SACADA Database Code: 61

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 #61)		1.911		1.122	159.9	54.8	8.2	SACADA[1]
1-Yne			0.416		69.8			doi: 10.1016/j.ssc.2013.07.001

Elasticity tensor (kBar)[1]

4897.0931	1217.0727	200.2737	23.1387	-37.3190	-2.0385
1217.0727	4925.7871	149.8426	5.4763	49.8397	1.5029
200.2737	149.8426	2542.7157	-7.6642	-20.7080	-0.0199
23.1387	5.4763	-7.6642	228.7420	2.4528	-3.4708
-37.3190	49.8397	-20.7080	2.4528	153.4393	-0.1503
-2.0385	1.5029	-0.0199	-3.4708	-0.1503	155.4589

[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].