

## SACADA Database Code: 40

Topology: pcb (Allotrope with "sp" atoms)

# of independent nodes (IN): 1

Transitivity: [1222]

Space Group: Im-3m

Pearson: cI32

Coordination Number (CN): 2, 4 (1:1)

Year: 2012

## Data

Name	Pressure, GPa	Density, g/cm <sup>3</sup>	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pcb (SACADA #40)		1.327		1.519	135.7	44.4	6.7	SACADA <sup>1</sup>
supercubane C32								doi: <a href="https://doi.org/10.1021/jp3104479">10.1021/jp3104479</a> †

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

1471.7069	1299.8169	1299.8169	-0.0000	-0.0000	-0.0000
1299.8169	1471.7069	1299.8169	-0.0000	-0.0000	0.0000
1299.8169	1299.8169	1471.7069	-0.0000	-0.0000	0.0000
0.0000	0.0000	-0.0000	1103.2350	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	1103.2350	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	1103.2350

<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].