SACADA Database Code: 202

Topology: 4^3T138

# of independent nodes (IN): 3
Transitivity: -
Space Group: P6322
Pearson: hP36
Coordination Number (CN): 4

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^3T138 (SACADA #202)		2.981		1.240	337.1	317.5	54.7	SACADA[1]
β-C		1.53	3.07		521		71.8	doi: 10.1016/j.physleta.2015.06.037

Elasticity tensor (kBar)[1]

7484.7928	1829.8397	531.4402	-0.0000	0.0000	-0.0000
1829.8397	7484.7928	531.4402	-0.0000	-0.0000	0.0000
531.4402	531.4402	9608.7555	-0.0000	0.0000	0.0000
-0.0000	-0.0000	-0.0000	2827.4766	-0.0000	-0.0000
0.0000	-0.0000	0.0000	-0.0000	3019.1262	-0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	3019.1262

[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].