**Applicant:** UltravioletChemicals

### Inventors:

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Chemical Product Formula: LiPF<sub>6</sub>

**Chemical Product Name:** Lithium Hexafluorophosphate

**Process Title: Swarts Reaction** 

### **EHS Summary:**

a. List the wastes generated and their quantity of generation.

The production of lithium hexafluorophosphate (LiPF6) using HF, LiCl, and PCl5 can generate various wastes, including:

- **Hydrogen fluoride (HF) waste:** The production of LiPF6 involves the use of HF, which is a hazardous and corrosive substance. Any unused or spent HF must be properly managed and disposed of according to local regulations.
- **Lithium chloride (LiCl) waste**: LiCl may be used as a starting material in the production of LiPF6. Any unused or spent LiCl must be properly managed and disposed of according to local regulations.
- **Phosphorus pentachloride (PCl5) waste**: PCl5 may be used as a starting material in the production of LiPF6. Any unused or spent PCl5 must be properly managed and disposed of according to local regulations.
- **Phosphorus Oxyflouride (POF<sub>3</sub>) waste**: The process produces a significant amount of waste as a by-product, which includes phosphorus oxyfluoride (POF<sub>3</sub>). The waste generated needs to be properly treated and disposed according to the local regulations.
- Solid waste: The production of LiPF6 may generate solid waste, such as byproducts or impurities, which must be properly managed and disposed of according to local regulations.
- **Waste water:** The production of LiPF6 may generate wastewater, which may contain HF, LiCl, PCl5, or other chemicals. Wastewater must be properly treated and disposed of according to local regulations to prevent environmental contamination.

The amount of waste generated can range from several hundred kilograms to several tons per ton of LiPF6 produced, depending on the specific conditions of the reaction. In one study, it was reported that the Swarts reaction for producing LiPF6 can generate up to 1.8 tons of waste per ton of LiPF6 produced, with the majority of the waste consisting of POF3 and HF.

Efficient reaction conditions, high-quality starting materials, and effective waste management practices can help reduce the amount of waste generated. In addition, the use of advanced purification methods can help increase the yield and purity of the final product, further reducing waste.

b. What the current regulations for the above waste materials. (Limits to which it can be disposed in the environment)

The disposal of various chemicals in India is regulated under the Hazardous and Other Wastes (Management and Transboundary Movement) Rules, 2016.

- **Hydrogen fluoride (HF) waste:** As per the Hazardous and Other Wastes (Management and Transboundary Movement) Rules, 2016, the permissible limit for hydrogen fluoride in wastewater is 2 mg/l. However, the disposal of hydrogen fluoride is generally not permitted unless it is treated and neutralized to meet the prescribed limits.
- **Lithium chloride (LiCl) waste**: Lithium chloride is classified as a hazardous waste and its disposal is subject to strict regulations under the rules. The permissible limit for lithium chloride in wastewater is 5 mg/l as per the rules.
- **Phosphorus pentachloride (PCl5) waste:** As per the rules, PCl5 is classified as a Schedule I waste, which means that it is highly toxic and poses a severe threat to human health and the environment. The permissible limit for PCl5 in wastewater is 0.1 mg/l.
- Phosphorus Oxy-flouride (POF<sub>3</sub>) waste:
- Solid waste :

Permissible limits for pollutants in landfill leachate:

o pH: 6.5 to 8.5

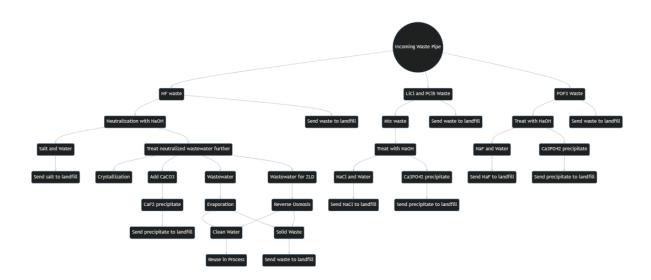
Biochemical Oxygen Demand (BOD): 100 mg/l

Chemical Oxygen Demand (COD): 250 mg/l

Total Suspended Solids (TSS): 100 mg/l

Total Dissolved Solids (TDS): 2100 mg/l

c. Describe the treatment procedure for wastes with block diagram. Your chemical plant must be a zero liquid discharge plant.



d. Are there any safety concerns for the chemicals. Give exposure limits: Time Weighted Average (TWA) for 8 hours and short-term exposure limit (STEL) for 15 minutes.

Some of the safety concerns related to the production of LiPF6 include:

- **Toxicity:** LiPF6 is toxic and exposure to the chemical can cause respiratory, skin, and eye irritation, as well as other adverse health effects. Workers involved in the production process must be trained on the proper handling and use of LiPF6 and be provided with appropriate personal protective equipment (PPE) to minimize the risk of exposure.
- **Flammability**: LiPF6 is a flammable material and can pose a fire hazard if not handled properly. The production process must be designed and operated to minimize the risk of fire, and workers must be trained on fire prevention and response procedures.
- **Reactivity**: LiPF6 can react violently with water, air, and other chemicals, which can lead to the release of toxic gases and cause fires or explosions. The production process must be carefully controlled to prevent these types of reactions from occurring.
- **Corrosivity**: LiPF6 can be corrosive to certain materials, such as aluminum, which can lead to equipment damage and failure. The production process must be designed to minimize contact between LiPF6 and incompatible materials, and equipment must be constructed from materials that are compatible with the chemical.

**TWA** exposure limit: 2.5 mg/m<sup>3</sup>

**STEL** exposure limit: 5 mg/m<sup>3</sup>

### References:

- 1. <u>LiPF6 SDS.pdf (mtixtl.com)</u>
- 2. <u>Lithium hexafluorophosphate 98 21324-40-3 (sigmaaldrich.com)</u>

# List the contributions of each author:

- Author 1 determined the waste generation quantity.
- Author 1 and 2 carried out the literature search and found the current regulations.
- Authors 2 and 3 found necessary treatment steps and prepared the block diagram.
- Author 3 obtained TWA and STEL data.

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