**SACADA Database Code: 325**

Topology: $3,4^{11}T2$

# of independent nodes (IN): 12
Transitivity: [(12)(19)(17)(10)]
Space Group: C2/m
Pearson: mS48
Coordination Number (CN): 3, 4 (1:11)

Year: 2013

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| $3,4^{11}T2$ (SACADA #325) | | 3.481 | | 0.675 | 420.6 | 481.1 | 90.6 | SACADA[1] |
| 24C | 20 | | | | | | | doi: 10.1103/PhysRevB.88.014102 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 11362.2562 | 710.9584 | 965.2161 | -0.0000 | -0.0000 | 558.4779 |
| 710.9584 | 10366.5921 | 564.1226 | -0.0000 | 0.0000 | -345.2129 |
| 965.2161 | 564.1226 | 11717.3908 | -0.0000 | -0.0000 | -309.3049 |
| -0.0000 | -0.0000 | -0.0000 | 4293.6215 | -382.6450 | 0.0000 |
| -0.0000 | 0.0000 | -0.0000 | -382.6450 | 4347.3095 | -0.0000 |
| 558.4779 | -345.2129 | -309.3049 | 0.0000 | -0.0000 | 5116.1710 |

[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].