Project Number **861985**	Title **Identification of main release sources of perovskites in PeroCUBE devices**	Deliverable Number **D7.3**
		Version **1.1**

H2020-NMBP-TR-IND-2019

PeroCUBE – High-Performance Large Area Organic Perovskite devices for lighting, energy and Pervasive Communications

Deliverable 7.3

Human Health Risk Assessment for perovskite materials in PeroCUBE devices

WP 7 – Human health risk assessment and life cycle assessment

Authors: Neeraj Shandilya (TNO), Bernice Scholten (TNO), Lia de Simon (TNO), Tom Ligthart (TNO), Susan Dekkers (TNO), Wouter Fransman (TNO)

Lead participant: TNO

Delivery date: 23 May 2023

Dissemination level: Public

Type: Report

The PeroCUBE project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 861985.

Revision History

Author Name, Partner short name	Description	Version	Date
Neeraj Shandilya (TNO), Bernice Scholten (TNO), Lia de Simon (TNO), Tom Ligthart (TNO), Susan Dekkers (TNO), Wouter Fransman (TNO)	First draft deliverable for internal review	V1.0	12/05/2023
Zhongcheng Yuan (UOXF)	Internal review	V1.0	18/05/2023
Quentin Jeangros (CSEM)	Coordinator review	V1.0	18/05/2023
Neeraj Shandilya (TNO)	Final draft deliverable (post internal and partners reviews)	V1.1	23/05/2023

Contents

Executive Summary

This deliverable presents a tier-2 quantitative risk assessment of the perovskite-based devices based on the human health impacts arising due to exposure to potentially toxic substances that have been emitted/released to different environmental compartments (including air, water and soil) over the course of the life cycle of these devices. It is the output of T7.3.

Need for the Deliverable

The overall objective of WP7 is to assess the potential human health risks and to provide a life cycle assessment to balance the risks and benefits of the application of perovskites in lighting and energy harvesting applications. These risks mainly arise from the release of hazardous substances (including materials and solvents) during the production, use or disposal of the perovskite-based devices. Following the tier-0 and tier-1 assessments, potential risks and benefits were identified which were further refined based on the release hotspots. A tier-2 assessment is now needed to quantitatively assess the human health risk based on these identified potential risks and release hotspots. Such tiered approach allows a pro-active approach towards the elimination of any potential risk at an early stage of product development and thus enables a better product design or gives guidelines for an improved value chain design.

Objectives of the Deliverable

The objectives of this deliverable include:

- Presentation of the concept and methodology used for the quantitative human health risk assessment of perovskite-based devices;
- Identification of the chemical compound(s), life cycle stage(s) and environmental compartment(s) which are of potentially high concern for the human health;
- Perform the quantitative human health risk assessment of selected perovskite-based devices.

Outcomes

In the present task, USEtox was employed to calculate the Human Health Impact (expressed as the impact score (IS)) for a variety of (in)organic chemical compounds and perovskite crystals over the course of the entire life cycle of the perovskite-based devices, manufactured at a lab scale with 10 cm^2 of perovskite crystal film. The output *IS* is measured in terms of disability-adjusted life years[1] (DALY) which is the sum of the years of life lost to due to premature mortality and the years lived with a disability due to the toxicity of the substance to which a person is exposed. One DALY represents the loss of the equivalent of one year of full health. The main challenge to calculate the relevant *IS* values was the lack of data on environmental fate, human exposure factors and human toxicity of these compounds in the USEtox database. Consequently, a series of sources were extensively consulted to retrieve the missing information/data as much as possible. This included exploration of different online databases, Safety Data Sheets, PubMed screening of the relevant scientific literature, QSAR and read-

[1] https://www.who.int/data/gho/indicator-metadata-registry/imr-details/158#:~:text=Definition%3A-,One%20DALY%20represents%20the%20loss%20of%20the%20equivalent%20of%20one,health%20condition%20in%20a%20population

across. Based on this, compounds like Formamidinium iodide, 1,3-Di-tert-butylimidazolium tetrafluoroborate, N-Butylammonium bromide, 3-Butenylamine hydrochloride and 2,2'-(Ethylenedioxy)bis(ethylamine) were screened-off from the current risk assessment because either risk assessment is not needed for them (e.g. due to the absence of toxic alerts) for certain exposure routes or no data could be retrieved to calculate their fate, exposure and toxicity factors, despite such an extensive effort. Therefore, extra information needs to be retrieved to perform their risk assessment.

For the rest of the compounds, the human health risk assessment estimated that the impact on the human health is highest during end-of-life phase of the devices' life cycle (IS= 4.99E-10 DALY), compared to other life cycle stages. This is followed by the precursor ink formulation stage during production phase. During the precursor ink formulation stage of the devices, the decreasing order of human health impact obtained for different chemical compounds is CsI (*IS*= 7.32E-11 DALY) > CsBr (*IS*= 3.05E-11 DALY) > PbI_2 (*IS*= 2.30E-11 DALY). During precursor ink formulation and end-of-life, the *IS*, and thus the risk to the human health, is highest through contaminated water. During the devices fabrication and use phase, despite the released amounts are 10 times higher for the water, the *IS* is still higher for the soil which indicates that the risk is primarily dependent on the toxicity factor of the exposure route and the intake availability of a certain compound from an environmental compartment and less dependent on its released amount.

In terms of worker exposure due to the inhalation of the indoor air during the production and disposal of perovskite-based devices at lab scale, all estimated exposure concentrations for relevant compounds were observed to be lower than their corresponding Occupational Exposure Limit (OEL) which signify occupational risk to be unlikely due to the inhalation of released substances in the indoor air at lab scale. The released mass, m, which has been considered from D7.2, and calculated CF are mainly based on the substance-intrinsic properties (e.g. vapor pressure) and assume a "passive" release from the product. For the occupational indoor air situation, we know that this is not the case and a lot of release/exposure scenarios (or process categories) depend on the activity rather than the substance properties. This is a clear deficit of the USEtox model. Thus, onsite experimental measurement data are always needed to be certain before completely ruling out occupational risk likeliness.

It should be noted that the *IS* values reported in this study correspond to the production of 10 cm^2 of perovskite crystal surface (representing lab-scale production). The *IS* values will increase in case of higher crystal surface (e.g. 100 cm^2). Therefore, a new risk assessment will be needed for a perovskite crystal surface area other than 10 cm^2.

The calculated *IS*, were observed to be much lower than the *IS* of the noncommunicable diseases representative for the world caused by the human exposure to toxic chemicals. An incredible amount of perovskite crystals (442,292 kg) needs to be produced for it to be equal to the reported average value (= 2.7 DALY) for non-carcinogenic, yet grave, effects on humans. Even though the production of 442,292 kg of perovskite crystals is way beyond the current scope of the PeroCUBE project (which is limited to lab scale production of perovskite-based devices), it can be a realistic scenario upon devices' production upscaling to mass level, especially considering the current global silicon wafers mass production scale (9 million metric tons approx.[2]) for conventional photovoltaic cells in 2022. Therefore, for such large production scale, human health risks are expected to be significant (e.g. loss of 2.7 years or more of healthy human life per person). Thus, the innovators need to consider alternatives to the material design in their methodology to make it safe to the human health before the perovskite-based technology becomes large enough to be comparable with current silicon wafers production. Such

[2] Global silicon production 2022 | Statista

alternatives include, for example, substitution of lead and caesium halides with tin metal without compromising with high efficiency and stability of the device (Cao and Yan 2021)[3], chemical absorption of lead upon leaking (Li et al. 2021), replacing the use of hazardous solvents like dimethylformamide with dimethyl sulfoxide (Küffner et al. 2021) which has 100 times lesser health impact than dimethylformamide and better devices recycling options (e.g. Chen et al. 2021) and as discussed in more details in D7.2.

The lab scale production of 10 cm^2 sized perovskite film surfaces (with 2 mg approx. of perovskite content), as considered within the PeroCUBE project, does not present any human health risk and thus does not need any such alternative. In fact, no REACH registration is even needed to produce perovskite crystals at such a small scale.

Next steps

The assessed potential impacts of chemical compounds release in this task, providing characterization factors as substance-specific measures of relative impact potential, will be used in a comparative context of Life Cycle Assessment within T7.4. Compounds like lead and caesium halides, life cycle stage of end-of-life and environmental compartment of water have been expected to be elements of potentially high concern upon upscaling which will be integrated in the LCA (T7.4) in order to obtain accurate results on the full spectrum of environmental and human impact categories.

The LCA process is comprised of four steps:

1. goal and scope definition,
2. inventory,
3. impact assessment,
4. interpretation of the results.

The impact assessment phase is the core of the LCA calculation as it is the part that links the masses of the substances emitted to the environment to the relevant impact category. There are different methods that can be used for the life cycle impact assessment, such as ReCiPe[4], Environmental prices[5] or USEtox 2[6]. Each method considers different impact categories and has different characterization factors for each category. Due to the novelty of the considered materials, all possible impacts on the environment and characterisation factors for all the released substances are not possible to determine. For this reason, to fully assess the human toxicity of these materials within the LCA framework, the findings from the human health risk assessment in T7.3 are essential for input to T7.4, as shown in Figure 1.

[3] Although the study claims that the use of tin halide (instead of lead or caesium halide) does not compromise with the efficiency and stability of the device, the PeroCUBE partners argue that it is not completely true and thus there is no efficient alternative to lead at this stage.

[4] LCIA: the ReCiPe model | RIVM

[5] Environmental Prices Handbook EU28 version - CE Delft - EN

[6] USEtox® 2.0 Documentation | USEtox®

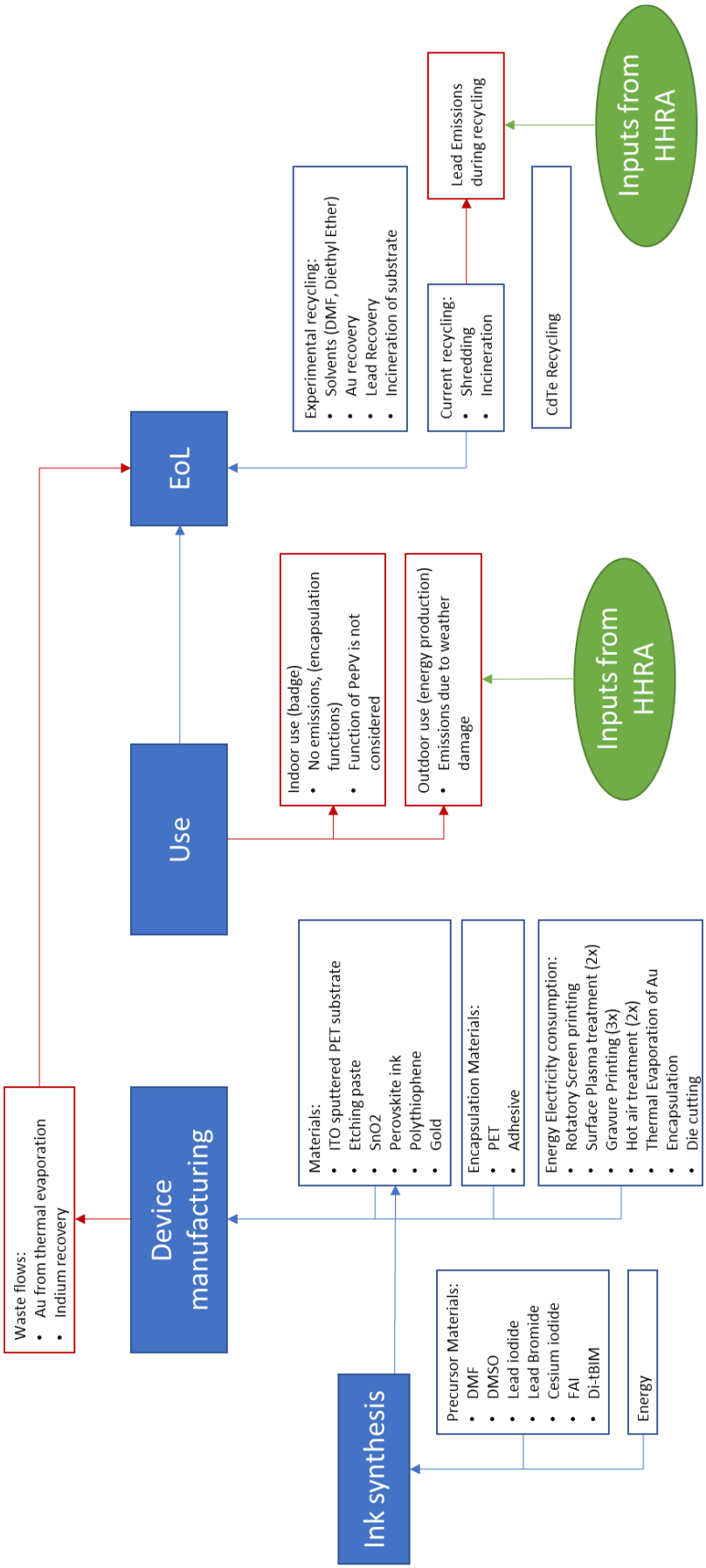

Figure 1: System boundaries for the LCA and the integration point of the HHRA outcomes

1 Introduction

The objective of WP7 is to assess the potential human health risks and to provide a life cycle assessment to balance the risks and benefits of the application of perovskites in lighting and energy harvesting applications. To achieve these goals, a tiered approach is followed, going initially from a qualitative approach (with relatively low input needs and higher uncertainty) to a full quantitative life cycle assessment (LCA) at the end of the project, when the applications will be better defined.

The first task in the WP7, i.e. task 7.1, was to qualitatively assess the benefits and risks of perovskite-based devices compared with their conventional technological counterparts. The assessment was based on a qualitative approach (tier-0) using the LICARA Innovation Scan tool (https://diamonds.tno.nl/#licara). Low to moderate risks and moderate benefits for these perovskite-base devices were observed over their entire life cycle which put the devices development in a transit 'yellow zone' of the tool, signifying them as promising developments. However, they needed additional benefits and even lower risks. The use of hazardous lead halide compounds and volatile solvents and their potential emissions during different life cycle stages were identified and reported as major concerns.

The second task, T7.2, was focused on the identification and quantification of such harmful emissions to different workplace, consumer and environmental compartments (including air, water and soil) over the devices' entire life cycle to highlight potential sources of human and/or environmental exposures. This was done using Hotspot Scan which is a tier-1 assessment tool (https://diamonds.tno.nl/#hotspotscan). The emission of lead ions which occurs throughout the life cycle of the devices and end-of-life stage (in which the majority to environmental emissions take place) were identified as major focal points for human and environmental exposure during the life cycle of the perovskite-based devices.

In the third and current task, T7.3, we focus on a tier-2 quantitative human health risk assessment of the following 3 perovskite-based devices:

- **Perovskite-based photovoltaic (PePV)**: PePV is a type of solar cell or a photovoltaic that uses organo-metallic compounds to produce electricity from sunlight through the photovoltaic effect. The perovskites used in this project are various lead halide compounds. The PePVs act as energy harvesting devices, i.e. devices which are able to capture energy from external sources (e.g. sunlight) and make it available for power applications.
- **Perovskite-based light emitting diodes (PeLED)**: PeLED utilize lead halide perovskite for electroluminescence in the red, green and blue region in the visible light range with potentially high-colour purity and low-cost light emission. They have an optical bandgap that can be tuned in the visible to infrared regions, which makes them very promising for a range of optoelectronics applications.
- **Perovskite-based wearable (PeW)**: PeW mainly serves as a demonstrator for the perovskite-based technology application and the devices using it in the form of a watch/bracelet. It is generally produced using an in-mould integration technology where a flexible foil containing the light emitting PeLED areas, printed conductors and the solar energy harvesting PePV are integrated into one seamless part via injection moulding process.

In this task, we follow a complete life cycle approach for these 3 devices to characterise the release amounts of different chemical compounds (based on T7.2), their environmental distribution and fate in the compartments of air, water and soil, the consequent human exposure through these environmental compartments and toxicity-related effects associated with this human exposure. This

is done using USEtox tool. Through this assessment, relevant compounds, environmental compartments and life cycle stages are sorted in terms of their potential human health impact, which facilitates the integration of this HHRA in the LCA in T7.4.

2 Methodology

In this section, information on different elements in the risk assessment is provided which includes considered perovskite-based devices, life cycle stages of these devices, inventory of different substances used and released per life cycle stage and USEtox tool.

2.1 Perovskite-based devices

As discussed above, following 3 perovskite-based devices are considered in the risk assessment:

- Perovskite-based photovoltaic (PePV)
- Perovskite-based light emitting diodes (PeLED)
- Perovskite-based wearable (PeW)

2.2 Life cycle

This section presents the relevant life cycle stages of a perovskite-based device (e.g. PePV, PeLED). A schematic overview is shown in Figure 2.

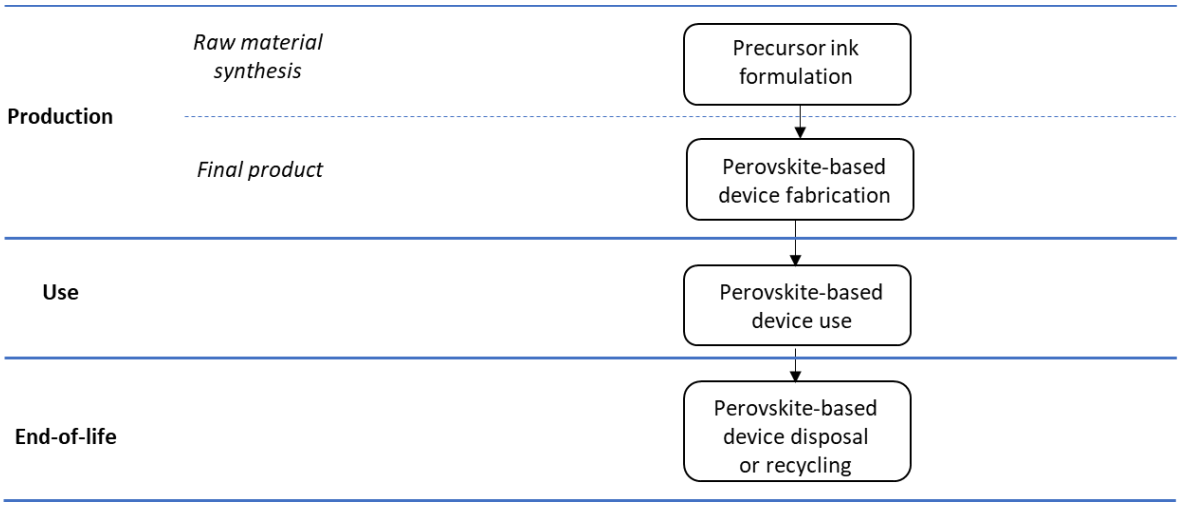

Figure 2: Life cycle stages of a perovskite-based device

The life cycle is considered to start from the device production stage which in itself consists of devices fabrication after the precursor ink formulation. Once the devices are fabricated, they are used, for instance within domestic settings of a house, for energy harvesting and energy emission purposes. Based on the lifetime of the device, they are used for a certain period of time by the consumers and finally are disposed of after their use. The following sections give a detailed overview of the different life cycle stages of the perovskite-based devices.

2.2.1 Production phase

Precursor ink formulation

To formulate the precursor inks, two respective recipes from UOXF and VTT were received for PePV and three respective recipes for red, green and blue PeLED were received from UOXF. These recipes have been optimised over the course of the project to ensure possibly maximum device stability. For PePV, the two respective recipes from UOXF and VTT are very similar to each other in composition except for the (i) Br-content which is lower in the VTT recipe; (ii) use of DMSO which is the only solvent

in the VTT recipe against UOXF recipe in which two solvents, DMSO and DMF, are used and (iii) use of starch as a rheological additive in VTT recipe which is absent in UOXF recipe. Table 1 provides a list of compounds which were ultimately considered (based on the received recipes) for the risk assessment purpose in this task. Since the PeW is assumed to be a bracelet/watch with an integrated PePV and PeLED system, the list of compounds in its case are same as the PePV and PeLED.

Table 1: List of the compounds used for the respective precursor inks formulation for PePV and PeLED

PePV	PeLED		
	Green	Blue	Red
Dimethylformamide (DMF)	Dimethyl Sulfoxide (DMSO)	Dimethyl Sulfoxide (DMSO)	Dimethylformamide (DMF)
Dimethyl Sulfoxide (DMSO)	N-Butylammonium bromide (n-BABr)	3-Butenylamine hydrochloride (BEACl)	Formamidinium iodide (FAI)
1,3-Di-tert-butylimidazolium tetrafluoroborate, 97% (Di-tBIM)	18-crown-6	18-crown-6	2,2'-(Ethylenedioxy)bis(ethylamine) (EDEA)
Formamidinium iodide (FAI)	Lead bromide	Lead bromide	Lead iodide
Methylammonium chloride (MACl)	Cesium bromide (CsBr)	Cesium bromide (CsBr)	Cesium bromide (CsBr)
Lead iodide (PbI_2)			
Lead bromide ($PbBr_2$)			
Cesium iodide (CsI)			

Device fabrication

During the process of production of perovskite-based devices, a thin layer of lead halide perovskite is synthesised from the precursor ink while printing it on a substrate (i.e. in-situ synthesis of perovskite crystalline thin films). The deposition or printing technique is selected depending on the substrate onto which the perovskite thin film is to be deposited. For instance, the deposition of the perovskite film on flexible and rigid substrates takes place by roll to roll (R2R) and sheet to sheet techniques respectively. In general, the bulk density of the deposited perovskite crystalline film is estimated to be in the order of 4.03 g/cm^3 for PePV. Considering a 500 nm-thick layer of perovskite crystalline film, the surface density of the film is equal to 2.015 g/m^2. Since the molar content of lead represents 32.83% of the total molecular weight of the film, its surface density is equal to 0.67 g/m^2 in the film. For PeLEDs, the average film thickness is much lower and estimated to be around 40 nm which corresponds to a surface density of 0.17 g/m^2 for the perovskite film and 0.06 g/m^2 for the lead in the film. These estimations are also valid for PeW.

At the current stage of the project, the potential manufacturing scale (lab, pilot or massive) of the perovskite devices is still uncertain which makes it difficult to carry out the risk assessment for a certain amount of perovskite produced during the devices fabrication stage. Nevertheless, based on the intended applications, approximate amounts of perovskites that are likely to be present in a perovskite-based device can be estimated.

As top boundary, the PePV application for energy production was considered. In this case, a reference unit of 1 kilowatt-peak (1 kWp) is common to compare technologies. Since the potential efficiency of the PePV is currently unknown at this moment, , it is assumed to be 20%, based on the NREL reported

efficiencies of the last years[7]. For a 20% efficient PePV, under standard test conditions, the area corresponding to 1 kWp is 5m^2. This means that 1 kWp of PePV will roughly contain 10 g of perovskite crystals. In case of PeLED, the amount of perovskite is comparatively less than in a PePV. If this estimate is considered for PeLED, it would be a worst-case scenario for a large surface application containing perovskite crystals. Looking at other intended applications of PePV and PeLED, these include small surface applications for energy harvesting, PeW or medical devices or a portable lamp. In these cases, the surface of the PeroCUBE devices is expected to be between 1 and 100 cm^2. In this case, the amounts of perovskite crystals contained in the device vary from 0.06 mg (1 cm^2 LED device) and 20 mg (100 cm^2 PV device). Looking at these rough estimates, it can be seen that the perovskite amounts expected to be found in the PeroCUBE devices vary between less than 1 mg to ~10g. For this reason, the risk assessment for large scale production (e.g. 1000kg) of perovskite crystals (see D7.2) was not carried out as this amount is too far from the intended applications, and such a risk assessment would not deliver useful insights for the project at hand. The risk assessment focuses instead on devices with 10 cm^2 of perovskite crystal surface (representing lab scale production) which correspond to 2 mg and 0.18 mg of perovskite crystals in PePV and PeLED respectively. In addition, the materials used during technology demonstration or application (e.g. substrate itself, aluminium for the PePV mounting, parts of the watch/bracelet for PeW) are kept excluded from the current risk assessment which is focussed only on the perovskites and compounds mentioned in Table 1.

2.2.2 Use phase

PePV

In D7.2, issues of hygroscopicity and potential perovskite crystals run-off in ground and surface water were explained which may affect the lifetime of the PePV and thus its potential eventual risks to the human population upon exposure. In addition, the issue of device encapsulation layer was also considered based on the available literature. At this stage of the project, PeroCUBE partners are still working on different encapsulation techniques (polymeric/glass) to determine the most effective way of keeping the device intact during its use in outdoor conditions which are frequented by rain, hail and temperature fluctuations. To accommodate this factor in our assessment comprehensively, we thus consider four potential scenarios:

(i) Scenario 1: Encapsulation layer remains completely intact and there is no leaching from the device;

(ii) Scenario 2: Slight wear of the encapsulation layer and 5% of the substances from the perovskite crystals in PePV leach to the ground water and soil;

(iii) Scenario 3: Significant wear of the encapsulation layer and 50% of the substances from the perovskite crystals in PePV leach to the ground water and soil;

(iv) Scenario 4: Complete breach of the of the encapsulation layer and all substances from the perovskite crystals in PePV leach to the ground water and soil.

PeLED

When the PeLED is used inside the controlled and moderate environment or ambience of a consumer household, it is believed that, unlike PePV, PeLED is not subjected to any harsh weather or mechanical damage. Consequently an indoor use of the PeLED is believed to not impart the release of perovskite during the use phase. On the other hand, when used outdoors, it is subjected to the same weather or

[7] Best Research-Cell Efficiency Chart (nrel.gov)

mechanical damage as a PePV and is assumed to leach the same amount of lead in the environment per square meter as PePV. For the current risk assessment, we consider that the PeLED is being used indoor applications, e.g. large surface lighting and thus there is no leaching to the environment.

PeW

Similar to PeLED, PeW is also believed to be not subjected to any outside weather and thus not impart any release of perovskite to the environmental compartments during its use. Even though a PeW is excepted to be worn outside and subjected to sweat, movement or friction which may induce perovskite crystals release, any potential release during the use phase is expected to still remain limited into the housing of the perovskite crystals and will not be in direct contact with any of the environmental compartments.

2.2.3 End-of-life phase

Similarly as described in D7.2, three different End-of-life (EoL) routes are considered in this HHRA for the perovskite-based devices: recycling, landfilling and incineration. The issues and ongoing research regarding the recycling and (safe) disposal of the perovskite devices and other electronic waste through these three routes were also explained in detail in D7.2. Following the same approach, as was considered in D7.2, we consider in this HHRA that 41%, 14% and 45% of the left-off perovskite crystals from all perovskite-based devices use will be recycled, landfilled and incinerated respectively.

The 4 potential scenarios of the PePV use phase have direct consequences on the quantity of perovskite crystals reaching their EoL phase. Thus, the EoL phase, also has 4 potential scenarios, each scenario as a result of the use phase scenario:

(i) Scenario 1: Encapsulation layer remains completely intact and 100% of perovskite crystals reach EoL phase;

(ii) Scenario 2: Slight wear of the encapsulation layer and 95% of perovskite crystals reach EoL phase;

(iii) Scenario 3: Significant wear of the encapsulation layer and 50% of perovskite crystals reach EoL phase;

(iv) Scenario 4: Complete breach of the of the encapsulation layer and all perovskite crystals are lost to the ground water and soil before they reach EoL phase.

2.3 USEtox 2.0 model

The USEtox model is used to characterize human toxicological impacts and ecotoxicity in life cycle assessment. It has been developed by a team of researchers from the Task Force on Toxic Impacts under the UNEP-SETAC Life Cycle Initiative (Hauschild et al. 2008, Rosenbaum et al. 2008). It calculates an Impact Score (IS) which is, in case of human impacts, a measure of human health impact of the individual emissions in life cycle inventories of different products. *IS* is calculated using a weighted summation of the releases of substances of a product system with help of characterization factors (eq 1).

$$IS = \sum_{i} \sum_{x} CF_{x,i} \times m_{x,i} \qquad (1)$$

In the present context, IS is the human health impact score (measured in terms of disability-adjusted life years, DALY); $CF_{x,i}$ is the human toxicity characterization factor of substance x emitted to compartment i (DALY/$kg_{emitted}$) and $m_{x,i}$ is the released mass of substance x to compartment i

($kg_{emitted}$). DALY is the sum of the years of life lost to due to premature mortality and the years lived with a disability due to the toxicity of the substance to which a person is exposed. One DALY represents the loss of the equivalent of one year of full health.

In our risk assessment, we consider an aggregated CF which combines both carcinogenic and non-carcinogenic impacts for substance emissions to several environmental compartments. In the context of this project, these environmental compartments are industrial/occupational indoor air, outside air (including urban and continental air), water (including fresh and sea water) and soil (including natural and agricultural soil). USEtox calculates characterization factors for human toxicity of relevant organic and inorganic substances as shown in Figure 3.

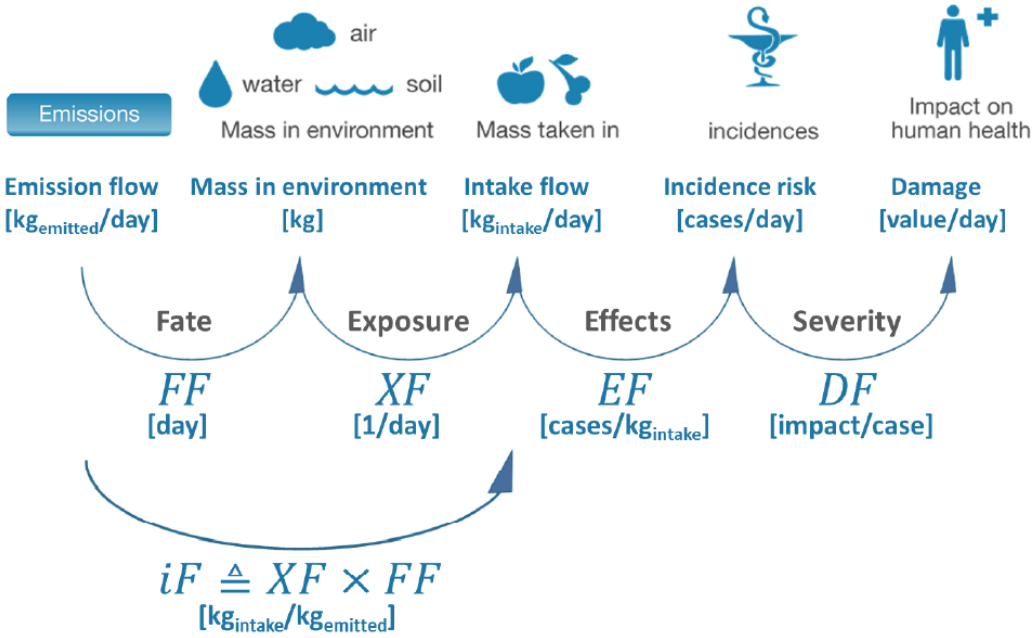

Figure 3: Framework for characterizing human toxicity in USEtox 2.0 (Fantke 2017)

In USEtox, substances that have a potential to increase human disease have a human health characterization factor that is derived from the product of three matrices including fate factors (FF), human exposure factors (XF), and human toxicological effect factors (EF), as shown in equation 2.

$$\boldsymbol{CF = EF.XF.FF} \qquad (2)$$

The product of the fate factor matrix FF and the human exposure factor matrix XF results in the matrix containing human intake fractions (iF). The intake fraction represents the fraction of the mass emitted into a specific compartment that is taken in by the human population (eq 3).

$$\boldsymbol{iF = XF.FF} \qquad (3)$$

In USEtox, intake through inhalation and ingestion routes are considered in iF calculations. Dermal route remains excluded. The fate factors (FF) link the quantity released into the environment to the chemical masses (or concentrations) in a given compartment. Apart from the fate factors and exposure factors, effect factors are also required in the calculation of human-toxicological characterization factors. The effect factor (EF) reflects the change in life time disease probability due to change in life time intake of a pollutant (cases/kg). USEtox determines effect factors for carcinogenic and noncarcinogenic chemicals separately. Data for effects after inhalation and oral (ingestion) exposure are also determined separately.

2.3.1 Substance data use

The fate and human exposure module of USEtox which accounts for removal processes and intermediate transport processes of substances in the environment (e.g. biodegradation by micro-organisms, burial into the sediment, leaching to the groundwater), requires a set of substance-specific input physio-chemical parameters which are shown in Table 2. Human exposure factor reflects the rate at which a substance is able to transfer from a receiving compartment into the human population through a series of exposure pathways based on substance-specific input parameters (Table 2). In USEtox, several human exposure pathways are modelled: Inhalation (of air); Drinking water (ingestion); (Ingestion of) above-ground products (leaf crops, including fruit and cereals); (Ingestion of) below-ground products (root and tuber crops); (Ingestion of) meat; (Ingestion of) dairy products; (Ingestion of) fish; and (Ingestion of) crop residues (from application of agricultural pesticides). The human exposure factor of a substance depends on (i) the properties of the substance, (ii) the selected receiving compartment (e.g. fresh water at the continental scale) and (iii) the exposure pathway (e.g. ingestion of drinking water).

Table 2: Substance-specific data in USEtox for calculating fate and human exposure factors

Factor	Unit	Factor	Unit
Molar mass, MW	g/mol	Dissolved organic carbon and water partitioning coefficient, K_{DOC}	L/kg
Octanol-water partitioning coefficient, K_{OW}	L/L	Rate of constant degradation in air, k_{degA}	1/s
Organic carbon-water partitioning coefficient, K_{OC}	L/kg	Rate of constant degradation in water, k_{degW}	1/s
Henry constant (at 25°C), K_{H25C}	Pa·m³/mol	Rate of constant degradation in sediment, k_{degSd}	1/s
Vapor pressure (at 25°C), P_{vap25}	Pa	Rate of constant degradation in soil, k_{degSl}	1/s
Solubility (at 25°C), Sol_{25}	mg/L	Rate of constant dissipation in above-ground plant tissues, k_{dissP}	1/s
Individual human inhalation/ingestion rate, IR	m³/day	Compartment volume, *V*	m³
Population, *P*	-	Mixing factor, *Mix*	(-)
Total removal rate, *K*	h^{-1}	Bioaccumulation factor for root, BAF_{root}	$kg_{veg}.kg_{soil}^{-1}$
Biotransfer factor for milk, BTF_{milk}	d/kg	Bioaccumulation factor for leaf, BAF_{leaf}	$kg_{veg}.kg_{soil}^{-1}$
Biotransfer factor for meat, BTF_{meat}	d/kg		

Estimation Programs Interface (EPI) Suite is used as a default database by USEtox for the derivation of physio-chemical parameters in Table 2. It uses both experimental and estimated data and, as a general rule, these experimental data are favoured by USEtox over any estimated data. Using this method, data for DMF, PbI_2, $PbBr_2$, CsI and CsBr were retrieved (see the list of compounds in Table 1). For FAI, DMSO and MACl, experimental/estimated data are unavailable in EPI Suite database, due to which USEtox internal estimation routines were applied, as implemented in the sheet «Fate» of the USEtox model file. There are several other compounds in Table 1, i.e. Di-tBIM, n-BABr, 18-crown-6, BEACl and EDEA, for which even the USEtox internal estimation routines are unavailable and thus the corresponding physio-chemical parameters (from Table 2) could not be retrieved. For these

compounds, OECD QSAR toolbox was partly employed (for MW, data was simply retrieved from Safety data sheets of these compounds which are available at the websites of their respective vendors).

OECD QSAR toolbox is a software application intended to fill in the gaps regarding data needed for assessing the risk of chemicals. It incorporates information and tools from various sources into a logical workflow and groups chemicals into different categories. For the aforementioned compounds for which the OECD QSAR toolbox is used, it fills in the relevant data gaps based on the –

- identification of relevant structural characteristics and potential mechanism or mode of action of a target chemical;
- identification of other chemicals that have the same structural characteristics and/or mechanism or mode of action;
- use of existing experimental data.

In addition, other consulted substance inventories include (i) C&L Inventory[8] which contains classification and labelling information on approx. 4,400 substances received from their manufacturers and importers; (ii) REACH factsheets[9] of substances which have been registered and can be placed on the EEA market by those companies with a valid registration; (iii) ChemSpider[10] which is a chemical structure database. Further information specific to each physio-chemical parameter is provided in Table 3 using which information on missing data was retrieved as much as possible.

Table 3: Parameter specific methodology to retrieve the information for different compounds which was missing in the USEtox database (valid unless a specific source to derive the parameter value is mentioned in Table 5)

Parameter	Based on
Octanol-water partitioning coefficient	OECD QSAR (A 'fragment constant' methodology is applied in which the compound structure is divided into fragments (atoms or larger functional groups, whatever option has known coefficient) and their respective values are added together); ChemSpider
Henry constant	ChemSpider; $(P_{vap25} \times MW)/Sol_{25}$;
Vapor pressure	Leistra 2011 ; ChemSpider
Solubility	OECD QSAR; C&L Inventory; ChemSpider; Peng et al. 2021
Dissolved organic carbon and water partitioning coefficient	ChemSpider; REACH factsheet
Degradation rates in air, water, soil and sediment	Footprint 2015 and Sinkkonen and Paasivirta 2000 ; ChemSpider; Horváth et al. 2021; Mallick et al. 2023
Rate constant dissipation in above-ground plant tissues	Fantke et al. 2014
Individual human inhalation/ingestion rate	EPA 2011
Population	Rosenbaum et al. 2008
Compartment volume	Rosenbaum et al. 2015
Mixing factor	Rosenbaum et al. 2015
Total removal rate	Rosenbaum et al. 2015

[8] https://echa.europa.eu/information-on-chemicals/cl-inventory-database
[9] https://echa.europa.eu/information-on-chemicals/registered-substances
[10] ChemSpider | Search and share chemistry

Bioaccumulation factor for root	USEtox database
Bioaccumulation factor for leaf	USEtox database
Biotransfer factor for milk	USEtox database
Biotransfer factor for meat	USEtox database

2.3.2 Human toxicity

The human toxicological effect factor (EF) reflects the change in life time disease probability due to change in life time intake of a pollutant (cases/kg_{intake}). For carcinogenic and non-carcinogenic effects, the effective dose affecting 50% of exposed individuals (ED_{50}) for a defined health endpoint for humans related to inhalation or oral (ingestion) exposure (kg/person/lifetime) is calculated from the daily dose for animal (e.g. rat) and exposure duration (e.g. sub-chronic) per kg body weight that causes a disease probability of 50% for a specific exposure route (mg/kg/d).

Within the USEtox database, ED_{50} values for carcinogenic effects are estimated from the carcinogenic low-dose slope factor (q*) by a 1/q*-to-ED_{50} conversion factor of 0.8, based on animal data, where q* is the carcinogenic, low-dose, slope factor for animal (e.g. rat) and exposure duration (e.g. chronic) for a specific exposure route (kg.day/mg or m^3/mg). In the case of effects other than cancer, the ED_{50} has been estimated from no-observed effect level (NOEL) by a NOEL-to-ED_{50} conversion factor of 9. In case only a LOEL was available, a LOEL-to-ED_{50} conversion factor of 2.25 has been applied. USEtox derives NOELs and LOELs from the IRIS database (http://www.epa.gov/iris/).

For several substances for which no ED_{50} value is derived within the USEtox database, a manual search was performed to derive ED_{50} values: firstly for all substances information was derived on the molecular formula, the molecular weight (MW), CAS number, the SMILES code, and on commonly used synonyms[11].

Subsequently the hazard assessment was conducted by first screening the ECHA database for potential classification and labelling, and to verify if a REACH dossier was present. In addition, the EPA IRIS database was consulted, and a PubMed screening was performed by using the following queries: "*compound name*" AND ("genotox*" OR "carcinogen*" OR "tox*"). If toxicity data could become available from these approaches, a decision was made on the most relevant study to derive a no observed adverse effect level (NOAEL). This was mainly based on the lowest reported NOAEL, unless this study was deemed insufficient. Note that we did not investigate the possibility of applying dose-response modelling, because this work concerns a quick scan on hazards. Based on the NOAEL, a conversion was made to an ED_{50} value (as input for Usetox) based on the Usetox instructions, i.e. the units were converted to kg/person/lifetime, using a default lifetime of 70 years and a default body weight of 70 kg for ingestion and a default inhalation rate of 13 m^3/day and a default lifetime of 70 years for inhalation, all per person (UNEP/SETAC, 2018). We furthermore searched for basic physical and chemical properties, for example by looking into safety data sheets, to obtain information on the physical appearance of the chemical. This could, for example, provide information on whether inhalation exposure is relevant.

[11] The databases and websites used for retrieving this information were: ChemicalBook - Chemical Search Engine, PubChem (nih.gov), ChemSpider | Search and share chemistry

If no data on genotoxicity or carcinogenicity could be found based on the aforementioned approach, a QSAR was performed to give an indication if genotoxicity or mutagenicity should be taken into account. For this purpose the four VEGA models for carcinogenicity (i.e. Antares, ISSCAN-CGX, CAESAR, ISS) were used. Based on the evaluation of their performance by Van Vugt-Lussenburg et al. (2019), the priority order for use of the models is: 1. ISS, 2. ISSCAN-CGX, 3. Antares and 4. CAESAR. In addition, the VEGA consensus model for four SARs for mutagenicity were used (i.e. CAESAR, SARPy/IRFMN, ISS, KNN/Read-Across).

If there was no toxicity data available from the abovementioned sources, the possibilities for read across were explored by using the USEPA comptox chemical dashboard (the GenRA module). The GenRa procedure offers the opportunity to look for similars in the USEPA chemical inventory using a nearest neighbour approach based on chemical, biological or toxicological fingerprints. By filtering on ToxRef[12] data, the search results were limited to potential source chemicals with at least some in vivo data. If there was a good-enough read across candidate (this was based on expert judgement), an additional toxicity search was conducted for the alternative candidate, in line with the approach as described above. In certain cases it was decided to use one part of the compound (i.e., for cesium bromide the ED_{50} value was based on bromide (sodium bromide). If read across was based on compounds which are included in Usetox, the ED_{50} values as derived by USEtox was used.

Because read across did not always result in useful alternatives, we also explored the possibility of using a TTC (Threshold of Toxicological Concern) approach. However due to the general limitations of this approach, including the fact that TTC is only regulatory accepted for oral exposure and the approach is very conservative (i.e., the TTC refers to the fifth percentile of all available NOELs for a certain class of chemicals), we decided that TTC is not a suitable approach. In addition, we considered the fact that for other chemicals in the USEtox database for which no data is available to derive an ED_{50} value, the TTC approach is not applied, so applying the TTC to only the chemicals considered in this work would be inconsistent.

2.3.3 Substance release into environment

The released mass of substance, to be used in equation 1, is considered from D7.2 in which the hotspot scan of the perovskite-based devices was reported. As described in details in D7.2, release of the substances from perovskite-based devices to different workplace, consumer and environmental compartments (including air, water and soil) over the devices' entire life cycle were assessed based on the available scientific papers, Best Available Techniques reference documents, (specific) environmental release categories (spERC/ERC) defined for the EUSES risk assessment used for REACH, Waste Electrical and Electronic Equipment (WEEE) directive, complemented with expert judgement. The released mass of the substances were calculated in D7.2 to produce a reference amount of 1,000 kg of perovskite crystals. For the present task 7.3, those values are extrapolated to produce, use and dispose a reference of 10 cm^2 surface of perovskite crystal film. Also, it is assumed that when a substance releases to air (during production and EoL phase), it is mainly an indoor air release and its remaining fraction is filtered before it reaches the outdoors. Thus, there is no exposure risk or health impact to be expected based on the inhalation of the outside air.

[12] ToxRef is the in vivo toxicity database of USEPA

2.3.4 Occupational exposure and comparison with Occupational Exposure Limits

Following standard practices, the risk due to the worker exposure to the indoor air release of substances is also assessed by comparing it with established Occupational Exposure Limit (OEL) for a substance. OELs are regulatory values which indicate levels of exposure that are considered to be safe (health-based) for a chemical substance in the air of a workplace. Such limits are set by regulatory authorities at EU and national levels, taking into account the available information and most recent data on the hazards of a substance, particularly with respect to carcinogenicity, mutagenicity, toxicity to reproduction and repeated dose toxicity, but also to effects from short-term exposure.[13] To make comparison with OEL, the substance released into indoor air compartment (reported in terms of mass) during production and EoL phases are considered from D7.2, as mentioned previously. The released amounts are converted into exposure amounts by multiplying them with the USEtox calculated *XF* which are then converted into mass-based concentrations (mass per unit volume) by dividing the exposure amounts (in mass) with the archetypical volume of industrial settings (= 350 m^3) for manufacturing facilities in OECD countries (Rosenbaum et al. 2015). The calculations assume presence of one worker during the activity and daily time at work to be equal to 8h. Other details on the used values to calculate *XF* are provided in Table 5.

[13] Occupational exposure limits - ECHA (europa.eu)

3 Results

3.1 Human toxicity factors derivation

Table 4 provides a summary of the derived ED_{50} values for the compounds studied in this work to calculate $\boldsymbol{EF}$. For each compound a detailed explanation is given in the Annex for the rationale of deriving an ED_{50} value.

Table 4. Summary of derived ED_{50} values (kg/person/life time) for cancer and non-cancer endpoints.

Compound	ED_{50} non-cancer (kg/person/lifetime)		Based on	ED_{50} cancer (kg/person/lifetime)		Based on
	Ingestion	Inhalation		Ingestion	Inhalation	
DMSO	2012	1495	Toxicity data	Not required because of lack of genotoxic potential		Toxicity data
Di-tBIM	No data	No data	-	Not required because of the absence of alerts in the QSAR for mutagenicity		QSAR
FAI	No data	No data	-	Not required because of the absence of alerts in the QSAR for mutagenicity		QSAR
MACl	982	No data	-	Not required because of lack of genotoxic potential		QSAR + in vitro assay
n-BABr	No data	No data	-	Not required because of the absence of alerts in the QSAR for mutagenicity		QSAR
CsI	4.3	No data	Read across to sodium iodide	Not required because of the absence of alerts in the QSAR for mutagenicity		QSAR
CsBr	488	No data	Read across to sodium bromide	Not required because of the absence of alerts in the QSAR for mutagenicity		QSAR
18-crown-6	No data	No data	-	50	50	Read across to 1,4 dioxane
BEACl	No data	No data	-	Not required because of the absence of alerts in the QSAR for mutagenicity		QSAR
EDEA	No data	No data	-	Not required because of the absence of alerts in the QSAR for mutagenicity		QSAR
Perovskite crystals (PePV)	0.2*	0.2*	USEtox database for Pb	61.9*	61.9*	USEtox database for Pb
Perovskite crystals (PeLED)	0.1*	0.1*	USEtox database for Pb	50.2*	50.2*	USEtox database for Pb
DMF	5.90	5,90	USEtox database	Not required because of lack of carcinogenic effects		USEtox database

** As reported in D7.2, For the molar Pb content is 32.8% for the application in PePV and it is 40.4% for the application in PeLED.*

Table 5: Derived fate and exposure factors to be used for IS calculation; n/a: not applicable

Compound	Fate factors										Exposure factors					
	MW (g/mol)	K_{OW} (L/L)	K_{H25C} (Pa·m³/mol)	P_{vap25} (Pa)	Sol_{25} (mg/L)	K_{DOC} (L/kg)	k_{degA} (1/s)	k_{degW} (1/s)	k_{degSd} (1/s)	k_{degSl} (1/s)	k_{dissP} (1/s)	IR (m³/day)	P (-)	V (m³)	Mix (-)	K^ (-)
DMF	73.1	0.097	0,007	515.99	1.E+06	n/a	1.31E-05	5.35E-07	5.94E-08	2.67E-07	6.80E-06					
Pb^{2+}*	207.2	n/a	1.00E-20	2.40E-23	not required	4.79E+06	1.E-20	1.E-20	1.E-20	1.E-20	1.E-20					
Cs^{+}#	132.91	n/a	1.00E-20	2.11E-04	not required	8.54E+02	1.E-20	1.E-20	1.E-20	1.E-20	1.E-20					
DMSO	78.13	0.044	1.53E-04	8.13E+01	1.E+06	n/a	4.65E-05	5.35E-07	5.94E-08	2.67E-07	6.94E-06					
MACl	67.52	4.57E+04	2.04E-06	3.11E-09	1.E+03	n/a	3.47E-05	5.35E-07	5.94E-08	2.67E-07	3.25E-07					
18-crown-6	264.31	2.09E-01	1.E-05	8.89E-03	7.5E+04	n/a	7.94E-05	3.09E-07	3.43E-08	1.54E-07	2.85E-07	Inh: 60 Ing: 1.4	6E+9	350	1	12
$CH_3NH_3PbI_3$ Perovskite crystal	620	No data	1.51E-44	1.12E-42	4.6E+04$	n/a	1.E-10@	3.44E-06	1.93E-10	1.93E-10	1.87E-07					
FAI	171.97	No data	No data	1.2E+03	No data	n/a	No data	No data	No data	No data	No data					
Di-tBIM	268.1	No data	No data	No data	No data	n/a	No data	No data	No data	No data	No data					
n-BABr	154.05	No data	No data	No data	No data	n/a	No data	No data	No data	No data	No data					
BEACl	107.58	No data	No data	No data	No data	n/a	No data	No data	No data	No data	No data					
EDEA	148.20	6.76E-03	7.41E-04	0.5	1.E+06	n/a	9.4E-7	1.72E-04	1.55E-03	3.45E-04	No data					

** Both PbI_2 and $PbBr_2$ dissociate into Pb^{2+} ions and halide ions during their intermedia transport processes in the environment. Also, it is the Pb^{2+} which accounts for their toxicity upon exposure. Therefore, both fate and human exposure factors for these two compounds are accounted by Pb^{2+} ion.*

 # Both CsI and CsBr dissociate into Cs^{+} ions and halide ions during their intermedia transport processes in the environment. Also, it is the Cs^{+} which accounts for their toxicity upon exposure. Therefore, both fate and human exposure factors for these two compounds are accounted by Cs^{+} ion.

$ Based on the solubility of $CsPbBr_3$ perovskite crystal (Peng et al. 2021)

@Approximated using the general degradation rate of flexible PET in the air ($<10^{-10}$ s^{-1}) (Chamas et al. 2020; Fantke et al. 2017)

Inh: Inhalation; Ing: Ingestion

^ Total removal rate, K, is the summation of air exchange rate in the building (=12 h^{-1}), removal rate due to indoor air degradation (= 0 h^{-1}) and removal rate due to surface adsorption and degradation (= 0 h^{-1})

3.2 Fate and exposure factors derivation

Values of derived fate and exposure factors for the compounds are provided in Table 5 which constitute $\boldsymbol{FF}$ and $\boldsymbol{XF}$ respectively to calculate $\boldsymbol{iF}$. Depending on the type of compound (organic/inorganic), some of the factors are not applicable (denoted as "n/a" in Table 5). For several compounds like FAI, Di-tBIM, n-BABr, BEACl and EDEA, respective ED_{50} values are either unknown (due to lack of data) or are redundant, as shown in Table 4. Moreover, the fate and exposure factors are also sparsely available for these compounds. Consequently, derivation of $\boldsymbol{CF}$ is not possible for these compounds and they have been kept excluded from further assessment.

Table 5 (contd.): Derived fate and exposure factors to be used for IS calculation

Compound	Exposure factors			
	BAF_{root} ($kg_{veg}.kg_{soil}^{-1}$)	BAF_{leaf} ($kg_{veg}.kg_{soil}^{-1}$)	BTF_{milk} (d/kg)	BTF_{meat} (d/kg)
DMF	1.24	5.52E-03	7.94E-06	4.33E-05
Pb^{2+}*	3.00E-03	1.10E-02	1.90E-04	7.00E-04
$Cs^{+\#}$	8.40E-03	2.90E-02	4.60E-03	2.20E-02
DMSO	1.23	3.32E-03	7.94E-06	4.33E-05
MACl	1.77E+02	6.22E-02	3.63E-04	1.98E-03
18-crown-6	1.24	1.62E-01	7.94E-06	4.33E-05
$CH_3NH_3PbI_3$ Perovskite crystal	3.53	2.13	7.94E-06	4.33E-05
FAI	No data	No data	No data	No data
Di-tBIM	No data	No data	No data	No data
n-BABr	No data	No data	No data	No data
BEACl	No data	No data	No data	No data
EDEA	1.23	2.13E-03	7.94E-06	4.33E-05

** Both PbI_2 and $PbBr_2$ dissociate into Pb^{2+} ions and halide ions during their intermedia transport processes in the environment. Also, it is the Pb^{2+} which accounts for their toxicity upon exposure. Therefore, both fate and human exposure factors for these two compounds are accounted by Pb^{2+} ion.*

\# Both CsI and CsBr dissociate into Cs^+ ions and halide ions during their intermedia transport processes in the environment. Also, it is the Cs^+ which accounts for their toxicity upon exposure. Therefore, both fate and human exposure factors for these two compounds are accounted by Cs^+ ion.

3.3 Risk assessment during production phase

3.3.1 Precursor ink formulation

In Table 6, calculated *IS*, expressed as *DALY*, are shown for different compounds used during the precursor ink formulation for PePV. DMF and DMSO, being solvents, are the only compounds that release mass into the industrial indoor air and thus have a direct impact on human health upon direct worker exposure through aerosols. The highest human health impact is observed for CsI (total *IS*= 7.32E-11 DALY) mainly based on the release to water (due to its higher persistence and insolubility) and secondly for PbI_2 (total *IS*=2.30E-11 DALY) mainly based on the release to soil (due to its low degradation rate in the soil). The total *IS* is observed to be highest for the water compartment, which shows that it is the most likely route to impact the human health to show any carcinogenic/non-

carcinogenic effect depending on the compound. When all environmental compartments are combined, the overall *IS* of the precursor ink formulation stage is estimated to be equal to 1.04E-10 DALY (Figure 4). In Table 7, worker exposure concentration is estimated to be equal to 9.98E-10 mg/m^3 and 2.49 E-10 mg/m^3 for DMF and DMSO respectively. Both of these exposure concentrations are below their respective OELs[14, 15]. There is no release into the indoor air and thus no worker exposure to the rest of the compounds, i.e. MACl, PbI_2, $PbBr_2$ and CsI. Although it has been noted for MACl, that it decomposes into Methylamine and HCl during thermal annealing process. Due to this, the worker is prone to the inhalation exposure of Methylamine particularly. However, we do not expect its released amount to be greater than its OEL (= 12 mg/m^3).

For PeLEDs, the *IS* are lower than PePV in general terms, as shown in Table 8, Table 10 and Table 12. DMSO is the only compound that has *IS* relevant to the release into air for green and blue PeLEDs (=3.36E-16 DALY and 2.86E-16 DALY respectively). The worker exposure concentrations of DMSO are estimated to be equal to 1.56E-09 mg/m^3 and 1.33E-09 mg/m^3 respectively (Table 9 and Table 11) which are both below the OEL. For red PeLED, it is the DMF that has *IS* relevant to the release into air (=7.59E-14 DALY) and its worker exposure concentration is estimated at 1.25E-09 mg/m^3 (Table 13) which is also below its OEL. Similar to PePV, Caesium halide and Lead halide are the compounds with highest *IS* based on their release to water and soil respectively. And with the highest total *IS*, the water compartment is most likely to show any human health impact upon contamination compared to air and soil. When all environmental compartments are combined (Figure 4), the overall *IS* of the precursor ink formulation stage is estimated to be equal to 1.28E-10 DALY (=3.29E-11 DALY for green PeLED + 3.21E-11 DALY for blue PeLED + 6.26E-11 DALY for red PeLED).

IS values for the PeW is estimated to be the sum of individual PePV and PeLED *IS* values (as shown in Figure 4) and all aforementioned compound and environmental compartments related observations remain valid for the PeW.

3.3.2 Device fabrication

The *IS* for the exposure to perovskite crystals during PePV and PeLED (RGB) fabrication are shown in Table 14. Given the greater density of perovskite film in PePV than in PeLED, *IS* is higher for PePV than PeLED, with soil being the environmental compartment with highest total *IS* for both devices. Since the Pb^{2+} ions from the perovskite crystals tend to adsorb to the upper soil layers (Amadi et al. 2018 and Lu et al. 2016), the lead intake by the human body (through ingestion) becomes highly likely and thus has the highest impact. When all environmental compartments are combined, the overall *IS* is estimated to be equal to 6.45E-13 DALY and 1.15E-13 DALY for PePV and PeLED fabrications respectively (Figure 4). The worker exposure concentration is estimated to be equal to 5.73E-11 mg/m^3 and 5.10E-12 mg/m^3 during PePV and PeLED fabrications respectively, both of which are below the OEL for lead metal (=0.1 mg/m^3)[16].

Since the PeW is essentially an integration of PePV and PeLED into one device, its *IS* for each environmental compartment during its fabrication is simply the sum of their individual *IS* values, as shown in Table 14 and Figure 4.

[14] https://nj.gov/health/eoh/rtkweb/documents/fs/0759.pdf
[15] https://www.ilo.org/dyn/icsc/showcard.display?p_lang=en&p_card_id=0459&p_version=2
[16] https://www.ncbi.nlm.nih.gov/books/NBK206974/

3.4 Risk assessment during use phase

In Table 16, calculated IS are shown for the 4 potential scenarios during use phase of the PePV devices. Among the 4 potential scenarios, as expected, scenario 4 has the highest total *IS* (= 2.45E-10 DALY) in which there is assumed to be 100% breach of the encapsulation layer, while scenario 1 has the least total IS (=0) in which there is assumed to be no breach in the encapsulation layer. When the two compartments are compared, the human health impact through soil is consistently higher for all 4 scenarios despite greater release amounts to water. This observation is supported by Mallick et al. 2023 which demonstrated that, upon leaching, Pb^{2+} ions from the perovskite crystals are strongly retained into the soil and thus are more available for human intake than from water. This shows that soil is the compartment to most likely have the greater human health impact upon contamination than water. For PeLED and PeW, due to the absence of any perovskite release, any risk to the human health is highly unlikely and thus the *IS* is equal to 0 for both devices.

3.5 Risk assessment during end-of-life phase

The use phase of the PePV has direct consequences on the *IS* calculation during its EoL phase. The 4 potential scenarios have different perovskite crystals amounts reaching the device's EoL. Thus, the EoL phase, also has 4 potential scenarios, each scenario as a result of the use phase scenario (Table 17). Scenario 1 in which it is assumed that 100% of the perovskite crystals reach their EoL has the highest total *IS* equal to 1.45E-10 DALY with all environmental compartments combined, followed by scenario 2 with total *IS* equal to 1.38E-10 DALY (Figure 4). On the other hand, scenario 4 with no perovskite available (assuming 100% of it leached out during use phase), has the least *IS* (=0). For all 4 scenarios, there is no expected emission to soil and compared to air, the higher impact is through water for which impact on the human health is consistently seen to be higher due to perovskite leaching during landfilling. For outside air, *IS* values are calculated to be in the order of 10^{-16} DALY during landfilling. The worker exposure concentration during PePV incineration is expected to be highest during scenario 1 (=9.35E-11 mg/m^3) but it is lower than the OEL for lead (Table 18).

For the PeLED (RGB), since all perovskite content reaches EoL, there is only one scenario in which highest *IS* (= 1.73E-11 DALY) is calculated for water during landfilling (Table 19). In terms of magnitude, this *IS* value is even lower than the *IS* for scenario 3 of the PePV (= 7.24E-11 DALY) in which 50% of the perovskite reaches to the EoL. When all environmental compartments are combined, the overall *IS* of the EoL phase for the PeLED is estimated to be equal to 2.57E-11 DALY. The worker exposure concentration during PeLED (RGB) incineration is estimated to be equal to 8.39E-12 mg/m^3 (Table 20) which is lower than the OEL for lead.

For the PeW too, all perovskite content reaches the end of life. Therefore, combined estimations from scenario 1 of the PePV and PeLED remain valid for the PeW.

Table 6: Calculated Impact scores (in terms of DALY) for exposure to compounds relevant during precursor ink formulation for PePV; $IS = CF \times m$

Compound	Industrial indoor air			Outside air			Water			Soil			Total IS per compound (y)
	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	
DMF	5.24E-05	1.76E-09	9.22E-14	1.16E-05	0	0	8.92E-06	3.52E-08	3.14E-13	1.24E-05	1.76E-10	2.17E-15	4.08E-13
DMSO	1.22E-07	4.39E-10	5.37E-17	2.95E-08	0	0	2.69E-08	8.79E-09	2.37E-16	3.78E-08	4.39E-11	1.66E-18	2.92E-16
MACl	1.36E-07	0	0	6.38E-08	0	0	5.52E-08	9.02E-08	4.98E-15	7.87E-08	4.43E-10	3.49E-17	5.01E-15
PbI_2	4.61E-02	0	0	8.80E-02	0	0	1.65E-04	2.55E-08	4.22E-12	1.47E-01	1.28E-10	1.88E-11	2.30E-11
$PbBr_2$	4.61E-02	0	0	8.80E-02	0	0	1.65E-04	8.55E-09	1.41E-12	1.47E-01	4.27E-11	6.29E-12	7.70E-12
CsI	7.80E-03	0	0	1.58E-02	0	0	1.98E-02	3.68E-09	7.29E-11	1.57E-02	1.84E-11	2.90E-13	7.32E-11
		Total IS	6.04E-14		Total IS	0		Total IS	7.89E-11		Total IS	2.54E-11	

Table 7: Calculated worker exposure concentration during precursor ink formulation stage for PePV

Compound	Released mass, $mg_{emitted}$	*XF* (-)	Exposed mass, $mg_{exposed}$	Exposure concentration (mg/m^3)	OEL (mg/m^3)	<OEL?
DMF	1.76E-03	1.98E-04	3.49E-07	9.98E-10	29.9	Yes
DMSO	4.39E-04	1.98E-04	8.71E-08	2.49E-10	160	Yes

Table 8: Calculated Impact scores (in terms of DALY) for exposure to compounds relevant during precursor ink formulation for green PeLED; $IS = CF \times m$

Compound	Industrial indoor air			Outside air			Water			Soil			Total IS per compound (y)
	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	
DMSO	1.22E-07	2.75E-09	3.36E-16	2.95E-08	0	0	2.69E-08	5.50E-08	1.48E-15	3.78E-08	2.75E-10	1.04E-17	1.83E-15
18-crown-6	1.67E-05	0	0	6.64E-06	0	0	7.06E-06	2.00E-10	1.41E-15	8.75E-06	1.00E-12	8.76E-18	1.42E-15
$PbBr_2$	4.61E-02	0	0	8.80E-02	0	0	1.65E-04	2.63E-09	4.35E-13	1.47E-01	1.32E-11	1.94E-12	2.37E-12
CsBr	7.80E-03	0	0	1.58E-02	0	0	1.98E-02	1.54E-09	3.04E-11	1.57E-02	7.68E-12	1.21E-13	3.05E-11
		Total IS	3.36E-16		Total IS	0		Total IS	3.08E-11		Total IS	2.06E-12	

Table 9: Calculated worker exposure concentration during precursor ink formulation stage for green PeLED

Compound	Released mass, $mg_{emitted}$	*XF* (-)	Exposed mass, $mg_{exposed}$	Exposure concentration (mg/m^3)	OEL (mg/m^3)	<OEL?
DMSO	2.75E-03	1.98E-04	5.46E-07	1.56E-09	160	Yes

Table 10: Calculated Impact scores (in terms of DALY) for exposure to compounds relevant during precursor ink formulation for blue PeLED; $IS = CF \times m$

Compound	Industrial indoor air			Outside air			Water			Soil			Total IS per compound (y)
	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	
DMSO	1.22E-07	2.34E-09	2.86E-16	2.95E-08	0	0	2.69E-08	4.69E-08	1.26E-15	3.78E-08	2.34E-10	8.87E-18	1.56E-15
18-crown-6	1.67E-05	0	0	6.64E-06	0	0	7.06E-06	1.70E-10	1.20E-15	8.75E-06	8.52E-13	7.46E-18	1.21E-15
$PbBr_2$	4.61E-02	0	0	8.80E-02	0	0	1.65E-04	2.58E-09	4.27E-13	1.47E-01	1.29E-11	1.90E-12	2.33E-12
CsBr	7.80E-03	0	0	1.58E-02	0	0	1.98E-02	1.50E-09	2.97E-11	1.57E-02	7.49E-12	1.18E-13	2.98E-11
		Total IS	2.86E-16		Total IS	0		Total IS	3.01E-11		Total IS	2.02E-12	

Table 11: Calculated worker exposure concentration during precursor ink formulation stage for blue PeLED

Compound	Released mass, $mg_{emitted}$	*XF* (-)	Exposed mass, $mg_{exposed}$	Exposure concentration (mg/m^3)	OEL (mg/m^3)	<OEL?
DMSO	2.34E-03	1.98E-04	4.64E-07	1.33E-09	160	Yes

Table 12: Calculated Impact scores (in terms of DALY) for exposure to compounds relevant during precursor ink formulation for red PeLED; $IS = CF \times m$

Compound	Industrial indoor air			Outside air			Water			Soil			Total IS per compound (y)
	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	
DMF	3.43E-05	2.21E-09	7.59E-14	1.16E-05	0	0	8.92E-06	4.42E-08	3.95E-13	1.24E-05	2.21E-10	2.73E-15	4.73E-13
PbI_2	4.61E-02	0	0	8.80E-02	0	0	1.65E-04	3.24E-09	5.36E-13	1.47E-01	1.62E-11	2.38E-12	2.92E-12
CsBr	7.80E-03	0	0	1.58E-02	0	0	1.98E-02	2.98E-09	5.90E-11	1.57E-02	1.49E-11	2.34E-13	5.92E-11
		Total IS	7.59E-14		Total IS	0		Total IS	5.99E-11		Total IS	2.62E-12	

Table 13: Calculated worker exposure concentration during precursor ink formulation stage for red PeLED

Compound	Released mass $mg_{emitted}$	*XF* (-)	Exposed mass, $mg_{exposed}$	Exposure concentration (mg/m^3)	OEL (mg/m^3)	<OEL?
DMF	2.21E-03	1.98E-04	4.38E-07	1.25E-09	29.9	Yes

Table 14: Calculated Impact scores (in terms of DALY) for exposure to perovskite crystals during PePV and PeLED (RGB) fabrication; $IS = CF \times m$

Device	Industrial indoor air			Outside air			Water			Soil		
	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)
PePV	3.26E-03	1.01E-10	3.28E-13	3.77E-03	0	0	4.83E-05	2.01E-10	9.73E-15	1.53E-03	2.01E-10	3.08E-13
PeLED	6.48E-03	9E-12	5.83E-14	7.51E-03	0	0	9.61E-05	1.8E-11	1.73E-15	3.04E-03	1.8E-11	5.47E-14

Table 15: Calculated worker exposure concentration to perovskite crystals during PePV and PeLED (RGB) fabrication

Device	Released mass, $mg_{emitted}$	*XF* (-)	Exposed mass, $mg_{exposed}$	Exposure concentration (mg/m^3)	OEL (mg/m^3)	<OEL?
PePV	1.01E-04	1.98E-04	2.00E-08	5.73E-11	0.1	Yes
PeLED	9.00E-06	1.98E-04	1.79E-09	5.10E-12	0.1	Yes

Table 16: Calculated Impact scores (in terms of DALY) for exposure to perovskite crystals during the use of PePV device; $IS = CF \times m$; Scenario 1: Encapsulation layer remains completely intact and there is no leaching from the device; Scenario 2: Slight wear of the encapsulation layer and 5% of the substances from the perovskite crystals in PePV leach to the ground water and soil; Scenario 3: Significant wear of the encapsulation layer and 50% of the substances from the perovskite crystals in PePV leach to the ground water and soil; Scenario 4: Complete breach of the of the encapsulation layer and all substances from the perovskite crystals in PePV leach to the ground water and soil.

Scenario	Water			Soil			Total IS per scenario (y)
	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	
1	4.83E-05	0	0	1.53E-03	0	0	0
2	4.83E-05	4.66E-08	2.25E-12	1.53E-03	6.55E-09	1.00E-11	1.23E-11
3	4.83E-05	4.66E-07	2.25E-11	1.53E-03	6.55E-08	1,00E-10	1.23E-10
4	4.83E-05	9.33E-07	4.51E-11	1.53E-03	1.31E-07	2,00E-10	2.45E-10

Table 17: Calculated Impact scores (in terms of DALY) for exposure to perovskite crystals during the EoL of PePV device; $IS = CF \times m$; Scenario 1: Encapsulation layer remains completely intact and 100% of perovskite crystals reach EoL phase; Scenario 2: Slight wear of the encapsulation layer and 95% of perovskite crystals reach EoL phase; Scenario 3: Significant wear of the encapsulation layer and 50% of perovskite crystals reach EoL phase; Scenario 4: Complete breach of the of the encapsulation layer and all perovskite crystals are lost to the ground water and soil before they reach EoL phase.

Scenario	Industrial indoor air			Outside air						Water						Total IS per scenario (y)
	Incineration			Incineration			Landfilling			Incineration			Landfilling			
	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$	m ($kg_{emitted}$)	IS (DALY)	
1	3.26E-03	1.65E-10	5.38E-13	3.77E-03	0	0	3.77E-03	4.03E-14	1.52E-16	4.83E-05	9.73E-07	4.70E-11	4.83E-05	2.01E-06	9.72E-11	1.45E-10
2	3.26E-03	1.57E-10	5.11E-13	3.77E-03	0	0	3.77E-03	3.83E-14	1.45E-16	4.83E-05	9.25E-07	4.47E-11	4.83E-05	1.91E-06	9.24E-11	1.38E-10
3	3.26E-03	8.26E-11	2.69E-13	3.77E-03	0	0	3.77E-03	2.02E-14	7.61E-17	4.83E-05	4.87E-07	2.35E-11	4.83E-05	1.01E-06	4.86E-11	7.24E-11
4	3.26E-03	0	0	3.77E-03	0	0	3.77E-03	0	0	4.83E-05	0	0	4.83E-05	0	0	0

Table 18: Calculated worker exposure concentration to perovskite crystals during the EoL of PePV device; Scenario 1: Encapsulation layer remains completely intact and 100% of perovskite crystals reach EoL phase; Scenario 2: Slight wear of the encapsulation layer and 95% of perovskite crystals reach EoL phase; Scenario 3: Significant wear of the encapsulation layer and 50% of perovskite crystals reach EoL phase; Scenario 4: Complete breach of the of the encapsulation layer and all perovskite crystals are lost to the ground water and soil before they reach EoL phase.

Scenario	Released mass, $mg_{emitted}$	*XF* (-)	Exposed mass, $mg_{exposed}$	Exposure concentration (mg/m^3)	OEL (mg/m^3)	<OEL?
1	1.65E-04	1.98E-04	3.27E-08	9.35E-11	0.1	Yes
2	1.57E-04	1.98E-04	3.12E-08	8.90E-11	0.1	Yes
3	8.26E-05	1.98E-04	1.64E-08	4.68E-11	0.1	Yes
4	0	1.98E-04	0	0	0.1	Yes

Table 19: Calculated Impact scores (in terms of DALY) for exposure to perovskite crystals during the EoL of PeLED (RGB) device; $IS = CF \times m$

Industrial indoor air			Outside air						Water					
Incineration			Incineration			Landfilling			Incineration			Landfilling		
CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$)	m ($kg_{emitted}$)	IS (DALY)	CF (DALY/ $kg_{emitted}$	m ($kg_{emitted}$)	IS (DALY)
6.48E-03	1.48E-11	9.56E-14	7.51E-03	0	0	7.51E-03	3.6E-15	2.70E-17	9.61E-05	8.69E-08	8.35E-12	9.61E-05	1.80E-07*	1.73E-11

** It is a worst case estimate as it assumes that in a landfill 99.9% of the lead is emitted*

Table 20: Calculated worker exposure concentration to perovskite crystals during the EoL of PeLED (RGB) device

Released mass $mg_{emitted}$	*XF* (-)	Exposed mass, $mg_{exposed}$	Exposure concentration (mg/m^3)	OEL (mg/m^3)	<OEL?
1.48E-05	1.98E-04	2.94E-09	8.39E-12	0.1	Yes

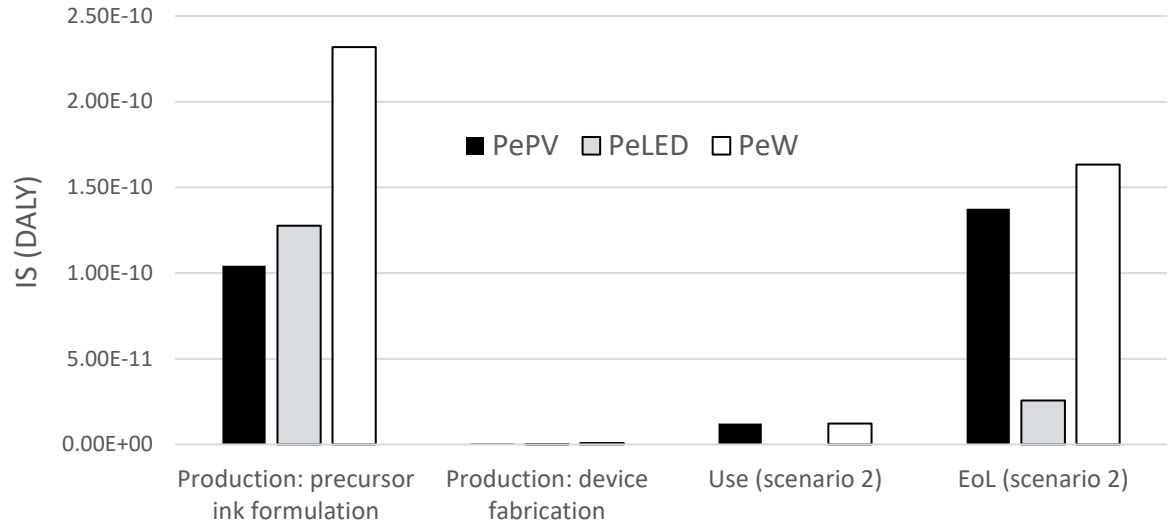

Figure 4: Overall Impact Score per life cycle stage with all environmental compartments combined for the three perovskite-based devices

3.6 Representativeness to other diseases

Huijbregts et al. 2005 in their analysis to derive human damage on a world level for 1990, calculated average *IS* value for carcinogenic and noncarcinogenic effects from human exposure to toxic chemicals to be equal to 11.5 DALY and 2.7 DALY respectively. The study considers approx. 1,200 substances (including non-ionic organic chemicals, ionic organic chemicals, metals, and inorganic chemicals) and 49 non-communicable diseases in its evaluation. Compared to these two values, the calculated *IS* value to produce, use and dispose 10 cm^2 sized perovskite films in PePV and PeLED are very low.

For the use scenario 2, in which a slight wear of the encapsulation layer is assumed (5% perovskite loss), the *IS* is calculated to be equal to 1.23E-11 DALY. An *IS* equal to 2.7 DALY to generate even non-carcinogenic effects would mount to 21.95×10^{11} cm^2 (= 10 cm^2 x 2.7 DALY / 1.23E-11 DALY) of perovskite crystal film which would contain 442,292 kg of perovskite crystals in PePV (= 2.015 g/m^2 x 21.95 x 10^{11} cm^2). Producing this much amount of perovskite crystals is highly unlikely for the current scope of the PeroCUBE project.

Although the average disease burden considered by Huijbregts et al. 2005 would have reduced since 1990 due to the better disease cure with advances in human health care, and the reported *DALY* by Huijbregts et al. 2005 are bound to be lower if reconsidered in the present times, we expect that the *IS* values for producing 10 cm^2 sized perovskite crystals would still be much lower than noncommunicable diseases representative for the world.

4 Conclusions & Discussion

In the present task, USEtox was employed to calculate the Human Health Impact (expressed as the impact score (IS)) for a variety of (in)organic chemical compounds and perovskite crystals over the course of entire life cycle of the perovskite-based devices, manufactured at a lab scale with 10 cm^2 of perovskite crystal film. The output *IS* is measured in terms of disability-adjusted life years, DALY, which is the sum of the years of life lost due to premature mortality and the years lived with a disability due to the toxicity of the substance to which a person is exposed. One DALY represents the loss of the equivalent of one year of full health. The main challenge to calculate the relevant *IS* values was the lack of data on environmental fate, human exposure factors and human toxicity of these compounds in the USEtox database. Consequently, a series of sources were extensively consulted to retrieve the missing information/data as much as possible. This included exploration of different online databases, Safety Data Sheets, PubMed screening of the relevant scientific literature, QSAR and read-across. Based on this, compounds like Formamidinium iodide, 1,3-Di-tert-butylimidazolium tetrafluoroborate, N-Butylammonium bromide, 3-Butenylamine hydrochloride and 2,2'-(Ethylenedioxy)bis(ethylamine) were screened-off from the current risk assessment because either risk assessment is not needed for them (e.g. due to the absence of toxic alerts) for certain exposure routes or no data could be retrieved to calculate their fate, exposure and toxicity factors, despite such an extensive effort. Therefore, extra information needs to be retrieved to perform their risk assessment.

For the rest of the compounds, the human health risk assessment estimated that the impact on the human health is highest during EoL phase of the devices' life cycle (IS= 4.99E-10 DALY), compared to other life cycle stages. This is followed by the precursor ink formulation stage during production phase. The decreasing order of human health impact obtained for different chemical compounds employed during the precursor ink formulation stage of the devices is CsI (*IS*= 7.32E-11 DALY) > CsBr (*IS*= 3.05E-11 DALY) > PbI_2 (*IS*= 2.30E-11 DALY). During precursor ink formulation and EoL, the *IS*, and thus the risk to the human health, is highest through contaminated water. During the devices fabrication and use phase, despite the released amounts are 10 times higher for the water, the *IS* is still higher for the soil which indicates that the risk is primarily dependent on the toxicity factor of the exposure route and the intake availability of a certain compound from an environmental compartment and less dependent on its released amount.

In terms of worker exposure due to the inhalation of the indoor air during the production and disposal of perovskite-based devices at lab scale, all estimated exposure concentrations for relevant compounds were observed to be lower than their corresponding OEL which signify occupational risk to be unlikely due to the inhalation of released substances in the indoor air at lab production scale. The released mass, *m*, which has been considered from D7.2, and calculated *CF* are mainly based on the substance-intrinsic properties (e.g. vapor pressure) and assume a "passive" release from the product. For the occupational indoor air situation, we know that this is not the case and a lot of release/exposure scenarios (or process categories) depend on the activity rather than the substance properties. This is a clear deficit of the USEtox model. Thus, onsite experimental measurement data are always needed to be certain before completely ruling out occupational risk likeliness.

It should be noted that the *IS* values, reported in this study, correspond to the production of 10 cm^2 of perovskite crystal surface (representing lab-scale production). The *IS* values will increase in case of higher crystal surface (e.g. 100 cm^2). Therefore, a new risk assessment will be needed for a perovskite crystal surface area other than 10 cm^2.

The calculated *IS*, were observed to be much lower than the *IS* of the noncommunicable diseases representative for the world caused by the human exposure to toxic chemicals. An incredible amount of perovskite crystals (442,292 kg) needs to be produced for it to be equal to the reported average

value (= 2.7 DALY) for non-carcinogenic, yet grave, effects on humans. Even though 442,292 kg of perovskite crystals is way beyond the current scope of the PeroCUBE project (which is limited to lab scale production of perovskite-based devices), it can be a realistic scenario upon devices' production upscaling to mass level, especially considering the current global silicon wafers mass production scale (9 million metric tons approx.[17]) for conventional photovoltaic cells in 2022. Therefore, for such large production scale, human health risks are expected to be significant (e.g. loss of 2.7 years or more of healthy human life per person). Thus, the innovators need to consider alternatives to the material design in their methodology to make it safe to the human health before the perovskite-based technology becomes large enough to be comparable with current silicon wafers production. Such alternatives include, for example, substitution of lead and caesium halides with tin metal without compromising with high efficiency and stability of the device (Cao and Yan 2021), chemical absorption of lead upon leaking (Li et al. 2021), replacing the use of hazardous solvents like dimethylformamide with dimethyl sulfoxide (Küffner et al. 2021) which has 100 times lesser health impact than dimethylformamide and better devices recycling options (e.g. Chen et al. 2021) and as discussed in more details in D7.2.

The lab scale production of 10 cm^2 sized perovskite crystal surfaces (with approx. 2 mg of perovskite content), as considered within the PeroCUBE project, do not present any human health risk and thus do not need any such alternative. In fact, no REACH registration is even needed to produce perovskite crystals at such a small scale.

Nevertheless, the assessed potential impacts of chemical compounds released in this task, providing characterization factors as substance-specific measures of relative impact potential, will be used in a comparative context of LCA within T7.4. Compounds like lead and caesium halides, life cycle stage of EoL and environmental compartment of water have been expected to be elements of potentially high concern upon upscaling which can be definitely of interest for their full impact using LCA.

[17] Global silicon production 2022 | Statista

5 References

Amadi, A.A., Osinubi, K.J., 2018. Transport parameters of lead (Pb) Ions migrating through saturated lateritic soil-bentonite column. Int J Geotech Eng 12 (3), 302–308.

Cao J and Yan F (2021) Recent progress in tin-based perovskite solar cells. Energy Environ. Sci. 14, 1286-1325

Chamas A, Moon H, Zheng J, Qiu Y, Tabassum T, Jang JH, Abu-Omar M, Scott SL, Suh S (2020) Degradation Rates of Plastics in the Environment. ACS Sustainable Chem. Eng. 2020, 8, 9, 3494–3511

Chen B, Fei C, Chen S, Gu H, Xiao X, Huang J (2021) Recycling lead and transparent conductors from perovskite solar modules. Nature Communications 12, 5859

EPA (2011) Exposure Factors Handbook: 2011 Edition. National Center for Environmental Assessment, Washington, DC; EPA/600/R-09/052F. Access link: https://ordspub.epa.gov/ords/eims/eimscomm.getfile?p_download_id=522996

Fantke P, Gillespie B, Juraske R, Jolliet O (2014): Estimating half-lives for pesticide dissipation from plants. Environmental Science and Technology 48: 8588-8602

Fantke, P., Bijster, M., Guignard, C., Hauschild, M., Huijbregts, M., Jolliet, O., Kounina, A., Magaud, V., Margni, M., McKone, T.E., Posthuma, L., Rosenbaum, R.K., van de Meent, D., van Zelm, R., 2017. USEtox® 2.0 Documentation (Version 1), http://usetox.org

Footprint (2015): The Pesticide Properties Database (PPDB 2.0) of the Footprint Project

Hauschild MZ, Huijbregts MAJ, Jolliet O, Macleod M, Margni MD, van de Meent D, Rosenbaum RK, McKone TE (2008): Building a model based on scientific consensus for life cycle impact assessment of chemicals: The search for harmony and parsimony. Environmental Science and Technology 42: 7032-7037

Horváth E, Kollár M, Andričević P, Rossi L, Mettan X, Forró L (2021) Fighting Health Hazards in Lead Halide Perovskite Optoelectronic Devices with Transparent Phosphate Salts. ACS Appl. Mater. Interfaces 2021, 13, 33995−34002

Huijbregts MAJ, Rombouts LJA, Ragas MJ, van de Meent D (2005) Human-Toxicological Effect and Damage Factors of Carcinogenic and Noncarcinogenic Chemicals for Life Cycle Impact Assessment. Integrated Environmental Assessment and Management 1: 181–244

Küffner J, Hanisch J, Wahl T, Zillner J, Ahlswede E, Powalla M (2021) One-Step Blade Coating of Inverted Double-Cation Perovskite Solar Cells from a Green Precursor Solvent. ACS Appl. Energy Mater. 4, 10, 11700–11710

Leistra M (2011) Methods for estimating the vapour pressure of organic chemicals, Alterra report 2215, Wageningen

Li X, Zhang F, Wang J, Tong J, Xu T, Zhu K (2021) On-device lead-absorbing tapes for sustainable perovskite solar cells. Nature Sustainability 4, 1038–1041

Lu, C., Wu, Y., Hu, S., Zhang, X., Fu, Y., 2016. Distribution and transport of residual lead and copper along soil profiles in a mining region of North China. Pedosphere 26 (6), 848–860.

Mallick A, Mendez-Lopez RD, Arye G, Cahen D, Visoly-Fisher I (2023) Soil adsorption and transport of lead in the presence of perovskite solar cell-derived organic cations. Journal of Hazardous Materials 451: 131147

Peng J, Xia CQ, Xu Y, Li R, Cui L, Clegg JK, Herz LM, Johnston MB, Lin Q (2021) Crystallization of CsPbBr3 single crystals in water for X-ray detection, Nature Communications 12: 1531

Rosenbaum RK, Bachmann TM, Gold LS, Huijbregts MAJ, Jolliet O, Juraske R, Koehler A, Larsen HF, MacLeod M, Margni MD, McKone TE, Payet J, Schuhmacher M, van de Meent D, Hauschild MZ (2008): USEtox - The UNEP-SETAC toxicity model: Recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment. The International Journal of Life Cycle Assessment 13: 532-546

Rosenbaum RK, Meijer A, Demou E, Hellweg S, Jolliet O, Lam NL, Margni M, McKone TE (2015): Indoor air pollutant exposure for life cycle assessment: Regional health impact factors for households. Environmental Science and Technology 49: 12823-12831

Sinkkonen S, Paasivirta J (2000): Degradation half-life times of PCDDs, PCDFs and PCBs for environmental fate modeling. Chemosphere 40: 943-949

van Vugt-Lussenburg B, van der Burg B, Kroese D, Buist H, Meima M (2019). D4.3 - An innovative, cost-effective integrated testing strategy to evaluate toxicological safety issues of candidate solvents. EU Horizon 2020 Project Resolve , project number 745450.

6 Appendix

6.1 Dimethyl Sulfoxide

Substance information

- Molecular formula: C2H6OS
- Organic/ inorganic compound: organic
- Cas number: 67-68-5
- SMILES: CS(=O)C

Hazard assessment

In 2008 the OECD published a report on dimethyl sulfoxide (BIAC/ ICCA, 2008). In the SIDS initial assessment profile summary conclusions are described on human health. In general DMSO is of low acute toxicity. For inhalation, the lowest NOAEC is described for respiratory tract irritation: according to the results of a 13 -week inhalation toxicity study compliant with the OECD TG 413, the No Adverse Effects Concentration (NOAEC) for DMSO could be established at ca. 1000 mg/m^3 for respiratory tract irritation.

For oral exposure the lowest NOAEC is described for a developmental toxicity study. In this study, performed according to the OECD TG 414, oral administration of DMSO to pregnant female rats or rabbits during the period of organogenesis was not teratogenic. The NOAELs for maternal toxicity were 1000 and 300 mg/kg bw/d in rats and rabbits, respectively.

Non-carcinogenicity ED50: Based on the Usetox manual for organic substances, the NOEL values were converted to ED50 values, based on Huijbregts et al. (2005).

Summary

<u>Non-cancer inhalation:</u>

- The OECD TG 413 is a sub-chronic study, so a conversion factor to extrapolate from sub-chronic to chronic of 2 is applied.
    - 1000 mg/m^3 /2= 500 mg/m^3
- Since it concerns an inhalation study, there was no allometric scaling factor applied
- Subsequently a factor of 9 is applied to convert a NOAEC to an ED50 value
    - 500mg/m^3 x 9= 4500 mg/m^3
- Convert the value to kg/person/lifetime
    - **ED50: 1495 kg/ person/life time**

<u>Non-cancer oral:</u>

- The OECD TG 414 is a chronic study, so no conversion factor needed.
- Since it concerns a rabbit study, an interspecies conversion factor (CF) of 2.4 is applied
    - 300 mg/kg bw/d / 2.4 = 125 mg/kg bw/d
- Subsequently a factor of 9 is applied to convert a NOAEC to an ED50 value
    - 125 mg/kg bw/d x 9 = 1125 mg/kg bw/d
- Convert the value to kg/person/lifetime

- **ED50: 2012 kg/ person/life time**

The OECD report described that, with a few exceptions, a large battery of *in vitro* and *in vivo* non-guideline studies confirmed the lack of genotoxic potential. There is no valid carcinogenicity study conducted with DMSO.

Cancer: **no ED50 necessary**

6.2 1,3-Di-tert-butylimidazolium tetrafluoroborate (Di-tBIM)

Substance information

- Cas number: 263163-17-3
- Molecular formula: $C_{11}H_{21}BF_4N_2$
- smiles:
  - F[B-](F)(F)F.CCIIn1cc[n+](c1)CIIC
  - [B-](F)(F)(F)F.CCIIN1C=C[N+](=C1)CIIC
  - [B-](F)(F)(F)F.CCIIn1cc[n+](c1)CIIC
- Pubchem CID: 16217979
- Organic/ inorganic compound: organic
- Basic physical and chemical properties:
  - Physical state: Solid. Melting point/range: 157 - 198°C[18]

Hazard assessment

Based on the ECHA dossier of this chemical there is a classification for 1,3-Di-tert-butylimidazolium tetrafluoroborate for the following endpoints: skin irrit.2, eye irrit.2, and STOT SE 3. There is no data available for these classifications (i.e. no dossier)[19]. For all other endpoints data is lacking. In addition a search was performed for only "1,3-Di-tert-butylimidazolium" (i.e., excluding tetrafluoroborate), but this substance is not registered with ECHA.

Searching on "1,3-Di-tert-butylimidazolium tetrafluoroborate" in PubMed produced no results.

QSAR VEGA: Smiles code was not recognized.

Read-across

The GenRA module from the USEPA comptox chemical dashboard was used to explore feasible read across possibilities. Based on visual inspection of the structure (Annex A), read across appeared to be not feasible.

Summary

Non cancer:

[18] https://www.sigmaaldrich.com/NL/en/sds/aldrich/659983

[19] https://echa.europa.eu/nl/substance-information/-/substanceinfo/100.154.704

- Inhalation: Based on the fact that this concerns a solid compound with a high melting point, we consider inhalation exposure to vapours unlikely for the general population. However exposure via aerosols remains an option, this is especially a potential relevant route for workers. Because we cannot be conclusive on whether or not exposure is occurring, we conclude that there is not enough data available to derive a conclusion.
- Ingestion: no data available to derive an ED50.

Cancer:

Based on the absence of alerts in the QSAR for mutagenicity (*in vitro mutagenicity (Ames test) alerts by ISS)*, there is no need to derive a cancer ED50.

6.3 Formamidinium iodide (FAI)

Substance information

- Cas No: 879643-71-7
- Molecular formula: CH5IN2
- Smiles:
  - I.NC=N
  - C(=[NH2+])N.[I-]
- Inorganic/organic compound: organic
- Compound CID: 89906651
- Commonly used synonym: methanimidamide;hydroiodide
- Basic physical and chemical properties:
  - Physical state: powder. Melting point: 335°C[20]

Hazard assessment

Based on the ECHA dossier of this chemical there is a classification and labelling for methanimidamide;hydroiodide, i.e. for acute tox 4, skin irr 2, eye irr 2, stot se 3[21]. There is no dossier available. There is no data on Formamidinium iodide in IRIS EPA, nor for methanimidamide; hydroiodide. There are no relevant results for Formamidinium iodide in pubchem, nor for methanimidamide nor hydroiodide

Read across

The GenRA module from the USEPA comptox chemical dashboard was used to explore feasible read across possibilities. Based on visual inspection of the structure (Annex B) read across appeared to be not feasible.

QSAR VEGA: For both smiles code there is no QSAR available (an error is produced: "molecule has disconnected structure").

[20] https://www.sigmaaldrich.com/NL/en/sds/aldrich/806048

[21] https://echa.europa.eu/nl/substance-information/-/substanceinfo/100.262.499

Summary

Non cancer:

- Inhalation: Based on the fact that this concerns a solid compound with a high melting point, we consider inhalation exposure to vapours unlikely for the general population. However exposure via aerosols remains an option, this is especially a potential relevant route for workers. Because we cannot be conclusive on whether or not exposure is occurring, we conclude that there is not enough data available to derive a conclusion.
-
- Ingestion: no data available to derive an ED50.

Cancer:

Based on the absence of alerts in the QSAR for mutagenicity (*in vitro mutagenicity (Ames test) alerts by ISS)*, there is no need to derive a cancer ED50.

6.4 Methylammonium chloride

Substance information

- MF: CH_6ClN
- Compound CID: 11637
- Smiles:
  - CN.Cl
  - C[NH3+].[Cl-]
- Cas no: 593-51-1
- Organic/ inorganic compound: organic
- Synonym: Monomethylammonium chloride, Methylamine hydrochloride
- Basic physical and chemical properties:
  - Physical state: Crystals, Melting point/range: 209,3 – 215,3 °C[22]

Hazard assessment

There is a REACH dossier available for methylammonium chloride[23]. The lowest reported NOAEL in this dossier is based on a repeated dose toxicity study combined with a reproduction/developmental toxicity screening test. In that study male and female rats were treated with methylamine hydrochloride orally by gavage for 110 days. The study is performed according to OECD guideline 422 (there is no specification of GLP compliance). The NOAEL was considered to be 500 mg/kg bw/day for P1 generation (based on e.g. food consumption and body weight) and 1000 mg/kg bw/day for F1 generation.

[22] https://www.sigmaaldrich.com/NL/en/sds/mm/8.06020

[23] Substance Information - ECHA (europa.eu)

There is no data from IRIS EPA. There is no relevant data from pubmed on methylammonium chloride.

Based on the combined repeated dose toxicity study, an ED50 value can be derived.
Summary

Non-cancer oral:

- The OECD TG 422 is a subchronic study, so a conversion factor of 2 is needed:
  - 500/2 = 250 mg/kg bw/d.
- Since it concerns a rat study, an interspecies conversion factor (CF) of 4.1 is applied
  - 250 mg/kg bw/d / 4.1 = 61 mg/kg bw/d
- Subsequently a factor of 9 is applied to convert a NOAEC to an ED50 value
  - 61 mg/kg bw/d x 9 = 549 mg/kg bw/d
- Convert the value to kg/person/lifetime
  - **982 kg/ person/life time**

Non cancer inhalation:

- Based on the fact that this concerns a solid compound with a high melting point, we consider inhalation exposure to vapours unlikely for the general population. However exposure via aerosols remains an option, this is especially a potentially relevant route for workers. Because we cannot be conclusive on whether or not exposure is occurring, we conclude that there is not enough data available to derive a conclusion.

Cancer:

With regards to carcinogenicity. There is no classification of carcinogenicity or mutagenicity for methylammonium chloride. In the REACH dossier a reference is made to a study by Meshram et al. (1992), who performed a gene mutation toxicity study to determine the mutagenic nature of methylamine hydrochloride. Based on the results of the assay, methylamine hydrochloride failed to induce gene mutation in Salmonella typhimurium strain TA98, TA100 and TA104 both in the presence and absence of S9 metabolic activation system and hence is not likely to classify as a gene mutant in vitro.

QSAR VEGA: for both smiles codes there is no information available.

QSAR TTC: The *in vitro mutagenicity (Ames test) alerts by ISS* reported no alerts.

To conclude, based on this data, for cancer it appears there is no need for an ED50 value of methylammonium chloride.

6.5 N-Butylammonium bromide (n-BABr)

Substance information

- Cas no: 15567-09-6
- Molecular Formula: C4H12BrN
- Synonyms: Butylamine Hydrobromide
- Canonical smiles:
  - CCCCN.Br (computed by OEChem 2.3.0)

  - CCCC[NH3+].[Br-]
- Organic/ inorganic compound: organic
- Basic physical and chemical properties:
  - Physical state: solid (powder, crystal), melting point: 205°C[24]

Hazard assessment

Based on the ECHA dossier of this chemical there is a classification and labelling for Butylamine Hydrobromide, i.e. there are hazard statements for skin irr 2, eye irr 2[25]. There is no data available on these classifications. For all other endpoints the data is lacking. There is no relevant result from IRIS of the USEPA. A PubMed search also delivered no relevant results.

Read across

The GenRA module from the USEPA comptox chemical dashboard was used to explore feasible read across possibilities. Based on visual inspection of the structure (Annex C) read across appeared to be not feasible.

QSAR VEGA: Both smiles codes were not recognized by VEGA

Summary

Non cancer:

- Inhalation: Based on the fact that this concerns a solid compound with a high melting point, we consider inhalation exposure unlikely for the general population. Based on the fact that this concerns a solid compound with a high melting point, we consider inhalation exposure to vapours unlikely for the general population. However, exposure via aerosols remains an option, this is especially a potential relevant route for workers. Because we cannot be conclusive on whether or not exposure is occurring, we conclude that there is not enough data available to derive a conclusion.
- Ingestion: no data available to derive an ED50.

Cancer:

Based on the absence of alerts in the QSAR for mutagenicity (*in vitro mutagenicity (Ames test) alerts by ISS)*, there is no need to derive a cancer ED50.

6.6 Cesium iodide (CsI)

Substance information

- Compound CID: 24601
- MW: 259.809g/mol
- Isomeric smiles:
  - [I-].[Cs+]

[24] https://downloads.ossila.com/msds/n-butylammonium-bromide.pdf

[25] Substance Information - ECHA (europa.eu)

- Cas no: 7789-17-5
- Organic/ inorganic compound: inorganic
- Basic physical and chemical properties:
  - Physical state: solid, Melting point: 626°C[26]

Hazard assessment

- From ECHA no results
- From IRIS EPA no results
- Pubmed: no relevant results

In addition a search was conducted for only Cesium. There is a dossier available for cesium diiodide: it is stated that there are no hazard classifications for this compound[27]. For cesium acetate there is no information available from ECHA. A pubmed search for only cesium ("cesium" AND "tox*") delivered no relevant results. There is a REACH dossier available for sodium iodate, but this includes mainly studies that report on dermal effects, or lethal doses. There is also data on genotoxicity: cesium iodate did not have mutagenic activity in the Ames, micronucleus, or recessive lethal test. However it is not certain to which extent the effects of iodate could be extrapolated to iodide. It is known that Iodate is less soluble and more stable than iodide (both are generally referred to as iodized salt)[28].

There is a REACH dossier for **sodium iodide**[29], where iodide is the ion of toxicological concern. These data will be read-across to CsI, under the assumption that also in this case the iodide is of toxicological concern and not the Cs ion. The lowest reported effect is based on a subchronic repeated dose toxicity rats, based on oral exposure (via water). Based on the observations made, the LOAEL for repeated dose toxicity study was considered to be 100 mg/l (5 mg/kg/day).

Summary

Non-cancer oral:

- A conversion factor of 2 to convert from sub-chronic to chronic
  - 5 mg/kg/day / 2 = 2.5 mg/kg/day
- Since it concerns a rat study, an interspecies conversion factor (CF) of 4.1 is applied
  - 2.5 mg/kg bw/d / 4.1 = 0.6 mg/kg bw/d
- Since it concerns a LOAEL, the value needs to be divided by four
  - 0.6 mg/kg bw/d / 4 = 0.15 mg/kg bw/d[30]
- Subsequently a factor of 9 is applied to convert a NOAEC to an ED50 value
  - 0.15 mg/kg bw/d x 9 = 1.4 mg/kg bw/d
- Convert the value to kg/person/lifetime
  - ED50: 2.5 kg/ person/life time

[26] https://www.sisweb.com/referenc/msds/csi-sds.pdf
[27] Substance Information - ECHA (europa.eu)
[28] https://www.sciencedirect.com/science/article/pii/B9780323189071000913
[29] Substance Information - ECHA (europa.eu)
[30] A factor 4 is recommended by UseTOX (UNEP/SETAC, 2018)

- Recalculate ED50 value based on MW of read across candidate:
  - (MW I + MW Cs)/ (MW I + MW Na) = 1.74
- **ED50: 2.5 x 1.74 = 4.3 kg/ person/life time**

Non-cancer inhalation:

- There is no inhalation study available for sodium iodide because of the very low vapor pressure of sodium iodide.

Based on the absence of alerts in the QSAR for mutagenicity (*in vitro mutagenicity (Ames test) alerts by ISS)*, there is no need to derive a cancer ED50.

6.7 Cesium bromide (CsBr)

Substance information

- Cas no: 7787-69-1
- Smiles: [Br-].[Cs+]
- Organic/ inorganic compound: inorganic
- Basic physical and chemical properties:
  - Physical state: solid, Melting point: 636°C[31]

Hazard assessment

From the ECHA database there is a dossier available for cesium bromide with various classifications, but not on genotoxicity or carcinogenicity[32]. A search in pubmed delivered not relevant results.

Assuming cesium bromide is not covalently bound (based on the Smiles code), a search for information on cesium and bromide separately, was conducted. There is a REACH dossier available for **sodium bromide**[33]. As stated in that report, the ion of toxicological concern is the bromide ion. These data will be read-across to CsBr, under the assumption that also in this case the bromide is of toxicological concern and not the Cs ion. In this dossier a NOAEL of 60 mg/kg bw/day was derived based on a 90 days oral exposure study in rats. At this level there were no significant adverse effects on reproductive parameters found.

QSAR VEGA: there is no information available.

Summary

Non-cancer oral:

- This concerns a chronic study, so no conversion factor needed.
- Since it concerns a rat study, an interspecies conversion factor (CF) of 4.1 is applied

[31] https://www.fishersci.com/store/msds?partNumber=AC192061000&productDescription=CESIUM+BROMIDE+99.9%25+100GR&vendorId=VN00032119&countryCode=US&language=en

[32] Substance Information - ECHA (europa.eu)

[33] Substance Information - ECHA (europa.eu)

  - 60 mg/kg bw/d / 4.1 = 14.6 mg/kg bw/d
- Subsequently a factor of 9 is applied to convert a NOAEC to an ED50 value
  - 14.6 mg/kg bw/d x 9 = 132 mg/kg bw/d
- Convert the value to kg/person/lifetime
  - ED50: 236 kg/ person/life time
- Recalculate ED50 value based on MW of read across candidate:
  - (MW 80+ MW 133)/ (MW 80 + MW 23) = 2.1
- **ED50: 236 x 2.1 = 488 kg/ person/life time**

A search on cesium on pubmed("cesium" AND "tox*") delivered no relevant results.

Non cancer:

- Inhalation: Based on the fact that this concerns a solid with a high melting point, we consider inhalation exposure unlikely for the general population. Based on the fact that this concerns a solid compound with a high melting point, we consider inhalation exposure to vapours unlikely for the general population. However exposure via aerosols remains an option, this is especially a potential relevant route for workers. Because we cannot be conclusive on whether or not exposure is occurring, we conclude that there is not enough data available to derive a conclusion.

Cancer:

Based on the absence of alerts in the QSAR for mutagenicity (*in vitro mutagenicity (Ames test) alerts by ISS)*, there is no need to derive a cancer ED50.

6.8 18-crown-6

Substance information

- Molecular formula: $C_{12}H_{24}O_6$
- Smiles: C1COCCOCCOCCOCCOCCO1
- Cas no: 17455-13-9
- Compound CID: 28557
- Organic/ inorganic compound: organic
- Synonym (according to ECHA): 1,4,7,10,13,16-hexaoxacyclooctadecane
- Basic physical and chemical properties:
  - Physical state: solid, Melting point/range: 36 – 40 °C[34]

Hazard assessment

[34] https://www.fishersci.com/store/msds?partNumber=AC181565000&productDescription=18-CROWN-6%2C+99%25+500GR&vendorId=VN00032119&countryCode=US&language=en

From the ECHA database there is a dossier available for 18 crown 6 with various classifications for acute tox 4[35]. A Pubmed search provided no relevant results.

Read across

The GenRA module from the USEPA comptox chemical dashboard was used to explore feasible read across possibilities. Based on read across it appears that 1,4-dioxane 88% similar to 18-crown-6. Therefore 1,4-dioxane was read to 18-crown-6.

Summary

Non cancer:

- Inhalation: Based on the fact that this concerns a solid compound with a high melting point, we consider inhalation exposure to vapours unlikely for the general population. However, exposure via aerosols remains an option, this is especially a potential relevant route for workers. Because we cannot be conclusive on whether or not exposure is occurring, we conclude that there is not enough data available to derive a conclusion.
- Ingestion: no data available to derive an ED50.

Usetox already includes ED50 values for 1,4-dioxane for cancer endpoints. I.e.:

Cancer inhalation

- UseTox ED50: 50 kg/person/lifetime

Cancer oral

- UseTox ED50: 50 kg/person/lifetime

Since we did not find other similar molecules with toxicity data than 1,4-dioxane nor do we have data (e.g. relevant in vitro studies) to scale 18-crown-6 carcinogenicity to that of 1,4-dioxane, it is assumed they are equally toxic and the ED50's of 1,4-dioxane are attributed to 18-crown-6.

6.9 3-Butenylamine hydrochloride (BEACl)

Substance information

- Cas no: 17875-18-2
- Smiles:
  - C=CCCN.Cl
  - C=CCCN.Cl
- ECHA synonym: 1-Amino-3-butene hydrochloride
- Organic/ inorganic compound: organic
- Basic physical and chemical properties:
  - Physical state: solid, Melting point/range: 176 – 180 °C[36]

[35] Substance Information - ECHA (europa.eu)

[36] https://www.sigmaaldrich.com/NL/en/sds/aldrich/597678

Hazard assessment

Based on the ECHA dossier of this chemical there are various classifications for 3-Butenylamine hydrochloride, but not on genotoxicity or carcinogenicity[37]. A search in pubmed delivered not relevant results.

Read across

The GenRA module from the USEPA comptox chemical dashboard was used to explore feasible read across possibilities. Based on read across it appears that there are no good read across candidates (Annex D).

Summary

Non cancer:

- Inhalation: Based on the fact that this concerns a solid compound with a high melting point, we consider inhalation exposure to vapours unlikely for the general population. However exposure via aerosols remains an option, this is especially a potential relevant route for workers. Because we cannot be conclusive on whether or not exposure is occurring, we conclude that there is not enough data available to derive a conclusion.
- Ingestion: no data available to derive an ED50.

Cancer:

Based on the absence of alerts in the QSAR for mutagenicity (*in vitro mutagenicity (Ames test) alerts by ISS)*, there is no need to derive a cancer ED50.

6.10 2,2'-(Ethylenedioxy)bis(ethylamine) (EDEA)

Substance information

- Cas no: 929-59-9
- Synonym: ethylene glycol bis(2-aminoethyl) ether
- Smiles: C(COCCOCCN)N
- Name according to ECHA: 3,6-dioxaoctamethylenediamine
- Organic/ inorganic compound: organic
- Basic physical and chemical properties:
    - Physical state: liquid, Density: 1,015 g/cm^3 [38]

Hazard assessment

There is a dossier available for "3,6-dioxaoctamethylenediamine" (based on same Cas no)[39]. In this dossier information is available on genetic toxicity, it reads "A reliable bacterial reverse mutation assay and a Rat Hepatocyte Primary Culture /DNA repair test (UDS) are available. Both studies

[37] Substance Information - ECHA (europa.eu)
[38] https://www.sigmaaldrich.com/NL/en/sds/aldrich/385506
[39] Registration Dossier - ECHA (europa.eu)

indicate a negative result." Furthermore, the dossier includes studies that describe a LD50 and can thus not be used for derivation of an ED50.

Read across

The GenRA module from the USEPA comptox chemical dashboard was used to explore feasible read across possibilities. Based on read across it appears that there are no good read across candidates (Annex E).

QSAR VEGA:

- The results from the VEGA QSAR on mutagenicity and carcinogenicity are displayed below (Table 2).

QSAR outcome for 2,2'-(Ethylenedioxy)bis(ethylamine); Reliability is either good (3 out of 3 stars), moderate (2 out of 3 stars) or not moderate (1 out of 3 stars)

Model	**Outcome**	**Reliability**
CAESAR (2.1.13)	Non-mutagenic	Moderate
SARPy/IRFMN (1.0.7)	Non-mutagenic	Moderate
ISS (1.0.2)	Non-mutagenic	Moderate
KNN/Read-Across (1.0.0)	Mutagenic	Not reliable
CAESAR (2.1.9)	Carcinogen	Not reliable
ISS (1.0.2)	Non-carcinogen	Not reliable
IRFMN/Antares (1.0.0)	Possible non-carcinogen	Moderate
IRFMN/ISSCAN-CGX (1.0.0)	Possible non-carcinogen	Not reliable

Cancer:

Based on the absence of alerts in the QSAR for mutagenicity (*in vitro mutagenicity (Ames test) alerts by ISS)*, there is no need to derive a cancer ED50.

6.11 Lead based perovskite crystals

Substance information

For this particle we know that it concerns a nano-based material, so common approaches, like the application of QSARS are not applicable. Lead based perovskite crystals have a high solubility (personal communication, Tom Lighthart). In addition we received information on the composition of the particle (Annex F).

Hazard assessment

- Pubmed:
    - No relevant results for ""Lead based perovskite crystals"

Therefore an additional search is conducted to find toxicity data on perovskite crystals only.

- No results for ""perovskite" and "crystals" and "tox*""
- No relevant results for ""perovskite" and "crystals" and "health*""

- No results for “perovskite” and “tox*”
- “perovskite” and “genotox**”
  - Ecotoxicity and cytotoxicity studies

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6414526/

  - An in vitro study on human skin fibroblast cells
    https://pubmed.ncbi.nlm.nih.gov/35907160/

Because there is no information on the toxicity of perovskite crystals, we use the available ED50 for lead ions, since lead is known to be very toxic to humans and the ecosystem and therefore likely to be the most toxic moiety of Perovskite crystals (also based on expert knowledge of the other chemical constituents of the lead based perovskite crystal.

Non-cancer inhalation: 0.0579 kg Pb/person/lifetime

Non-cancer ingestion: 0.0579 kg Pb/person/lifetime

Cancer inhalation: 20.3 kg Pb/person/lifetime

Cancer ingestion: 20.3 kg Pb/person/lifetime

Note that it is known that the Pb content in the perovskite crystals depends on the application in which the crystals are being used. For the application in photovoltaic cells (PePV), the Pb content is 32.8%. It is 40.4% for the application in LED device (PeLED).

This results in the following calculation:

- ED50 non-cancer inhalation/ ingestion **for PePV:**
  - 0.0579 kg Pb/person/lifetime
  - 0.0579 x (100/32.8) = **0.2 kg Pb/person/lifetime**
- ED50 cancer inhalation/ ingestion for **PePV**:
  - 20.3 Pb/person/lifetime
  - 20.3 x (100/32.8) **= 61.9 kg Pb/person/lifetime**
- ED50 non-cancer inhalation/ ingestion **for PeLED:**
  - 0.0579 x (100/ 40.4) = **0.1 kg Pb/person/lifetime**
- ED50 cancer inhalation/ ingestion for **PeLED**:
  - 20.3 x (100/40.4) = **50.2 kg Pb/person/lifetime**