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Systematic Optimization of High Activity Neutralization Materials for Bulk Chemical Agent Detoxification

Bulk detoxification of chemical warfare agents (CWAs) presents unique operational and logistical challenges. Typical surface decontamination processes rely on large excesses of reagents to fully neutralize CWAs; however, at large scale, the quantity of decontaminants (bleach, oxidizers, etc.) becomes prohibitively cumbersome. High-activity neutralization reagents are required in order to reduce the overall logistical burden. Ideally, such materials would be sufficiently stable and safe for operators to use/transport, easily introduced to bulk CWAs, and not require additional infrastructure during or after use. The 12 Principles of Green Chemistry were used to evaluate candidate processes and determine the most operationally effective method. Prevention of exposure was the cardinal goal, supported by reaction optimization to minimize product toxicity. Operational goals were addressed by optimizing for atom economy to minimize operator and environmental exposure, at the expense of using small quantities of highly reactive metal salts (Li_3N). The efficacy of this system, evaluated against other options such as amine substitution using the 12 Principles of Green Chemistry, will be discussed in detail.

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