SACADA Database Code: 277

Topology: mgz-x-d

# of independent nodes (IN): 7
Transitivity: [7(11)83]
Space Group: P63/mmc
Pearson: hP68
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
mgz-x-d (SACADA #277)		3.062		0.675	383.7	425.7	79.6	SACADA[1]
Clathrate V								doi: 10.1021/jp205676p
Clathrate V		3.03	3.84		366.5		82.5	doi: 10.1021/ic102178d
L5		3.05	6.0		403			doi: 10.1007/s11224-012-0040-0
KVII		3.05			403			doi: 10.1063/1.4802002
Clathrate II-2H								doi: 10.1002/cphc.201300133

Elasticity tensor (kBar)[1]

9470.8035	1040.3387	980.5831	-0.0000	0.0000	0.0000
1040.3387	9470.8035	980.5831	-0.0000	-0.0000	0.0000
980.5831	980.5831	9582.6154	-0.0000	-0.0000	-0.0000
-0.0000	-0.0000	-0.0000	4215.2324	-0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	4282.4395	-0.0000
-0.0000	0.0000	-0.0000	0.0000	-0.0000	4282.4395

[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].