**SACADA Database Code: 81**

Topology: cag

# of independent nodes (IN): 1
Transitivity: [1431]
Space Group: Cmcm
Pearson: oS16
Coordination Number (CN): 4

Year: 2011

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| cag (SACADA #81) | | 3.357 | | 0.220 | 415.5 | 428.2 | 78.0 | SACADA[1] |
| LA5 | | | | | | | | doi: 10.1134/s1063776111060173 |
| LA5 | | | | | | | | link |
| Y-carbon | | | | | | | | doi: 10.1103/PhysRevB.85.201407 |
| Y-carbon | | | | | | | | doi: 10.3103/s1063457612060093 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 9770.6978 | 1155.2565 | 1532.6075 | -0.0000 | 0.0000 | -0.0000 |
| 1155.2565 | 11303.0756 | 757.1142 | 0.0000 | 0.0000 | 0.0000 |
| 1532.6075 | 757.1142 | 9482.1218 | -0.0000 | -0.0000 | -0.0000 |
| -0.0000 | 0.0000 | -0.0000 | 4866.8297 | -0.0000 | 0.0000 |
| 0.0000 | 0.0000 | -0.0000 | -0.0000 | 4340.8059 | 0.0000 |
| -0.0000 | 0.0000 | -0.0000 | 0.0000 | -0.0000 | 3383.7450 |

[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].