SACADA Database Code: 198

Topology: 3^2,4T203

# of independent nodes (IN): 3
Transitivity: -
Space Group: P63/mcm
Pearson: hP36
Coordination Number (CN): 3, 4 (2:1)

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T203 (SACADA #198)		2.257		0.663	262.3	211.1	30.0	SACADA[1]
h-Carbon	0-20	2.30	2.13		267.1	221.5	34.0	doi: 10.1016/j.carbon.2015.05.027

Elasticity tensor (kBar)[1]

4439.7391	1684.5110	640.8152	-0.0000	0.0000	0.0000
1684.5110	4439.7391	640.8152	0.0000	-0.0000	-0.0000
640.8152	640.8152	9516.6721	-0.0000	0.0000	0.0000
-0.0000	0.0000	-0.0000	1377.6140	-0.0000	-0.0000
0.0000	0.0000	0.0000	-0.0000	2415.5047	-0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	2415.5047

[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].