

Synthesis and Theoretical Study of New Guanylated Cyclophosphazenes and Their Use in the CO₂ Fixation into Styrene Carbonate

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Abstract

Three new guanylated cyclophosphazenes G1–G3 have been synthesized through the catalytic guanylation of three different bi, tetra and hexa (p-aminophenoxy)-cyclophosphazenes by using N,N'-diisopropylcarbodiimide as guanylating agent, ZnEt₂ as catalyst and dry tetrahydrofuran as solvent. The resulting products have been characterized by ¹H, ¹³C{¹H} and ³¹P{¹H} NMR spectroscopy. The hexaguanylated cyclophosphazenes exhibit a deep purple colour, unusual for this type of compounds. The electronic structure of these compounds was investigated by carrying out density functional calculations at PBE-D3(BJ)/TZP level of theory. The molecular structural analysis reveals that aromatic rings are stacked and time dependent density functional calculations show that a charge transfer electronic transition occurs between the aromatic rings which absorb light around 500–700 nm. Finally, the catalytic usefulness of guanylated cyclophosphazene compounds G1–G3 has been proven by the preparation of styrene carbonate from the reaction between styrene oxide and carbon dioxide. © 2022, The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature.

Author keywords

Cyclophosphazene; Guanidine; Organocatalyst; Styrene carbonate