**SACADA Database Code: 476**

Topology: $4^3$T181

# of independent nodes (IN): 3
Transitivity: [3763]
Space Group: C2/c
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 |
|---|---|---|---|---|---|---|---|---|
| $4^3$T181 (SACADA #476) | | 3.323 | | 0.994 | 369.5 | 396.6 | 73.4 | SACADA[1] |
| G184 | | | | | | | | doi: 10.1002/cphc.201700151 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 9781.0185 | 1113.5317 | 700.4480 | -0.0000 | -0.0000 | -525.1872 |
| 1113.5317 | 9272.7492 | 512.3681 | -0.0000 | -0.0000 | 531.9750 |
| 700.4480 | 512.3681 | 9566.1665 | -0.0000 | -0.0000 | -101.6177 |
| -0.0000 | -0.0000 | -0.0000 | 4263.8821 | -55.1226 | 0.0000 |
| -0.0000 | -0.0000 | 0.0000 | -55.1226 | 2866.3989 | -0.0000 |
| -525.1872 | 531.9750 | -101.6177 | 0.0000 | -0.0000 | 4210.3667 |

[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].