SACADA Database Code: 63

Topology: crb (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1232]
Space Group: I4/mmm
Pearson: tI40
Coordination Number (CN): 2, 4 (4:1)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
crb (SACADA #63)		.864		1.223	31.9	1.5	0.2	SACADA[1]
3-Yne			4.168		40.80			doi: 10.1016/j.ssc.2013.07.001

Elasticity tensor (kBar)[1]

705.9905	692.2859	844.5137	12.8522	-10.4745	-5.3095
692.2859	729.5300	813.2358	1.7367	13.8115	6.8558
844.5137	813.2358	1011.6602	-11.7506	-14.7153	2.1644
12.8522	1.7367	-11.7506	74.8500	2.5500	-2.7011
-10.4745	13.8115	-14.7153	2.5500	29.0649	0.2993
-5.3095	6.8558	2.1644	-2.7011	0.2993	29.2133

[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].