

## SACADA Database Code: 424

Topology: 4<sup>8</sup>T33

# of independent nodes (IN): 8

Transitivity: [8(19)(12)3]

Space Group: P-1

Pearson: aP16

Coordination Number (CN): 4

Year: 2017

## 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>8</sup> T33 (SACADA #424) |               | 3.411                      |         | 0.963                    | 384.8     | 440.5      | 82.9         | SACADA <sup>1</sup>   |
| G124                             |               |                            |         |                          |           |            |              | doi: <a href="https://doi.org/10.1002/cphc.201700151">10.1002/cphc.201700151</a><br>✉ |

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

|           |           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|-----------|
| 9147.8381 | 1258.5202 | 1049.7790 | -419.1390 | -115.4534 | -488.7982 |
| 1258.5202 | 9709.9718 | 602.7033  | -584.6571 | -183.3269 | -4.1902   |
| 1049.7790 | 602.7033  | 9953.3618 | 173.0811  | 531.8542  | -282.8831 |
| -419.1390 | -584.6571 | 173.0811  | 4516.3334 | -191.9367 | 41.1391   |
| -115.4534 | -183.3269 | 531.8542  | -191.9367 | 4164.3975 | 79.2383   |
| -488.7982 | -4.1902   | -282.8831 | 41.1391   | 79.2383   | 4796.5585 |

<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].