SACADA Database Code: 345

Topology: ajk6

# of independent nodes (IN): 19
Transitivity: [(19)(29)(20)7]
Space Group: P63/mmc
Pearson: hP204
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ajk6 (SACADA #345)		3.063		0.670	371.1	415.0	77.7	SACADA[1]
Clathrate II-6H								doi: 10.1002/cphc.201300133

Elasticity tensor (kBar)[1]

9242.3317	955.3439	926.4090	-0.0000	-0.0000	-0.0000
955.3439	9242.3317	926.4090	-0.0000	0.0000	-0.0000
926.4090	926.4090	9298.8784	0.0000	0.0000	0.0000
-0.0000	0.0000	0.0000	4143.4939	0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	4141.5846	-0.0000
-0.0000	-0.0000	0.0000	0.0000	-0.0000	4141.5846

[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].