## **SACADA Database Code: 568**

Topology: 4<sup>3</sup>T75-CA

# of independent nodes (IN): 3

Transitivity: [3773] Space Group: Imma

Pearson: ol24

Coordination Number (CN): 4

Year: 2021

## **Data**

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 <sup>3</sup> T75-CA (SACADA #568)		3.391		0.199	415.0	439.2	80.9	SACADA <sup>1</sup>
4 <sup>3</sup> T75-CA								doi: 10.1038/s41524-021-00491-y

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

10186.5496	494.2718	2209.0968	-0.0000	-0.0000	-0.0000
494.2718	11217.1910	888.6193	-0.0000	-0.0000	0.0000
2209.0968	888.6193	8796.5250	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	4165.3871	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	4867.5450	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	4259.7807

<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 Å<sup>-1</sup> 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].