

## Accepted Manuscript

Is the bonding cumulenic or polyacetylenic in nonatetraynylidene?

Venkatesan S. Thimmakondur, Baranitharan Sekar

PII: S2210-271X(16)30501-1

DOI: <http://dx.doi.org/10.1016/j.comptc.2016.12.015>

Reference: COMPTC 2332

To appear in: *Computational & Theoretical Chemistry*



Please cite this article as: V.S. Thimmakondur, B. Sekar, Is the bonding cumulenic or polyacetylenic in nonatetraynylidene?, *Computational & Theoretical Chemistry* (2016), doi: <http://dx.doi.org/10.1016/j.comptc.2016.12.015>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# Is the bonding cumulenenic or polyacetylenic in nonatetraynylidene?

Venkatesan S. Thimmakondur\*, Baranitharan Sekar

*Department of Chemistry, Birla Institute of Technology and Science, Pilani, K K Birla Goa Campus, Goa - 403 726, India.*

---

## Abstract

To answer the entitled question, the equilibrium geometry of the linear triplet ground electronic state ( $\tilde{X}^3\Sigma_g^-$ ) of nonatetraynylidene (**1**),  $\text{HC}_9\text{H}$ , 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 cumulenenic biradical.

**Keywords:** , Equilibrium geometry, Cumulenenic biradical, Polyacetylene,  $\text{HC}_9\text{H}$ , Nonatetraynylidene, Spin density

---



---

\*Corresponding author

Email address: [venkatesh@goa.bits-pilani.ac.in](mailto:venkatesh@goa.bits-pilani.ac.in) (Venkatesan S. Thimmakondur)

Download English Version:

<https://daneshyari.com/en/article/5392535>

Download Persian Version:

<https://daneshyari.com/article/5392535>

[Daneshyari.com](https://daneshyari.com)