SACADA Database Code: 303

Topology: $3^7,4^2T3$

# of independent nodes (IN): 3
Transitivity: [9(15)(10)4]
Space Group: P63/mmc
Pearson: hP160
Coordination Number (CN): 3, 4 (9:1)

Year: 2008

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^7,4^2T3$ (SACADA #303)		.960		1.110	26.3	19.0	2.3	SACADA[1]
HL C40		0.78	1.01		30.25			doi: 10.1103/PhysRevB.77.113402
HL C40		0.78			30.25			doi: 10.3103/s1063457610020012

Elasticity tensor (kBar)[1]

545.6381	139.5544	95.7990	-0.0000	0.0000	-0.0000
139.5544	545.6381	95.7990	-0.0000	0.0000	-0.0000
95.7990	95.7990	611.3978	-0.0000	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	203.0419	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	155.0151	-0.0000
-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	155.0151

[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].