SACADA Database Code: 39

Topology: pcb

# of independent nodes (IN): 1
Transitivity: [1222]
Space Group: Im-3m
Pearson: cI16
Coordination Number (CN): 4

Year: 1979

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pcb (SACADA #39)		2.791		1.245	311.0	218.1	25.6	SACADA[1]
C8								link
C8								link
C8								doi: 10.1021/ja00297a011
C8			6.5					doi: 10.1021/ja00185a004
supercubane								doi: 10.1016/0166-1280(95)04409-4
supercubane		2.9			319			doi: 10.1016/s0009-2614(98)00762-3
supercubane								doi: 10.1006/jssc.1999.8448
CA3								doi: 10.1134/s1063776111060173
CA3								link
Cubic-C16		2.75			309.1			doi: 10.1073/pnas.1311028110
pcb								doi: 10.1524/zkri.2013.1620
C8								doi: 10.1039/C6CE02635D

Elasticity tensor (kBar)[1]

5050.7278	2139.6478	2139.6478	0.0000	-0.0000	0.0000
2139.6478	5050.7278	2139.6478	0.0000	0.0000	-0.0000
2139.6478	2139.6478	5050.7278	-0.0000	-0.0000	0.0000
0.0000	0.0000	-0.0000	2862.4996	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	-0.0000	2862.4996	-0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	2862.4996

[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].