SACADA Database Code: 17

Topology: ths (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1211]
Space Group: I41/amd
Pearson: tI12
Coordination Number (CN): 2, 3 (1:1)

Year: 1984

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ths (SACADA #17)		2.559		1.555	179.6	56.8	8.7	SACADA[1]
allene carbon								doi: 10.1070/RC1984v053n07ABEH003084
allene carbon								doi: 10.1007/bf00749588
sp2/sp allotrope		2.72						link

Elasticity tensor (kBar)[1]

2712.8693	-712.8887	2404.4243	0.0000	-0.0000	0.0000
-712.8887	2712.8693	2404.4243	-0.0000	0.0000	0.0000
2404.4243	2404.4243	11897.5591	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	37.0553	0.0000	0.0000
-0.0000	0.0000	0.0000	0.0000	618.8612	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	618.8609

[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].