## **SACADA Database Code: 41**

Topology: pcb (Allotrope with "sp" atoms)

# of independent nodes (IN): 1

Transitivity: [1222] Space Group: Im-3m

Pearson: cl48

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

Year: 2012

## **Data**

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
pcb (SACADA #41)		.758		1.582	76.7	22.4	3.5	SACADA <sup>1</sup>
supercubane C48								doi: 10.1021/jp3104479

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

797.0976	751.8891	751.8891	-0.0000	-0.0000	0.0000
751.8891	797.0976	751.8891	-0.0000	-0.0000	0.0000
751.8891	751.8891	797.0976	0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	640.7269	0.0000	-0.0000
-0.0000	-0.0000	-0.0000	0.0000	640.7269	-0.0000
0.0000	0.0000	0.0000	-0.0000	-0.0000	640.7269

<sup>&</sup>lt;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  $2\pi \times 0.025 \, \text{Å}^{-1}$  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  $\text{Å}^{-1}$  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  $H_{\nu}$  has been estimated according to Oganov's model [9].