

SACADA Database Code: 19

Topology: ths (Allotrope with "sp" atoms)

of independent nodes (IN): 3

Transitivity: [1211]

Space Group: I41/amd

Pearson: tI32

Coordination Number (CN): 2, 3 (3:1)

Year: 2016

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ths (SACADA #19)		.546		1.029	-	-	-	SACADA ¹
Super graphyne			Metal					doi: 10.1016/j.carbon.2016.11.028 □

Elasticity tensor (kBar)¹

384.7086	306.6954	616.1424	-0.0000	0.0000	-0.0000
306.6954	384.7086	616.1424	-0.0000	-0.0000	-0.0000
616.1424	616.1424	1275.6471	0.0000	-0.0000	-0.0000
0.0000	-0.0000	0.0000	-4.6174	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	8.8931	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	-0.0000	8.8931

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 $2\pi \times 0.025 \text{ \AA}^{-1}$ 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 $\text{\AA}^{-1}$ 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].