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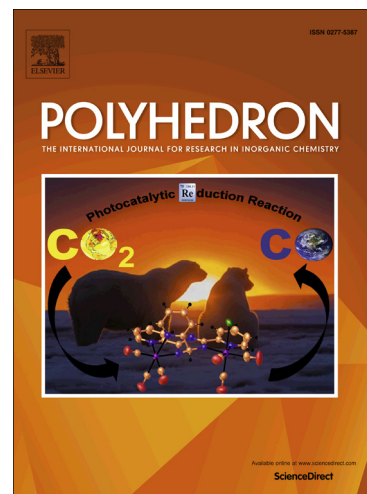
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Stabilization of Group 14 Tetrylene Compounds by an N-Heterocyclic Carbene: A Theoretical Study

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Abstract

The chemistry of stable tetrylenes (the heavier congeners of the group 14 elements) is an appealing target in main group chemistry because of their synthetic potential and industrial applications. The present work seeks to characterize, in the light of DFT calculations, the utilization of methylated N-heterocyclic carbene (NHC(CH₃)) as a Lewis base for the stabilization of ER₂ species as Lewis acids in the form of [NHC(CH₃)→ER₂]; (E = Ge, Sn, Pb; R = H, F, Cl, Br, CH₃) complexes. The structures of the latter complexes are investigated at the M05-2X /def2-TZVPP level of theory. The nature of the C→E bonds in the complexes is analyzed with NBO, AIM, EDA as well as ETS-NOCV at the mentioned level of theory.

The results confirm that the nature of the C→E bond interactions in [NHC(CH₃)→ER₂]; (E = Ge, Sn, Pb; R = H, F, Cl, Br, CH₃) complexes is largely electrostatic, with a contribution of about 57-67% of the total interaction energy. The orbital interaction (ΔE_{orb}) for the considered [NHC(CH₃)→ER₂] complexes arises from C→E σ -donation and C←E π -back donation, which is demonstrated by ETS-NOCV schemes.

Keywords: N-Heterocyclic carbene, Group 14 elements, M05-2x, EDA, ETS-NOCV

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