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Thermal fragmentation of spirodithiohydantoins: A novel route to NHCs

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Abstract

Spirodithiohydantoins undergo a two-step thermal fragmentation affording zwitterionic betaine intermediates and N-heterocyclic carbenes (NHCs) respectively. Such reactions are novel, occur under mild conditions and give NHCs in high yield and purity. This phenomenon was studied using various spectroscopic techniques and control experiments with elemental sulfur. Quantum chemical calculations were employed to provide a deeper understanding of such transformations.

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