SACADA Database Code: 210

Topology: $3,4^3T72$

# of independent nodes (IN): 4
Transitivity: [4554]
Space Group: Cmmm
Pearson: oS16
Coordination Number (CN): 3, 4 (1:3)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^3T72$ (SACADA #210)		3.326		0.192	394.9	315.0	44.1	SACADA[1]
oC16	16.7				391.3	318.8	42.9	doi: 10.1063/1.4952426

Elasticity tensor (kBar)[1]

10923.0992	1564.3878	1501.0299	0.0000	0.0000	0.0000
1564.3878	6974.8978	386.2587	-0.0000	0.0000	0.0000
1501.0299	386.2587	11817.3607	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	1216.4977	0.0000	-0.0000
0.0000	0.0000	0.0000	0.0000	2685.2416	0.0000
0.0000	0.0000	-0.0000	-0.0000	0.0000	5437.8910

[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].