**SACADA Database Code: 507**

Topology: $4^6$T45

# of independent nodes (IN): 6
Transitivity: [6(14)(14)6]
Space Group: Cm
Pearson: mS24
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 |
|---|---|---|---|---|---|---|---|---|
| $4^6$T45 (SACADA #507) | | 3.191 | | 0.968 | 355.6 | 337.2 | 58.4 | SACADA[1] |
| G220 | | | | | | | | doi: 10.1002/cphc.201700151 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 8689.1804 | 530.8637 | 1226.0942 | -0.0000 | 0.0000 | 279.4365 |
| 530.8637 | 8155.4814 | 1056.6724 | 0.0000 | -0.0000 | -38.5582 |
| 1226.0942 | 1056.6724 | 9703.6708 | 0.0000 | -0.0000 | -840.9900 |
| -0.0000 | 0.0000 | 0.0000 | 3214.8705 | -67.1057 | 0.0000 |
| 0.0000 | -0.0000 | -0.0000 | -67.1057 | 2382.5887 | -0.0000 |
| 279.4365 | -38.5582 | -840.9900 | 0.0000 | -0.0000 | 3671.0521 |

[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].