**SACADA Database Code: 231**

Topology: $4^4$T38

# of independent nodes (IN): 4
Transitivity: [49(12)9]
Space Group: Cmmm
Pearson: oS32
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 |
|---|---|---|---|---|---|---|---|---|
| $4^4$T38 (SACADA #231) | | 3.497 | | 0.646 | 440.2 | 501.0 | 94.2 | SACADA[1] |
| (RL3)2 | | | | | | | | doi: 10.1016/S0379-6779(97)81165-4 |
| oC32 | | | 3.00 | | 457.4 | 522.2 | 96.2 | doi: 10.1039/c3cp51746b |
| oC32 | | | | | | | | doi: 10.1088/0256-307x/32/9/096201 |
| oC32 | | | | | | | | doi: 10.1103/PhysRevB.93.085201 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 11570.0999 | 511.6592 | 1019.6583 | 0.0000 | -0.0000 | 0.0000 |
| 511.6592 | 12314.2485 | 251.1586 | -0.0000 | -0.0000 | -0.0000 |
| 1019.6583 | 251.1586 | 12178.6436 | -0.0000 | 0.0000 | -0.0000 |
| 0.0000 | -0.0000 | -0.0000 | 3972.5306 | 0.0000 | 0.0000 |
| -0.0000 | -0.0000 | 0.0000 | 0.0000 | 4597.9289 | 0.0000 |
| 0.0000 | -0.0000 | -0.0000 | 0.0000 | 0.0000 | 5318.2574 |

[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].