the recommendations for hydrolysis measurements after OECD TG 111). For soil and sediment, persistency tests are recommended to be carried out under aerobic or partially aerobic conditions, as solely anaerobic conditions are generally inappropriate, particularly for soil; however, persistency data obtained under anaerobic conditions may be used as part of the weight-of-evidence in the P/vP assessment. It is further noted that volatilization from surface water is not considered within the persistency assessment, as this process is only relevant for surface water transport, and not for groundwater and bank filtration transport.

Figure 1

Overview of the proposed assessment procedure to identify PMT/vPvM substances registered under REACH.



Source: Umweltbundesamt Section IV 2.3 Chemicals

A substance fulfils the persistence criterion (P) in any of the following situations:

- a the degradation half-life in marine water at 9 °C is higher than 60 days;
- b the degradation half-life in fresh or estuarine water at 12 °C and pH 4–9 is higher than 40 days;
- c the degradation half-life in marine sediment at 9 °C is higher than 180 days;
- d the degradation half-life in fresh or estuarine water sediment at 12 °C and pH 4–9 is higher than 120 days;
- e the degradation half-life in soil at 12 °C and pH 4–9 is higher than 120 days.

A substance fulfils the “very persistent” criterion (vP) in any of the following situations:

- a the degradation half-life in marine (9 °C), fresh or estuarine water (12 °C and pH 4–9) is higher than 60 days;
- b the degradation half-life in marine (9 °C) fresh or estuarine water sediment (12 °C and pH 4–9) is higher than 180 days;
- c the degradation half-life in soil (12 °C and pH 4–9) is higher than is higher than 180 days.

5.2 Mobility (M) and very mobile (vM)

For the PMT/vPvM assessment, the proposed mobility criterion (M) and “very mobile” criterion (vM) are introduced here, since criteria for mobility is not explicitly defined in REACH. We propose that only substances that meet the P or vP criterion need to be assessed for mobility. For consistency with the PBT assessment, the criteria presented below refer to terrestrial aquatic environments, at a temperature of 12 °C and values that result in the greatest mobility between a pH range of 4–9. For acids, this would be pH 9, for bases this would be pH 4, and for amphotropic substances this could be anywhere within this range. The intrinsic substance properties used as the basis of the mobility criteria are water solubility, the soil/sediment organic carbon-water partition coefficient (K_{oc}), and the pH-dependant octanol-water partition coefficient (D_{ow}).

The proposed water solubility cut-off criterion of > 0.15 mg/L is based on the minimum solubility a substance would need to have in order to leach through a soil column (Gustafson, 1989), as elaborated in an earlier UBA report (Kalberlah et al., 2014). The K_{oc} value is considered the best available quantifier of subsurface mobility; however, good quality K_{oc} data is not always available to registrants. Therefore, for practical considerations, the D_{ow} can be used when K_{oc} data is not available. D_{ow} can be obtained using the acid-dissociation constant, pK_a , and the octanol-water partition coefficient, K_{ow} (as described in the Appendix). For neutral compounds, K_{ow} is used instead of D_{ow} .

The log K_{oc} (or if not available, the log D_{ow}) we propose as a mobility cut-off in the criterion below is < 4.0 . This value is derived based on three main lines of reasoning. Firstly, a modelling study carried out by UBA reported that substances with a log K_{oc} as high as 4.5 can breakthrough sewage treatment plants and subsequently be emitted into the environment (Kalberlah et al., 2014). Secondly, ground water and drinking water source monitoring studies (Barnes et al., 2008; Lapworth et al., 2012; Loos et al., 2010; Wolter, 2016) reported the presence of compounds with log K_{oc} values as high as 4.0 to 4.5 (e.g. nonylphenol, galoxilide, 17 β -estradiol). However, the majority (ca. 95th percentile) of the substances found in these monitored ground water and drinking water sources had log K_{oc} and log D_{ow} values < 4.0 (see Appendix Tables A1-A2). Thirdly, the criteria are consistent with a draft screening study presented by DK which discovered that an estimated solubility of 0.15 mg/L equates to a log K_{oc} of 4.05.

A substance that fulfils the P or vP criterion also fulfils the mobility criterion (M) in any of the following situations:

- a the highest water solubility is ≥ 0.15 mg/L and the lowest log K_{oc} is ≤ 4.0 at environmentally relevant pH range of 4–9 and at a temperature of 12°C;
- b in the absence of log K_{oc} data, the highest water solubility is ≥ 0.15 mg/L and the lowest log D_{ow} is ≤ 4.0 at environmentally relevant pH range of 4–9 and at a temperature of 12°C.

A substance that fulfils the P or vP criterion also fulfils the “very mobile” criterion (vM) in any of the following situations:

- a the highest water solubility is ≥ 0.15 mg/L and the lowest log K_{oc} is ≤ 3.0 at environmentally relevant pH range of 4–9 and at a temperature of 12°C;
- b in the absence of log K_{oc} data, the highest water solubility is ≥ 0.15 mg/L and the lowest log D_{ow} is ≤ 3.0 at environmentally relevant pH range of 4–9 and at a temperature of 12°C.

5.3 Toxicity (T)

For the PMT/vPvM assessment, the proposed toxicity criterion (T) considers those mentioned in REACH Annex XIII (section 1.1.3) and extra criteria that specifically address concerns for chronic exposure of the general population via drinking water. These additional criteria include carcinogenic category 2, cell mutagenic category 2, effects on lactation, endocrine disruption and a Derived-No-Adverse-Effect-Level (DNEL) of ≤ 9 µg/kg/d (oral, long term, general population). The DNEL proposal is based on a study that derived “thresholds for toxicological concern” (TTC), and found that 9 µg/kg/d was the DNEL cut-off for 95 % of substances exhibiting “moderate or low biological activity” (i.e. CRAMER class II) (Barlow, 2005; Kalberlah et al., 2014).

A substance fulfils the toxicity criterion (T) in any of the following situations:

- a the long-term no-observed effect concentration (NOEC) or EC10 for marine or freshwater organisms is less than 0.01 mg/l;
- b the substance meets the criteria for classification as carcinogenic (category 1A, 1B or 2), germ cell mutagenic (category 1A, 1B or 2), or toxic for reproduction (category 1A, 1B, or 2) according to Regulation EC No 1272/2008;
- c there is other evidence of chronic toxicity, as identified by the substance meeting the criteria for classification: specific target organ toxicity after repeated exposure (STOT RE category 1 or 2) according to Regulation EC No 1272/2008;
- e the substance meets the criteria for classification as “additional category for effects on or via lactation”, according to Regulation EC No 1272/2008;
- f the Derived-No-Adverse-Effect-Level (DNEL) is ≤ 9 µg/kg/d (oral, long term, general population);
- g the substance acts as an endocrine disruptor in humans and/or wildlife species according to the WHO/IPCS definition of an endocrine disruptor. This is always the case if a substance can be identified as an endocrine disruptor for human health and/or the environment according to the criteria laid down in the draft of COMMISSION REGULATION (EU) .../... of XXX for setting out scientific criteria for the determination of endocrine disrupting properties and amending Annex II to Regulation (EC) 1107/2009.

6 The way forward for the protection of the sources of our drinking water

The establishment of criteria and an assessment procedure for identifying PMT/vPvM substances registered under REACH and the implementation of a PMT/vPvM assessment will enable all stakeholders together to protect the sources of our drinking water from REACH registered chemicals. This will bring benefits to each stakeholder.

6.1 Manufacturers, importers and downstream users

Registrants are already invited to perform voluntary PMT/vPvM assessments in the context of their CSA. This will allow the identification of PMT/vPvM substances during REACH registration, or during product development. If the data that is currently available for a PMT/vPvM assessment is of low quality, manufacturers, importers and downstream users should strive to obtain data of better quality in order to carry out a

more accurate assessment. When PMT/vPvM substances are identified, safer alternatives could be considered or RMM should be put into place to minimize emissions into the environment during the whole life cycle of the substance. This would assist industry in fulfilling their obligation under REACH to guarantee safe use of their registered substances.

6.2 Local authorities, water suppliers, and researchers

Such entities are invited to consider identified PMT/vPvM substances registered under REACH for their water monitoring programs, particularly if they have information about these being used in the catchment of the respective water supply. That being said, many PMT/vPvM substances are currently difficult to monitor in the aquatic environment because of a “gap” in suitable analytical methods (see Section 3.2); therefore, a published list of such substances would encourage the development of suitable techniques for their monitoring. Local authorities could use this list of identified PMT/vPvM substances registered under REACH to improve collaborations with local industry, to ensure that strategies to minimize emissions

into the environment are effective. In a worst-case scenario of a contamination of raw water with PMT/vPvM substances, such a list of identified PMT/vPvM substances registered under REACH could be used to enforce remediation action from the polluter.

6.3 ECHA and Member State authorities

ECHA and Member State authorities could provide guidance on the implementation of the PMT/vPvM criteria and assessment procedure. The proposed PMT/vPvM criteria and assessment procedure could be incorporated in ECHA's REACH guidance documents. This will help industry to identify all PMT/vPvM substances during registration under REACH. Only if voluntary measures by industry to minimize emissions into the environment are not effectively protecting the sources of our drinking water, would regulatory instruments need to be applied. Besides the option to propose restrictions, an alternative regulatory instrument is the authorization regime in cases where PMT/vPvM substances are identified as SVHC, following the “equivalent level of concern” criteria referred to in Article 57f of REACH.

7 Proposed plan for implementation

This revised proposal of PMT/vPvM criteria and assessment procedure to identify these substances is available for consultation, discussion and commenting.

In late 2017 the German Environment Agency (UBA) intends to publish an initial list of substances registered under REACH that are considered to fulfil the PMT/vPvM criteria or are candidate PMT/vPvM substances. This list will be based on the direct output of the comments received and revisions made to this document. This substance list will also be made available for consultation, discussion and commenting. If PMT/vPvM criteria are agreed on, the German competent authority intends to propose the first PMT/vPvM substances for candidate listing as SVHC in 2018.

A workshop will be held by the German Environment Agency in Berlin on March the 13–14th, 2018, to discuss how this initiative can best serve industry in fulfilling its obligations under REACH to use a precautionary approach to protect our drinking water. If you are interested in participating in this workshop, please contact the organizers Sarah Hale (sah@ngi.no) or Hans Peter Arp (hpa@ngi.no).

8 For commenting in writing by 04th of December 2017

8.1 On the initiative

Question 1

Does your MSCA, your organisation or you as an expert support the opinion of the German CA that REACH registered substances which are emitted into the environment and which have the intrinsic substance properties to be persistent in the environment, mobile in the aquatic environment, and toxic to environmental or human health (PMT substances) or very persistent in the environment and very mobile in the aquatic environment (vPvM substances) may cause a threat to the sources of our drinking water?

Question 2

Does your MSCA, your organisation or you as an expert support this initiative of the German CA to establish PMT/vPvM criteria and an assessment procedure under REACH?

Question 3

Does your MSCA, your organisation or you as an expert give priority to the establishment of PMT/vPvM criteria?

Question 4

Does your MSCA, your organisation or you as an expert consider that the hazard caused by PMT/vPvM substances, if emitted into the environment, is comparable to the hazard caused by PBT/vPvB substances, as justified in section 4?

8.2 On the proposed criteria

Question 5

Does your MSCA, your organisation or you as an expert support the establishment of the same P and vP criteria set out in Annex XIII of the REACH regulation for the PMT/vPvM assessment as put forward in section 5.1?

Question 6

Does your MSCA, your organisation or you as an expert support the establishment of the revised M and vM criteria for the PMT/vPvM assessment as put forward in section 5.2 and in the appendix?

Question 7

Does your MSCA, your organisation or you as an expert support the establishment of the revised T criteria for the PMT/vPvM assessment as put forward in section 5.3?

8.3 On the Impact

Question 8

Do you see that the implementation of a PMT/vPvM assessment under REACH will bring benefits for manufacturers, importers and downstream users? If yes, which benefits in particular?

Question 9

Do you expect the implementation of a PMT/vPvM assessment under REACH to bring benefits for local authorities, water suppliers and producers of drinking water, and researchers? If yes, which benefits in particular?

Question 10

Do you expect the implementation of a PMT/vPvM assessment under REACH to bring benefits for ECHA and Member State authorities? If yes, which benefits in particular?

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Appendix: Extra information related to the mobility criterion

The mobility criterion should account for neutral, ionic and ionizable substances over the relevant environmental pH range. Guidance tests, such as the recommended hydrolysis test in REACH (OECD TG 111), recommend that tests are done at pH values normally found in the environment (pH 4–9). Accounting for the fate of ionizable substances in soils over this pH range is complex, because the pH can change not only the substance properties but also the subsurface soil properties. Therefore, ideally for such compounds, K_{oc} data should be obtained over the relevant pH range of 4–9.

For practical considerations and as an alternative to K_{oc} values, the pH dependant octanol-water distribution coefficient ($\log D_{ow}$) can be used when K_{oc} information is not available. $\log D_{ow}$ should be reported as part of the Bioaccumulation criteria (B) in the PBT assessment. This parameter can be derived from the octanol-water partition coefficient (K_{ow}) and base-10 logarithm of the acid dissociation constant, pK_a :

$$D_{ow} = (1/(1+10^{(pH - pK_a)}))K_{ow}$$

(for monoprotic acids) (A1)

$$D_{ow} = (1 - 1/(1+10^{(pH - pK_a)}))K_{ow}$$

(for monoprotic bases) (A2)

It follows from these equations that for acids the D_{ow} at pH 9 would be the lowest (most mobile), and for bases the $\log D_{ow}$ at pH 4 would be the lowest (most mobile). However, there are some complex amphoteric substances that may have lower $\log D_{ow}$ at some point in between pH 4 and 9. For neutral compounds, K_{ow} is used instead of D_{ow} . It is noted that use of the D_{ow} may be problematic as surrogate for $\log K_{oc}$ for cations, which may have D_{ow} values that are orders of magnitude lower than K_{oc} values, because the majority of soils are negatively charged. Such considerations should be taken into account when assessing the mobility in the aquatic environment.

Table A1

List of groundwater and drinking water contaminants identified in multiple surveys, along with log K_{oc}, pK_a, log K_{ow} and minimum log D_{ow} values.

Contaminant	Study ^{a)}	Min log K _{oc}	Max log K _{oc}	log K _{oc} Reference ^{b)}	Acidic pK _a ^c	Basic pK _a ^c	log K _{ow} (neutral) ^d	log D _{ow} ^e (minimum)
DEET	A; D	2.1		Pubchem		-0.9	2.0	2.0
Caffeine	A; B; C; D	2.9	3.9	Pubchem		-1.2	-0.1	-0.1
PFOA	A	2.1		(Arp et al., 2006; Zareit-alabad et al., 2013)	-4.2		4.3	-8.9
Atrazine	A	1.7	3.1	Pubchem	14.5	3.2	2.6	2.5
Desethylatrazine	A	1.4	3.5	Pubchem	14.6	3.4	1.5	1.4
1H-Benzotriazole	A	2.2		Pubchem	8.6	0.6	1.4	0.9
PFOS	A	1.3	3.5	(Arp et al., 2006; Zareit-alabad et al., 2013)	-3.3		3.4	-8.9
Simazine	A	1.9	3.6	Pubchem	14.7	3.2	2.2	2.1
Carbamazepine	A; B; D	2.7		Pubchem	16.0	-3.8	2.5	2.4
Bisphenol A	A; D	2.5	3.2	(Staples et al., 1998)	9.8	-5.5	3.3	3.3
PFHxS	A	1.0		Pubchem	-3.3		3.2	-9.2
Terbutylazine	A	2.2		Pubchem	14.2	3.2	3.0	3.0
Bentazone	A	1.1		Pubchem	3.3d)	-9.7	2.8	-2.9
Propazine	A	1.9	2.7	Pubchem	14.3	3.2	2.9	2.9
2,4-Dinitrophenol	A	1.1		Pubchem	4.1 d	-8.1	1.7	-3.2
Diuron	A	2.6		(EC, 2005a)	13.2	-3.2	2.7	2.7
Sulfamethoxazole	A; B; C; D	1.9		Pubchem	6.2	2.0	0.9	-1.9
PFDA	A	2.7		(Schedin, 2013)	-5.2			-14.2
tert-Octylphenol	A	3.4		(EC, 2005c)	10.2	-5.4	3.0	3.0
Metolachlor	A	1.3	3.4	Pubchem	16.8	-4.1	3.1	3.1
Nitrophenol	A	1.2	2.7	Pubchem	7.1	-7.1	1.9	0.0
Isoproturon	A	1.6	2.4	(EC, 2002)	13.8	-3.1		
Hexazinone	A	1.7		Pubchem		-1.2	1.2	1.2
PFBS	A	2.3		Pubchem	1.1		1.8	-6.1
PFNA	A	2.0		(Schedin, 2013)	-6.5		5.5	-10.0
Mecoprop	A	0.7	1.6	Pubchem	3.5	-4.9	3.2	-2.3
Nonylphenol	A; D	3.7	4.5	(EC, 2005b), Pubchem	10.3	-5.5	5.8	5.7
Ketoprofen	A; B; D	0.4		Pubchem	3.9	-7.5	3.1	-2.0
Diazinon	A	2.3	3.3	Pubchem		4.2	3.8	3.4
MCPA	A	1.7	1.8	Pubchem	3.4	-4.9	3.3	-2.4
Chlortoluron	A	2.2	2.6	Pubchem	13.5	-3.2	2.4	2.4
Ibuprofen	A; B; C; D	2.3		(González-Naranjo et al., 2013)	4.9		4.0	-0.2
Methabenzthiazuron	A	2.7		See notef	5.0	1.8		
Dichlorprop	A	1.5	2.1	Pubchem	2.9	-5.0	3.4	-2.6
Diclofenac	A; B; D	2.4		Pubchem	4.0	-2.1	2.4	-2.6
Alachlor	A	2.1	3.3	Pubchem	16.6	-4.2	3.5	3.5
2,4-D	A	1.3	2.1	Pubchem	13.1	-3.6	2.8	2.8
2,4,5-T	A	1.9	2.4	Pubchem	2.6	-5.0	4.0	-2.4
EDTA	B	2.5		Pubchem	2.3	7.7	-3.9	-10.5
Diatrizoic acid	B	1.0		Pubchem	2.2	-4.2	1.4	-5.5
Linuron	A	2.7	3.0	Pubchem	11.9	-4.7	3.2	3.2

Triclosan	A; D	2.9	4.2	REACH dossier, Pubchem	7.7	-3.8	4.8	3.4
Estrone	A; D	2.7	4.3	Pubchem	10.3	-5.4	3.1	3.1
Gabapentin	B	1.7		Pubchem	4.6	9.9	-1.1	-7.0
Metformin	B	1.2		Pubchem		12.3	-2.6	-11.0
Paracetamol	B; C; D	1.3		Pubchem	9.5	-4.4	0.5	0.3
Clofibrilic acid	B; D	-2.1		(Gao and Deshusses, 2011; Scheytt et al., 2005)	3.4	-4.9	2.9	-2.7
Primidon	B; D	2.0		(Stevens-Garmon et al., 2011)	11.5	-6.2	1.1	1.1
Acetylsalicylic acid	B	2.0		Pubchem	3.4	-7.1	1.2	-4.4
Phenazone	B; D			Pubchem		0.5	0.4	0.4
Erythromycin	B	2.8		Pubchem	12.4	8.4	3.1	-1.3
Iopamidol	B	1.0		Pubchem	11.0	-2.8	2.5	2.5
Lincomycin	C; D	1.8		Pubchem	12.4	8.0	0.2	-3.8
sulfamethazine	C; D	1.7	2.2	Pubchem	7.0	2.0	0.1	-1.9
diltiazem	C			Pubchem	12.9	8.2	2.7	-1.5
1,7-dimethylxanthine	C	1.0		Pubchem	10.9	-1.1	-1.9	-1.9
cotinine	C; D	2.1		Pubchem		4.8	0.1	-0.8
cholesterol	C	4.2		Pubchem		-1.4	8.7	8.7
Iopamidol	D	1.0		Pubchem	11.0	-2.8	-2.4	-2.4
Propyphenazone	D			Pubchem		0.9	2.0	2.0
Salicylic acid	D	2.6		Pubchem	2.8	-6.3	2.3	-4.0
Galaxolide	D	3.9	4.6	Reach Dossier, Pubchem		-4.2	5.9	5.9
TCEP	D	2.0		(EU, 2009)	3.2	8.9	1.8	-4.0
17b-Estradiol	D	3.1	4.5	Pubchem, (Stumpe and Marschner, 2010)	10.3	-0.9	4.0	4.0

- a) **Study A.** „Emerging organic contaminants in groundwater: a review of sources, fate and occurrence“ conducted a review of various ground water surveys, and presented a list of organic substances that appeared on at least four independent studies, which is considered here (Lapworth et al., 2012).
- Study B.** „A national reconnaissance of pharmaceuticals and other organic wastewater contaminants in the United States—I Groundwater“ presents a survey of specified substances in remote groundwater sites through the United States. Substances that were detected in these sites were considered here (Barnes et al., 2008).
- Study C.** „Pan-European survey on the occurrence of selected polar organic persistent pollutants in ground water.“ Presents a survey of groundwater sites for drinking water abstraction throughout Europe, as suggested and selected by the „Joint Research Centre's Institute for Environment and Sustainability“. Substances that were detected at these drinking water abstraction sites were considered here (Loos et al., 2010).
- Study D.** A preliminary list of pharmaceuticals compiled by EU Groundwater Watch List, as of December 15, 2016, where the concentration in Europe was found to exceed 0.1 µg/L (Wolter, 2016)
- b) Data from „Pubchem“ were obtained from the NCBI PubChem database „<https://pubchem.ncbi.nlm.nih.gov/>“, accessed September 2017; Data from „REACH dossiers“ refer to the specific dossier for that substance, from „<https://echa.europa.eu/information-on-chemicals/registered-substances>“ accessed March 2015; other sources are given citations.
- c) Estimated values from the software ChemAxon (calculated September 2017), except where indicated.
- d) Data from „the NCBI PubChem database „<https://pubchem.ncbi.nlm.nih.gov/>“, accessed September 2017;
- e) Minimum log D_{ow} for the pH range 4 – 9, based on equations 1 and 2 in the text.
- f) Data from http://www.pesticideinfo.org/Detail_Chemical.jsp?Rec_Id=PC37799, accessed September 2017

Source: As given in the footnotes of Table A1.

Table A2

Selected statistics of the log K_{oc} , log K_{ow} and minimum log D_{ow} values presented in Table A1.

Statistic	log K_{oc} (minimum)	log K_{oc} (all values)	log K_{oc} (median values)	log K_{ow} (neutral)	lowest log D_{ow} (all species)
minimum	-2.1	-	-2.1	-3.9	-14.2
90 th percentile	2.9	3.9	3.4	4.0	3.4
95 th percentile	3.4a)	4.3a)	3.8	5.5	4.0
maximum	4.2	4.6	4.3	8.7	8.7

Source: Umweltbundesamt Section IV 2.3 Chemicals



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