

Si₆C₁₈: A Bispentalene Derivative with Two Planar tetracoordinate Carbons

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Abstract

Here we show that substituting the ten protons in the dianion of a bispentalene derivative (C₁₈H₁₀²⁻) by six Si²⁺ dications produces a minimum energy structure with two planar tetracoordinate carbons (ptC). In Si₆C₁₈, the ptCs are embedded in the terminal C₅ 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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