

SACADA Database Code: 373

Topology: 4⁶T30

of independent nodes (IN): 6

Transitivity: [6(14)(10)3]

Space Group: P-1

Pearson: aP12

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 ⁶ T30 (SACADA #373)		3.474		0.775	413.9	473.0	89.0	SACADA ¹
G40								doi: 10.1002/cphc.201700151 ✉

Elasticity tensor (kBar)¹

9504.0832	1494.9108	1247.7516	-3.3730	-6.7336	260.3509
1494.9108	9279.1997	902.7849	148.7196	129.8931	47.8352
1247.7516	902.7849	11257.0049	-147.9026	-203.3200	1.3424
-3.3730	148.7196	-147.9026	4874.2863	228.1023	-98.0809
-6.7336	129.8931	-203.3200	228.1023	4759.6094	74.2978
260.3509	47.8352	1.3424	-98.0809	74.2978	5354.9629

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].