SACADA Database Code: 199

Topology: 3^2,4T204

# of independent nodes (IN): 3
Transitivity: -
Space Group: P63/mcm
Pearson: hP36
Coordination Number (CN): 3, 4 (2:1)

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T204 (SACADA #199)		2.136		0.858	243.3	170.3	20.0	SACADA[1]
Hex-C36	0-20	2.179	1.57		244.7	176.3	24.7	doi: 10.1016/j.carbon.2015.05.027

Elasticity tensor (kBar)[1]

3972.8361	1595.5863	1016.1330	0.0000	0.0000	0.0000
1595.5863	3972.8361	1016.1330	0.0000	-0.0000	-0.0000
1016.1330	1016.1330	7105.7748	0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	1188.6249	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	1975.1980	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	1975.1980

[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].