SACADA Database Code: 177

Topology: $3,4^2T242$

# of independent nodes (IN): 3
Transitivity: [3566]
Space Group: P4/mbm
Pearson: tP20
Coordination Number (CN): 3, 4 (1:4)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^2T242$ (SACADA #177)		2.919		0.540	327.6	295.9	49.1	SACADA[1]
C_{20}-D		2.97	1.26					doi: 10.1016/j.carbon.2016.08.015

Elasticity tensor (kBar)[1]

5565.5531	2904.3856	332.4771	0.0000	-0.0000	0.0000
2904.3856	5565.5531	332.4771	-0.0000	0.0000	-0.0000
332.4771	332.4771	11616.1895	0.0000	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	3716.8809	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	3069.0863	0.0000
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	3069.0864

[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].