**SACADA Database Code: 157**

Topology: $3^3$T5

# of independent nodes (IN): 3
Transitivity: [3432]
Space Group: Cmmm
Pearson: oS12
Coordination Number (CN): 3

Year: 2001

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| $3^3$T5 (SACADA #157) | | 2.451 | | 1.203 | 144.9 | 88.2 | 10.2 | SACADA[1] |
| 6(3)3-26 | | 2.48 | 0.99 | | | | | doi: 10.1016/S0009-2614(01)00126-9 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 10206.3941 | 557.2014 | 1066.6531 | 0.0000 | 0.0000 | -0.0000 |
| 557.2014 | 5578.6099 | -19.1518 | 0.0000 | 0.0000 | 0.0000 |
| 1066.6531 | -19.1518 | 7089.5799 | -0.0000 | -0.0000 | -0.0000 |
| 0.0000 | 0.0000 | -0.0000 | 1085.6097 | -0.0000 | 0.0000 |
| 0.0000 | 0.0000 | -0.0000 | -0.0000 | 169.8197 | -0.0000 |
| 0.0000 | 0.0000 | -0.0000 | 0.0000 | -0.0000 | 468.2430 |

[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].