SACADA Database Code: 58

Topology: npo

# of independent nodes (IN): 1
Transitivity: [1232]
Space Group: P63/mmc
Pearson: hP6
Coordination Number (CN): 4

Year: 1999

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
npo (SACADA #58)		2.785		0.323	333.1	288.6	45.6	SACADA[1]
hcp-C3								doi: 10.1103/PhysRevB.59.733
TB								doi: 10.1134/s1063776111060173
hcp-C3								doi: 10.7498/aps.61.043103
								link
								doi: 10.1103/PhysRevLett.113.085501

Elasticity tensor (kBar)[1]

5927.2417	2104.9226	970.7463	-0.0000	-0.0000	0.0000
2104.9226	5927.2417	970.7463	-0.0000	0.0000	-0.0000
970.7463	970.7463	10503.4276	0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	1911.1596	0.0000	-0.0000
-0.0000	0.0000	-0.0000	0.0000	3640.0594	-0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	3640.0594

[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].