SACADA Database Code: 47

Topology: pbz (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1231]
Space Group: P-43m
Pearson: cP48
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
pbz (SACADA #47)		1.445		1.201	150.5	15.0	2.5	SACADA[1]
Cubic b-Graphyne		1.056	1.38					doi: 10.1016/0379-6779(93)90951-r

Elasticity tensor (kBar)[1]

1831.7325	1340.8149	1340.8149	-0.0000	-0.0000	0.0000
1340.8149	1831.7325	1340.8149	-0.0000	-0.0000	0.0000
1340.8149	1340.8149	1831.7325	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	107.3561	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	107.3561	0.0000
0.0000	-0.0000	0.0000	0.0000	0.0000	107.3561

[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].