

SACADA Database Code: 443

Topology: 4⁶T35

of independent nodes (IN): 6
Transitivity: [6(14)92]
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 T35 (SACADA #443)		3.255		0.876	380.7	393.8	71.9	SACADA ¹
G149								doi: 10.1002/cphc.201700151 ✉

Elasticity tensor (kBar)¹

8387.0738	1543.8941	908.3409	-36.6303	48.6463	-39.9975
1543.8941	8255.1687	1213.8835	80.5694	-53.1232	18.8295
908.3409	1213.8835	10406.6057	-202.7269	-435.1878	-146.9963
-36.6303	80.5694	-202.7269	3885.8067	314.1856	-112.4158
48.6463	-53.1232	-435.1878	314.1856	3566.2100	-118.5505
-39.9975	18.8295	-146.9963	-112.4158	-118.5505	4611.9632

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].