

## SACADA Database Code: 66

Topology: 4/5/t1

# of independent nodes (IN): 1

Transitivity: [1322]

Space Group: I41/a

Pearson: tI16

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
4/5/t1 (SACADA #66)		3.575		0.837	375.8	486.1	93.0	SACADA <sup>1</sup>
I41/a					346			doi: <a href="https://doi.org/10.1103/PhysRevB.91.214104">10.1103/PhysRevB.91.214104</a> †
BT8		3.508			333			doi: <a href="https://doi.org/10.1103/PhysRevB.94.174102">10.1103/PhysRevB.94.174102</a> †

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

10663.2199	420.1187	886.8770	23.5912	0.0000	0.0000
420.1187	10663.2199	886.8770	-23.5912	0.0000	0.0000
886.8770	886.8770	8257.6695	-0.0000	0.0000	-0.0000
23.5912	-23.5912	-0.0000	5178.4688	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	5070.2921	-0.0000
-0.0000	-0.0000	0.0000	0.0000	-0.0000	5070.2921

<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].

