SACADA Database Code: 160

Topology: 3^2,4T205

# of independent nodes (IN): 3
Transitivity: [3432]
Space Group: Immm
Pearson: oI16
Coordination Number (CN): 3, 4 (3:1)

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T205 (SACADA #160)		2.071		0.813	220.3	122.4	14.9	SACADA[1]
oI16-carbon			0.57		219.9	127.7	15.4	doi: 10.3103/s1063457614040042

Elasticity tensor (kBar)[1]

3996.2794	2185.9909	725.4701	-0.0000	0.0000	0.0000
2185.9909	2193.1208	573.5686	-0.0000	-0.0000	0.0000
725.4701	573.5686	9091.4127	0.0000	0.0000	-0.0000
-0.0000	-0.0000	0.0000	457.2629	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	1485.0142	-0.0000
0.0000	0.0000	-0.0000	0.0000	0.0000	2387.6743

[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].