SACADA Database Code: 16

Topology: ths (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1211]
Space Group: C2/c
Pearson: mS16
Coordination Number (CN): 2, 3 (1:1)

Year: 1993

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ths (SACADA #16)		1.581		1.351	95.8	38.4	5.5	SACADA[1]
Cis hinged polydiacetylene		1.564						doi: 10.1038/365735a0

Elasticity tensor (kBar)[1]

1016.9326	2006.8341	732.1545	0.0000	0.0000	359.7139
2006.8341	4191.0468	1329.7988	-0.0000	0.0000	599.0019
732.1545	1329.7988	2154.8584	0.0000	-0.0000	520.0840
0.0000	0.0000	0.0000	1562.9020	385.8434	0.0000
0.0000	0.0000	-0.0000	385.8434	404.0839	-0.0000
359.7139	599.0019	520.0840	0.0000	-0.0000	301.1903

[1] We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ Å^{-1} is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV Å^{-1} for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — have been calculated within the Voigt–Reuss–Hill [8] approximation. The Vicker's hardness H_v has been estimated according to Oganov's model [9].