SACADA Database Code: 148

Topology: 3,4T179

# of independent nodes (IN): 2
Transitivity: -
Space Group: P63/mcm
Pearson: hP24
Coordination Number (CN): 3, 4 (1:1)

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3,4T179 (SACADA #148)		2.790		0.744	329.7	277.3	42.1	SACADA[1]
Hex-C24		2.84	Metal		330.38	290.67	91.66	doi: 10.1039/c3tc32083a
Hex-C24		2.839			342	275		doi: 10.1021/acs.cgd.5b01490

Elasticity tensor (kBar)[1]

5917.6777	1997.7965	881.8805	0.0000	0.0000	-0.0000
1997.7965	5917.6777	881.8805	0.0000	-0.0000	-0.0000
881.8805	881.8805	10877.1295	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	1959.9406	-0.0000	0.0000
0.0000	-0.0000	-0.0000	-0.0000	3136.2342	-0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	3136.2342

[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].