

**SACADA Database Code: 618**

Topology: cjh41

# of independent nodes (IN): 2  
Transitivity: [2575]  
Space Group: I4/mmm  
Pearson: tI32  
Coordination Number (CN): 4

Year: 2021

**Data**

| Name                | Pressure, GPa | Density, g/cm <sup>3</sup> | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs                                                                                                                                                                            |
|---------------------|---------------|----------------------------|---------|--------------------------|-----------|------------|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| cjh41 (SACADA #618) |               | 3.094                      |         | 0.545                    | 352.6     | 314.1      | 51.3         | SACADA <sup>1</sup>                                                                                                                                                             |
| cjh41               |               |                            |         |                          |           |            |              | doi: <a href="https://doi.org/10.1038/s41524-021-00491-y">10.1038/s41524-021-00491-y</a><br> |

**Elasticity tensor (kBar)<sup>1</sup>**

|           |           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|-----------|
| 6813.8754 | 1520.6728 | 1395.5948 | 0.0000    | 0.0000    | -0.0000   |
| 1520.6728 | 6813.8754 | 1395.5948 | 0.0000    | 0.0000    | -0.0000   |
| 1395.5948 | 1395.5948 | 9858.6641 | -0.0000   | 0.0000    | 0.0000    |
| 0.0000    | 0.0000    | -0.0000   | 2713.0032 | 0.0000    | -0.0000   |
| 0.0000    | -0.0000   | 0.0000    | 0.0000    | 3390.9979 | 0.0000    |
| 0.0000    | -0.0000   | -0.0000   | -0.0000   | 0.0000    | 3390.9978 |

<sup>1</sup> 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  $\Gamma$ -centered k-points mesh with a reciprocal-space resolution of  $2\pi \times 0.025 \text{ \AA}^{-1}$  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  $\text{\AA}^{-1}$  for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young’s modulus, and the Poisson’s ratio  $\nu$  — 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].