Phosphorus, Sulfur and Silicon and the Related Elements 2016 vol.191 N11-12, pages 1480-1481

Thermal stability of primary and secondary phosphine oxides formed as a reaction of phosphine oxide with ketones

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Abstract

© 2016 Taylor & Francis Group, LLC.We present the study of reactivity of electrochemically generated in situ from white phosphorus P4 phosphine oxide H3PO toward various ketones (acetone, methylethylketone, methyl-n-propylketone). This interaction was found to give a selective formation of mono- and bis-(α -oxyalkyl)phosphine oxides RR'C(OH)P(O)H2 (1) and (RR'C(OH))2P(O)H (2) where R = Me; R' = Me, Et, n-Pr. Thermal properties of the formed primary and secondary phosphine oxides have been studied and quantum chemical calculations of thermodynamic stability of these compounds were performed.

http://dx.doi.org/10.1080/10426507.2016.1212047

Keywords

DFT calculations, Electrochemistry, ketones, phosphine oxide, white phosphorus