

Accepted Manuscript

Protomene: A new carbon allotrope

Francesco Delodovici, Nicola Manini, Richard S. Wittman, Daniel S. Choi, Mohamed Al Fahim, Larry A. Burchfield



PII: S0008-6223(17)31069-2

DOI: [10.1016/j.carbon.2017.10.069](https://doi.org/10.1016/j.carbon.2017.10.069)

Reference: CARBON 12496

To appear in: *Carbon*

Received Date: 8 August 2017

Revised Date: 7 October 2017

Accepted Date: 20 October 2017

Please cite this article as: F. Delodovici, N. Manini, R.S. Wittman, D.S. Choi, M. Al Fahim, L.A. Burchfield, Protomene: A new carbon allotrope, *Carbon* (2017), doi: 10.1016/j.carbon.2017.10.069.

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.

Protomene: a new carbon allotrope

Francesco Delodovici^a, Nicola Manini^a, Richard S Wittman^b, Daniel S. Choi^c, Mohamed Al Fahim^d, Larry A Burchfield^{*d}

^a*Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy*

^b*Pacific Northwest National Laboratory, 902 Battelle Blvd, Richland, WA 99354, USA*

^c*Mechanical and Materials Engineering Department, Masdar Institute of Science and Technology, A Part of Khalifa University of Science and Technology, PO Box 54224, Abu Dhabi, UAE*

^d*Alfields, Inc. PO Box 3091, Richland, WA 99354, USA*

Abstract

We introduce a new carbon allotrope named protomene. Its crystal structure is hexagonal, with a fully-relaxed primitive cell involving 48 atoms. Of these, 12 atoms have the potential to switch hybridization between sp^2 and sp^3 , forming dimers. By means of DFT simulations, we have identified the equilibrium structure of protomene, and estimate that it is 2% less bound than diamond. We have also estimated the amplitude of its direct band gap to be 3 eV, and predicted the X-ray diffraction pattern and phonon modes.

1. Introduction

Driven by the discovery of some of the most interesting new materials, namely fullerenes, nanotubes and graphene, the quest for new allotropes of carbon has been an increasingly active field of research for several decades [1]. This broad interest is fueled by the wide range of structural and electronic properties of carbon allotropes. Indeed, carbon possesses three energetically competitive different types of orbital hybridization (sp , sp^2 , and sp^3).

*Corresponding author. Tel: +971 50 5320 130. E-mail: info@alfields.co

Download English Version:

<https://daneshyari.com/en/article/7849207>

Download Persian Version:

<https://daneshyari.com/article/7849207>

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