SACADA Database Code: 150

Topology: cbs-3,4-C2m

# of independent nodes (IN): 2
Transitivity: -
Space Group: C2/m
Pearson: mS16
Coordination Number (CN): 3, 4 (1:1)

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
cbs-3,4-C2m (SACADA #150)		3.070		0.871	346.8	283.1	41.1	SACADA[1]
mC16-carbon			Metal		347.5	290.5	41.6	doi: 10.3103/s1063457614040042

Elasticity tensor (kBar)[1]

5185.5430	332.8057	862.0559	7.9115	-0.1837	-60.2911
332.8057	11257.6459	1964.2126	-7.1635	-1.8256	148.6476
862.0559	1964.2126	10994.5222	12.5579	3.2254	-600.7242
7.9115	-7.1635	12.5579	1639.1294	-322.3876	-1.5154
-0.1837	-1.8256	3.2254	-322.3876	4980.8458	1.8888
-60.2911	148.6476	-600.7242	-1.5154	1.8888	1446.7249

[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].