

SACADA Database Code: 492

Topology: 4¹⁶T23

of independent nodes (IN): 16

Transitivity: [(16)(32)(25)9]

Space Group: P1

Pearson: aP16

Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ¹⁶ T23 (SACADA #492)		3.341		0.827	392.9	427.3	79.4	SACADA ¹
G204								doi: 10.1002/cphc.201700151 cf

Elasticity tensor (kBar)¹

9587.5644	1066.2898	941.1971	417.3572	247.1466	61.5820
1066.2898	9835.8199	966.9374	178.8798	-259.0678	-176.0812
941.1971	966.9374	10009.1547	-213.5706	422.8764	-276.4767
417.3572	178.8798	-213.5706	4225.6704	8.7978	246.4825
247.1466	-259.0678	422.8764	8.7978	4223.3417	-44.3772
61.5820	-176.0812	-276.4767	246.4825	-44.3772	4152.1316

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].