SACADA Database Code: 690

Topology: 4^4T63-CA

# of independent nodes (IN): 4
Transitivity: [4(12)(11)7]
Space Group: P2/n
Pearson: mP16
Coordination Number (CN): 4

Year: 2023

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^4T63-CA (SACADA #690)		3.501		0.298	426.4	490.3	92.4	SACADA[1]
4^4T63-CA								doi: 10.1107/S205252062300255X

Elasticity tensor (kBar)[1]

11879.9235	623.1155	138.7436	0.0000	-0.0000	4.8545
623.1155	10663.4349	768.0346	-0.0000	-0.0000	-127.2276
138.7436	768.0346	12836.3026	0.0000	0.0000	-56.5091
0.0000	-0.0000	0.0000	4309.5821	-105.6015	-0.0000
-0.0000	-0.0000	0.0000	-105.6015	4607.8164	-0.0000
4.8545	-127.2276	-56.5091	-0.0000	-0.0000	4513.5637

[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].