SACADA Database Code: 46

Topology: pbz

# of independent nodes (IN): 1
Transitivity: [1231]
Space Group: Pn-3m
Pearson: cP24
Coordination Number (CN): 3

Year: 1946

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pbz (SACADA #46)		2.138		0.775	248.3	117.8	15.8	SACADA[1]
								doi: 10.1039/JR9460000456
6.8² D		2.19	3.4					doi: 10.1103/PhysRevLett.68.2325
Cubic Graphite		2.136	3.44		220			doi: 10.1016/0379-6779(93)90951-r
6.8² D								doi: 10.1098/rsta.1993.0045
6.8² D								doi: 10.1103/PhysRevB.47.1593
D688								doi: 10.1016/0009-2614(93)85009-d
D688		2.18			248			doi: 10.1016/0956-7151(94)90210-0
D688								doi: 10.1039/CS9952400341
6.8² D								doi: 10.1098/rsta.1996.0088
D688								doi: 10.1016/s0960-8974(97)00003-x
D688								doi: 10.1080/10641229809350239
SC24		2.14	3.45		325			doi: 10.1103/PhysRevB.57.R661
D688								doi: 10.1088/1367-2630/5/1/126
D688			2.9		325	131		doi: 10.1088/1367-2630/5/1/123
BTA_48								link
SC24		2.11	3.72					doi: 10.1103/PhysRevB.85.214104
pbz								doi: 10.1007/s11224-016-0782-1

Elasticity tensor (kBar)[1]

3456.1609	1995.6607	1995.6607	0.0000	0.0000	-0.0000

1995.6607	3456.1609	1995.6607	0.0000	0.0000	0.0000
1995.6607	1995.6607	3456.1609	-0.0000	0.0000	0.0000
0.0000	0.0000	-0.0000	1625.3846	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	1625.3846	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	1625.3846

[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].