SACADA Database Code: 27

Topology: pcu-h (Allotrope with "sp" atoms)

# of independent nodes (IN): 2
Transitivity: [1221]
Space Group: R-3m
Pearson: hR36
Coordination Number (CN): 2, 3 (1:1)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pcu-h (SACADA #27)		1.770		0.711	108.1	38.0	5.7	SACADA[1]
Rh12			Metal		195			doi: 10.1038/srep24665

Elasticity tensor (kBar)[1]

4851.1263	2648.7743	332.1053	-6.5036	235.5026	-10.5297
2648.7743	4921.7637	358.1626	28.4443	-247.6548	10.3718
332.1053	358.1626	300.8528	5.7351	-0.8451	-1.3428
-6.5036	28.4443	5.7351	1002.8804	10.4359	190.9582
235.5026	-247.6548	-0.8451	10.4359	89.2211	3.0845
-10.5297	10.3718	-1.3428	190.9582	3.0845	74.1427

[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].