

SACADA Database Code: 278

Topology: 4⁷T12

of independent nodes (IN): 7

Transitivity: [7(11)(10)6]

Space Group: Pnma

Pearson: oP28

Coordination Number (CN): 4

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ⁷ T12 (SACADA #278)		3.455		0.672	427.9	471.7	88.0	SACADA ¹
oP28	0-20	3.415	4.7		412		90.9	doi: 10.1039/c4cp04569f [†]

Elasticity tensor (kBar)¹

10136.3941	1056.2583	1723.3153	-0.0000	0.0000	0.0000
1056.2583	11390.4149	517.0127	0.0000	0.0000	0.0000
1723.3153	517.0127	10393.3491	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	5269.0132	-0.0000	-0.0000
0.0000	0.0000	0.0000	-0.0000	4252.3376	0.0000
0.0000	0.0000	-0.0000	-0.0000	0.0000	4637.7222

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].