SACADA Database Code: 15

Topology: ths

# of independent nodes (IN): 1
Transitivity: [1211]
Space Group: I41/amd
Pearson: tI8
Coordination Number (CN): 3

Year: 1983

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ths (SACADA #15)		2.900		1.077	348.2	146.1	20.7	SACADA[1]
A Hypothetical Metallic-Allotrope of Carbon		2.72	Metal					doi: 10.1021/ja00352a049
bct-4					362			doi: 10.1103/PhysRevB.45.4579
sp2 allotrope		2.97						link
Hinged polyacetylene		2.869						doi: 10.1038/365735a0
4(3)2		2.94						doi: 10.1016/S0009-2614(01)00126-9
bct-4								doi: 10.1007/978-94-010-1013-9_1
bct-4					354			doi: 10.1103/PhysRevB.78.125415
bct-4								link
bct-4		2.853	Metal					doi: 10.1039/c2cp43221h
Bct-C4								doi: 10.1088/0253-6102/64/2/237
cT16			Semimetal		216			nonelink

Elasticity tensor (kBar)[1]

7703.1624	535.0546	981.2768	0.0000	0.0000	0.0000
535.0546	7703.1624	981.2768	0.0000	-0.0000	0.0000
981.2768	981.2768	11638.8578	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	268.6571	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	1043.3743	-0.0000
0.0000	0.0000	-0.0000	0.0000	-0.0000	1043.3711

[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].