

Update 1 of: carbon in one dimension: structural analysis of the higher conjugated polyynes.

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The previous decade has witnessed an ongoing series of stunning breakthroughs in carbon allotrope chemistry.^{1,2} This field has attracted scientists from all disciplines and is playing a leading role in the nanotechnology boom. However, the polymeric sp carbon allotrope, often termed “carbyne”, remains an unsettled and somewhat controversial topic.³ This substance ranks in conceptual importance as a full equal of diamond, the polymeric, three-dimensional sp³ allotrope, and graphite, the polymeric, two-dimensional sp² allotrope. It should have a linear ground state, but remains difficult to generate, isolate, and characterize. All polymeric carbon allotropes must have some type of capping endgroup, and in this context carbyne has two limiting forms: one with dicoordinate terminal carbons (XC:) and consisting of alternating triple and single bonds, and another with tricoordinate terminal carbons (X₂C) and consisting solely of double bonds.

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