SACADA Database Code: 317

Topology: jcc33

# of independent nodes (IN): 10
Transitivity: [(10)(19)(15)6]
Space Group: Im
Pearson: mS32
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
jcc33 (SACADA #317)		3.315		0.747	393.3	402.8	73.2	SACADA[1]
Cm-32	24.0	3.268					83.1	doi: 10.1063/1.4794424

Elasticity tensor (kBar)[1]

9883.3736	1100.5527	1229.7485	-0.0000	-0.0000	247.3727
1100.5527	10286.2037	440.4351	0.0000	0.0000	161.4791
1229.7485	440.4351	9705.0205	0.0000	0.0000	-325.5114
-0.0000	0.0000	0.0000	3871.9137	101.1947	0.0000
-0.0000	-0.0000	0.0000	101.1947	3396.6286	-0.0000
247.3727	161.4791	-325.5114	0.0000	-0.0000	3968.2206

[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].