SACADA Database Code: 4

Topology: dia (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1111]
Space Group: Pn-3m
Pearson: P12
Coordination Number (CN): 2, 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
dia (SACADA #4)		1.780		1.794	167.5	20.0	3.3	SACADA[1]
Y-II carbon (2-fold)		1.77			171.2	28.1		doi: 10.1039/C4RA01962H

Elasticity tensor (kBar)[1]

1807.2433	1609.0825	1609.0825	-0.0000	0.0000	-0.0000
1609.0825	1807.2433	1609.0825	-0.0000	0.0000	-0.0000
1609.0825	1609.0825	1807.2433	-0.0000	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	316.7304	-0.0000	0.0000
0.0000	0.0000	-0.0000	-0.0000	316.7304	0.0000
-0.0000	-0.0000	-0.0000	0.0000	0.0000	316.7304

[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].