**SACADA Database Code: 625**

Topology: sqc8104

# of independent nodes (IN): 2
Transitivity: [2463]
Space Group: P42/mmc
Pearson: tP16
Coordination Number (CN): 4

Year: 2021

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| sqc8104 (SACADA #625) | | 2.701 | | 0.971 | 238.6 | 119.8 | 15.5 | SACADA[1] |
| sqc8104 | | | | | | | | doi: 10.1038/s41524-021-00491-y |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 3710.6288 | 963.9221 | 1459.0448 | -0.0000 | 0.0000 | 0.0000 |
| 963.9221 | 3710.6288 | 1459.0448 | -0.0000 | -0.0000 | -0.0000 |
| 1459.0448 | 1459.0448 | 7696.7619 | 0.0000 | 0.0000 | 0.0000 |
| -0.0000 | -0.0000 | 0.0000 | 599.3270 | 0.0000 | 0.0000 |
| 0.0000 | -0.0000 | 0.0000 | 0.0000 | 1128.1375 | 0.0000 |
| -0.0000 | -0.0000 | 0.0000 | 0.0000 | 0.0000 | 1128.1375 |

[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].