Sustainable phosphorus functionalization with disulfides

Useful monophosphorus products - e.g. hexafluorophosphate, are obtained from both white and red phosphorus. In contrast to the often inefficient and hazardous current multi-step methods, this invention provides access to diverse monophosphorus products and is both sustainable and economic. The reactions can operate as part of an (electro-)catalytic cycle, with excellent turnover numbers compared with other state-of-the-art direct methods. The inventive method is practically simple, requiring only very cheap, commercially available reagents.



IP RIGHTS
PCT application from
2024

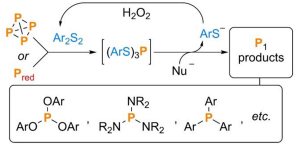
Direkt one-pot synthesis with high process safety

Our team of researchers set out to develop sustainable and efficient catalytic methods for the activation and transformation of P4. Such methods should mimic conceptually the commercial Cl2-based routes, achieving the same net transformations but with greater step economy and fewer hazardous reagents.

REFERENCES:
Downie, ChemSusChem 2024

01 One-pot reactions with simple reagents to obtain diverse valuable monophosphorus compounds
02 Minimal and only non-hazardous stoichiometric waste production, environmentally friendly
03 Sustainable closed-loop or (electro-) catalytic reactions routes possible
04 High process safety: no hazardous educts, intermediates or by-products

direct, oxidative P_4 functionalization



- One-pot
- High yields
- Simple reagents
- Minimal waste
- Closed loop or
- (electro-) catalysis

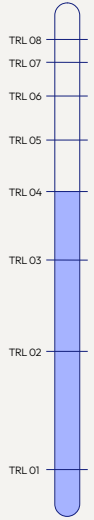
direct, one-step, low-waste oxidative functionalization from this invention, starting with elemental phosphorus. Nu indicates generic nucleophiles.

CHALLENGE

White phosphorus (P4) is the common starting point from which almost all commercially relevant monophosphorus compounds are prepared. Most current industrial synthesis routes rely on multiple reaction steps and/or extremely hazardous reagents, intermediates or waste. When developing new phosphorus functionalization routes, sustainability, simplicity, high yields and cost-effectiveness are all fundamental, ideally in the sense of a circular economy approach. Catalysis is a cornerstone in green approaches.

INNOVATION

Direct transformation of both white and red phosphorus into valuable monophosphorus products is done via initial oxidation by aryl disulfides followed by quenching with nucleophiles. The inventive process provides access routes to diverse P-C, P-N and P-O bonded products in good yields using inexpensive and easy-to-handle reagents. By isolating the thiolate by-products of these reactions, a simple, closed loop can be achieved that produces only minimal, benign waste byproducts, in contrast to other direct methods. This closed loop can even be elaborated into a true (electro-) catalytic cycle, which is extremely rare in the field of elemental phosphorus functionalization.



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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