IP RIGHTS
PCT application from 2024

Practical and safe fluorination of white phosphorus (P4)

The straightforward and safe fluorination of white phosphorus is disclosed. Possible products include the economically relevant hexafluorophosphate anion, key in the battery sector, and phosphorus trifluoride, an important synthetic P(III) synthon. A common organic oxidant assists the transformation via a P(III) intermediate. The reduced form of the oxidant can be re-oxidized, allowing its recycling. The invention avoids the handling of dangerous chlorine and hydrogen fluoride, in contrast to the traditional routes.

Safe and straightforward synthesis of a key battery component

The inventors have devised a sustainable and practical synthesis process that allows for high process safety. It creates a closed-loop system with minimal and harmless waste byproducts. Unlike established methods, this approach offers a safer and potentially catalytic pathway to accessing the PF6– anion.

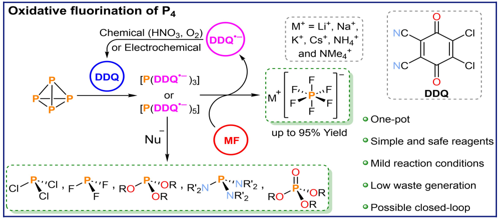
REFERENCES:
Horsley Downie et al., ChemSusChem 2024

01 Minimal and relatively unharmful waste production, associated only with the regeneration of the oxidant. e.g. KNO3.

02 One-pot reaction with simple and commercially available reagents.

03 Safe fluorination, circumventing the need for reactive and hazardous starting materials and intermediates.

04 Feasibility for a closed-loop or catalytic reaction development.



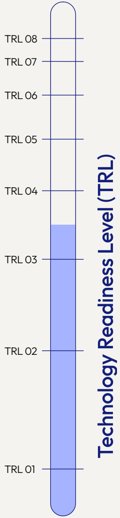
DDQ-mediated oxidative functionalization of P4. “Nu –” stands for a fluorine-, chlorine-, oxygen- or nitrogen-centered nucleophile.

CHALLENGE

The hexafluorophosphate anion is a key component in the most commonly used electrolyte in lithium-ion batteries, which is lithium hexafluorophosphate (LiPF6). Typically, LiPF6 is produced through a sequence of multi-step reactions involving white phosphorus, chlorine gas, and hydrogen fluoride. These processes require costly safety measures when carried out on an industrial scale, making them a significant factor in the overall production costs of batteries.

INNOVATION

The oxidative fluorination of phosphorus tetramer (P4) and its red allotrope is carried out using a common and easy-to-handle oxidant, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ). The reaction can proceed through either a phosphorus(III) or phosphorus(V) intermediate. Additionally, the phosphorus(III) intermediate can be functionalized by selected nucleophiles, such as alcohols or amines, resulting in the formation of phosphites or aminophosphines, respectively. The semi-hydroquinone radical anion form of DDQ (DDQ•–) can be isolated and re-oxidized back to DDQ using inexpensive oxidants such as oxygen or nitric acid, or through electrochemical means.



01 Basic principles observed · **02** Technology concept formulated · **03** Experimental proof of concept · **04** Technology validated in lab · **05** Technology validated in relevant environment · **06** Technology demonstrated in relevant environment · **07** System prototype demonstrated in operational environment · **08** System complete and qualified

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