SACADA Database Code: 22

Topology: bto

# of independent nodes (IN): 1
Transitivity: [1221]
Space Group: P6222
Pearson: hP6
Coordination Number (CN): 3

Year: 1990

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
bto (SACADA #22)		3.149		1.379	382.3	209.8	25.7	SACADA[1]
H-6		3.4	Metal		580			doi: 10.1557/JMR.1990.2273
H-6		3.17			372			doi: 10.1103/PhysRevB.43.6742
6(3)6-09		3.19						doi: 10.1016/S0009-2614(01)00126-9
H-6		3.16			370			doi: 10.1007/978-94-010-1013-9_1
H-6					384			doi: 10.1103/PhysRevB.78.125415
H-6								link
H-6		3.093	Metal					doi: 10.1039/c2cp43221h
H-6								doi: 10.1038/srep04339
H-6			Metal		273			doi: 10.1016/j.commatsci.2013.10.032
H-6								doi: 10.1039/c6ra10809a

Elasticity tensor (kBar)[1]

6016.8621	3359.7431	922.7967	0.0000	0.0000	0.0000
3359.7431	6016.8621	922.7967	0.0000	-0.0000	-0.0000
922.7967	922.7967	12494.5814	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	1328.5595	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	1992.7088	-0.0000
0.0000	-0.0000	-0.0000	0.0000	-0.0000	1992.7070

[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].