

SACADA Database Code: 230

Topology: 4⁴T36

of independent nodes (IN): 4
Transitivity: [49(10)7]
Space Group: Pmmn
Pearson: oP16
Coordination Number (CN): 4

Year: 2012

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ⁴ T36 (SACADA #230)		3.450		0.697	431.2	473.9	88.4	SACADA ¹
P-carbon								doi: 10.1021/ja304380p ↗
P-carbon		3.51	3.93		449.1	485.0	78.5	doi: 10.1103/PhysRevLett.108.135501 ↗
P-carbon					447			doi: 10.1016/j.carbon.2014.06.050 ↗
P-carbon								doi: 10.1088/0256-307x/32/9/096201 ↗
P-carbon								doi: 10.1103/PhysRevB.93.085201 ↗

Elasticity tensor (kBar)¹

12191.4713	385.2642	946.5946	-0.0000	0.0000	-0.0000
385.2642	11175.7049	976.9406	-0.0000	-0.0000	-0.0000
946.5946	976.9406	10847.0926	0.0000	0.0000	0.0000
-0.0000	-0.0000	0.0000	4593.9809	-0.0000	0.0000
0.0000	-0.0000	0.0000	-0.0000	3650.9212	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	-0.0000	5074.9125

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 [\[9\]](#).