

## SACADA Database Code: 264

Topology: 4<sup>6</sup>T17

# of independent nodes (IN): 6

Transitivity: [6(10)95]

Space Group: Pbam

Pearson: oP24-I

Coordination Number (CN): 4

Year: 2015

## Data

Name	Pressure, GPa	Density, g/cm <sup>3</sup>	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 <sup>6</sup> T17 (SACADA #264)		3.448		0.638	433.3	486.0	91.1	SACADA <sup>1</sup>
oP24-I	0-20	3.409	4.7		418		91.1	doi: <a href="https://doi.org/10.1039/c4cp04569f">10.1039/c4cp04569f</a>
Pbam			4.57		416			doi: <a href="https://doi.org/10.1103/PhysRevB.91.214104">10.1103/PhysRevB.91.214104</a>

## Elasticity tensor (kBar)<sup>1</sup>

10399.8163	1379.4777	1173.3015	-0.0000	0.0000	-0.0000
1379.4777	11349.1886	331.0372	0.0000	-0.0000	0.0000
1173.3015	331.0372	11478.7863	-0.0000	0.0000	0.0000
-0.0000	0.0000	-0.0000	4674.6189	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	4316.4320	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	5298.0653

<sup>1</sup> 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  $\Gamma$ -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  $\nu$  — 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].

