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RESEARCH ARTICLE

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Si_6C_{18}: 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 ($C_{18}H_{10}^{2-}$) by six Si^{2+} dications produces a minimum energy structure with two planar tetracoordinate carbons (ptC). In Si_6C_{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. Nevertheless, 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.

KEYWORDS
chemical bonding analysis, DFT computations, global minimum, planar tetracoordinate carbon, silicon-carbon clusters

1 | INTRODUCTION

Nowadays, molecules or clusters with planar hypercoordinate carbon (phC) are no longer a curiosity, given the experimental and theoretical effort to synthesize or design systems with these features [1–5]. The phCs isolation and experimental characterization initially seemed not feasible because they do not meet the apparent structural consequence of tetrahedral geometry in a tetracoordinate carbon, that is, they violate the van't Hoff and Le Bel principle. The pioneers to point out how to stabilize these systems was Monkhorst (1968), who evaluated the stereomutation of

