SACADA Database Code: 263

Topology: 3^6T5

# of independent nodes (IN): 6
Transitivity: [6(10)85]
Space Group: Pm-3m
Pearson: cP216
Coordination Number (CN): 3

Year: 1992

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^6T5 (SACADA #263)		1.030		0.763	101.6	43.5	6.1	SACADA[1]
P7par								doi: 10.1103/PhysRevB.46.1941
P7par								doi: 10.1038/355333a0
P7par								doi: 10.1103/PhysRevLett.69.921
P7par								doi: 10.1098/rsta.1993.0045
P7par					171			doi: 10.1016/0956-7151(94)90210-0
P7par								doi: 10.1021/jp9613201
P7par								doi: 10.1016/s0960-8974(97)00003-x
P7par								doi: 10.1088/1367-2630/5/1/126
P7par			1.3		126	45.1		doi: 10.1088/1367-2630/5/1/123
super-diamond								doi: 10.1021/nl0622202

Elasticity tensor (kBar)[1]

1449.1062	799.3636	799.3636	0.0000	-0.0000	-0.0000
799.3636	1449.1062	799.3636	-0.0000	0.0000	0.0000
799.3636	799.3636	1449.1062	0.0000	-0.0000	-0.0000
-0.0000	-0.0000	0.0000	527.5464	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	527.5464	0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	527.5464

[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].