**SACADA Database Code: 188**

Topology: $4^3$T87

# of independent nodes (IN): 3
Transitivity: [3785]
Space Group: Cmcm
Pearson: oS24
Coordination Number (CN): 4

Year: 1997

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| $4^3$T87 (SACADA #188) | | 3.420 | | 0.729 | 424.5 | 457.8 | 84.9 | SACADA[1] |
| (R2L)2 | | | | | | | | doi: 10.1016/S0379-6779(97)81165-4 |
| Z-carbon-9 | | | 2.86 | | 442 | | 90.2 | doi: 10.1021/ja301582d |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 12181.7601 | 905.2423 | 423.4585 | -0.0000 | 0.0000 | 0.0000 |
| 905.2423 | 10439.4518 | 1189.4308 | -0.0000 | -0.0000 | -0.0000 |
| 423.4585 | 1189.4308 | 10590.4672 | 0.0000 | 0.0000 | 0.0000 |
| -0.0000 | -0.0000 | 0.0000 | 4918.0268 | 0.0000 | -0.0000 |
| 0.0000 | -0.0000 | 0.0000 | 0.0000 | 3452.3182 | 0.0000 |
| 0.0000 | -0.0000 | 0.0000 | -0.0000 | 0.0000 | 4579.6579 |

[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].