SACADA Database Code: 44

Topology: pcb (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1222]
Space Group: Im-3m
Pearson: cI128
Coordination Number (CN): 2, 4 (7:1)

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pcb (SACADA #44)		.431		1.777	-	-	-	SACADA[1]
supercubane C128								doi: 10.1021/jp3104479

Elasticity tensor (kBar)[1]

395.3310	282.1709	282.1709	0.0000	0.0000	0.0000
282.1709	395.3310	282.1709	0.0000	-0.0000	0.0000
282.1709	282.1709	395.3310	-0.0000	0.0000	0.0000
0.0000	0.0000	-0.0000	-2.1085	0.0000	-0.0000
0.0000	-0.0000	0.0000	-0.0000	-2.1085	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	-2.1085

[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].