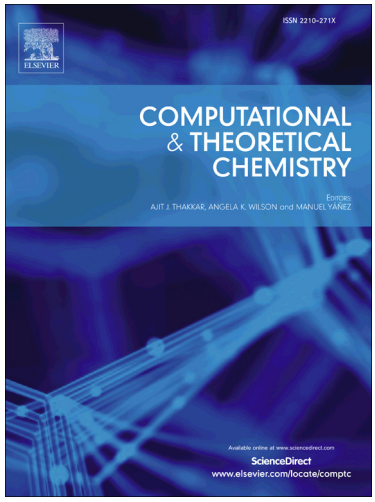

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Is the bonding cumulenic or polyacetylenic in nonatetraynylidene?

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Abstract

To answer the entitled question, the equilibrium geometry of the linear triplet ground electronic state ($\widetilde{X}^3\Sigma_g^-$) of nonatetraynylidene (**1**), HC_9H, has been theoretically investigated at various levels of theory. The relative energies, optimal geometry parameters, expectation values of S^2, rotational constant, spin densities, and harmonic vibrational frequencies with respect to both restricted open-shell Hartree-Fock (ROHF) and unrestricted HF (UHF) at different levels are examined. The methods employed are HF Self-Consistent Field (SCF), Møller-Plesset perturbation level of theory until second-order (MP2), coupled-cluster singles and doubles (CCSD), and CCSD with perturbative triple excitations (CCSD(T)). Correlation consistent polarized valence double and triple zeta (cc-pVXZ; X = D and T) basis sets are used in all calculations and frozen-core approximation is utilized in all post-SCF calculations. Population analysis of the spin densities at CC levels suggest that several valence structures are possible for **1** implying more polyacetylenic character rather than the cumulenic biradical.

Keywords: , Equilibrium geometry, Cumulenic biradical, Polyacetylene, HC_9H, Nonatetraynylidene, Spin density

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