**SACADA Database Code: 297**

Topology: $4^8$T6

# of independent nodes (IN): 8
Transitivity: [8(16)(13)5]
Space Group: P-3m1
Pearson: hP58
Coordination Number (CN): 4

Year: 2013

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| $4^8$T6 (SACADA #297) | | 2.974 | | 0.858 | 351.1 | 373.6 | 69.0 | SACADA[1] |
| KVIII | | 2.94 | 3.13 | | 338.8 | | 79.3 | doi: 10.1063/1.4802002 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 8585.7671 | 1097.1046 | 1032.0298 | 0.0000 | 99.0566 | 0.0000 |
| 1097.1046 | 8585.7671 | 1032.0298 | 0.0000 | -99.0566 | -0.0000 |
| 1032.0298 | 1032.0298 | 8120.9817 | 0.0000 | 0.0000 | -0.0000 |
| 0.0000 | 0.0000 | 0.0000 | 3744.3312 | -0.0000 | 99.0566 |
| 99.0566 | -99.0566 | 0.0000 | -0.0000 | 3784.9883 | 0.0000 |
| 0.0000 | -0.0000 | 0.0000 | 99.0566 | 0.0000 | 3784.9883 |

[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].