SACADA Database Code: 381

Topology: 4^7T23

# of independent nodes (IN): 7
Transitivity: [7(16)(12)5]
Space Group: P-1
Pearson: aP14
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^7T23 (SACADA #381)		3.385		0.919	387.5	429.0	80.2	SACADA[1]
G61								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

9271.5428	1026.8347	1500.8088	108.2427	-93.6719	-178.4653
1026.8347	10490.7617	705.7770	325.4987	174.2722	62.4460
1500.8088	705.7770	8694.5041	-51.7639	76.2552	-18.5038
108.2427	325.4987	-51.7639	4452.8379	6.4331	105.3304
-93.6719	174.2722	76.2552	6.4331	4007.2446	55.4528
-178.4653	62.4460	-18.5038	105.3304	55.4528	4682.7232

[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].