SACADA Database Code: 117

Topology: thj

# of independent nodes (IN): 2
Transitivity: [2342]
Space Group: I212121
Pearson: oI8
Coordination Number (CN): 4

Year: 2004

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
thj (SACADA #117)		3.436		2.115	383.5	390.0	70.6	SACADA[1]
J		3.391	1.5		330.6			doi: 10.1103/PhysRevB.70.045101

Elasticity tensor (kBar)[1]

10943.8332	46.3566	1676.8860	0.0000	0.0000	-0.0000
46.3566	12218.1393	991.1068	0.0000	0.0000	0.0000
1676.8860	991.1068	6620.2054	0.0000	0.0000	0.0000
-0.0000	0.0000	0.0000	3897.9902	-0.0000	-0.0000
0.0000	0.0000	0.0000	-0.0000	3691.5640	-0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	3409.5833

[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].