**SACADA Database Code: 495**

Topology: $4^4$T121

# of independent nodes (IN): 4
Transitivity: [4952]
Space Group: P2/m1
Pearson: mP16
Coordination Number (CN): 4

Year: 2017

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| $4^4$T121 (SACADA #495) | | 3.144 | | 0.942 | 364.6 | 335.0 | 56.5 | SACADA[1] |
| G207 | | | | | | | | doi: 10.1002/cphc.201700151 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 8832.6698 | 1028.4760 | 1234.3920 | -0.0000 | -0.0000 | 219.8477 |
| 1028.4760 | 8320.6368 | 1619.9845 | 0.0000 | -0.0000 | -233.1571 |
| 1234.3920 | 1619.9845 | 7901.4555 | -0.0000 | 0.0000 | 462.8358 |
| -0.0000 | 0.0000 | -0.0000 | 3274.1476 | 29.7644 | -0.0000 |
| -0.0000 | -0.0000 | -0.0000 | 29.7644 | 3906.8459 | 0.0000 |
| 219.8477 | -233.1571 | 462.8358 | -0.0000 | -0.0000 | 2670.0031 |

[1] 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 Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ 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$^{-1}$ for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — 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].