SACADA Database Code: 26

Topology: pcu-h

# of independent nodes (IN): 1
Transitivity: [1221]
Space Group: R-3m
Pearson: hR18
Coordination Number (CN): 3

Year: 2001

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pcu-h (SACADA #26)		2.561		1.032	184.1	97.1	12.2	SACADA[1]
6(3)1-10		2.49						doi: 10.1016/S0009-2614(01)00126-9
Rh6								doi: 10.1038/srep04339
Rh6					231	188		doi: 10.1038/srep21879
Rh6								doi: 10.1186/s40679-016-0024-z
Rh6								doi: 10.1016/j.carbon.2016.02.056
Rh6			0.47		299			doi: 10.1103/PhysRevLett.116.195501
Rh6								doi: 10.1038/srep24665

Elasticity tensor (kBar)[1]

6577.4724	3250.9796	1570.1598	-0.0000	-234.1870	0.0000
3250.9796	6577.4724	1570.1598	-0.0000	234.1870	-0.0000
1570.1598	1570.1598	880.7176	-0.0000	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	1663.2464	-0.0000	-234.1869
-234.1870	234.1870	-0.0000	-0.0000	1150.4049	-0.0000
0.0000	-0.0000	-0.0000	-234.1869	-0.0000	1150.4049

[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].