Si$_6$C$_{18}$: A Bispentalene Derivative with Two Planar tetracoordinate Carbons

Diego Inostroza$^1$, Luis Leyva-Parra$^1$, Osvaldo Yañez$^2$, J. César Cruz$^3$, Jorge Garza-Olguín$^4$, Victor García$^5$, Venkatesan Thimmakondu$^6$, and William Tiznado$^1$

$^1$Universidad Andres Bello
$^2$Universidad de Las Américas
$^3$Universidad Autónoma Metropolitana Iztapalapa
$^4$Universidad Autonoma Metropolitana Iztapalapa
$^5$Universidad Nacional Mayor de San Marcos
$^6$San Diego State University

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Abstract

Here we show that substituting the ten protons in the dianion of a bispentalene derivative (C$_{18}$H$_{10}$$^2-$) by six Si$^{2+}$ dications produces a minimum energy structure with two planar tetracoordinate carbons (ptC). In Si$_6$C$_{18}$, the ptCs are embedded in the terminal C$_5$ pentagonal rings and participate in a three-center, two-electron (3c-2e) Si-ptC-Si σ-bond. Our exploration of the potential energy surface identifies a triphenylene derivative as the putative global minimum. But robustness to Born-Oppenheimer molecular dynamics (BOMD) simulations at 900 and 1500 K supports bispentalene derivative kinetic stability. Chemical bonding analysis reveals ten delocalized π-bonds, which, according to Hückel’s 4n+2 π-electron rule, would classify it as an aromatic system. Magnetically induced current density analysis reveals the presence of intense local paratropic currents and a weakly global diatropic current, the latter agreeing with the possible global aromatic character of this specie.

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