

## SACADA Database Code: 448

Topology: nbo-x-d-4,4-C2/m-2

# of independent nodes (IN): 2

Transitivity: [2451]

Space Group: I2/m

Pearson: mS10

Coordination Number (CN): 4

Year: 2017

## Data

| Name                             | Pressure, GPa | Density, g/cm <sup>3</sup> | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs                                                                             |
|----------------------------------|---------------|----------------------------|---------|--------------------------|-----------|------------|--------------|----------------------------------------------------------------------------------|
| nbo-x-d-4,4-C2/m-2 (SACADA #448) |               | 3.213                      |         | 1.412                    | -         | -          | -            | SACADA <sup>1</sup>                                                              |
| G154                             |               |                            |         |                          |           |            |              | doi: <a href="https://doi.org/10.1002/cphc.201700151">10.1002/cphc.201700151</a> |

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

|            |           |           |            |           |            |
|------------|-----------|-----------|------------|-----------|------------|
| 5506.0921  | 877.1278  | 2538.1821 | 0.0000     | -0.0000   | -1430.6323 |
| 877.1278   | 9455.1530 | 21.3975   | -0.0000    | 0.0000    | -342.1346  |
| 2538.1821  | 21.3975   | 6523.6386 | -0.0000    | 0.0000    | 850.4886   |
| 0.0000     | -0.0000   | -0.0000   | -1298.9979 | 2404.8345 | 0.0000     |
| 0.0000     | 0.0000    | 0.0000    | 2404.8345  | 413.0896  | -0.0000    |
| -1430.6323 | -342.1346 | 850.4886  | 0.0000     | -0.0000   | 2297.3670  |

<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].