SACADA Database Code: 62

Topology: crb (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1232]
Space Group: I4/mmm
Pearson: tI24
Coordination Number (CN): 2, 4 (2:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
crb (SACADA #62)		1.650		1.015	114.8	45.4	6.6	SACADA[1]
2-Yne			2.646		71.7			doi: 10.1016/j.ssc.2013.07.001

Elasticity tensor (kBar)[1]

1209.1862	782.0057	1723.2609	0.0000	0.0000	0.0000
782.0057	1209.1862	1723.2609	0.0000	0.0000	0.0000
1723.2609	1723.2609	3968.5855	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	687.5621	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	681.1589	0.0000
-0.0000	-0.0000	-0.0000	0.0000	0.0000	681.1590

[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].