

## SACADA Database Code: 22

Topology: [bto](#) <sup>↗</sup>

# of independent nodes (IN): 1

Transitivity: [1221]

Space Group: P6222

Pearson: hP6

Coordination Number (CN): 3

Year: 1990

## Data

| Name             | Pressure, GPa | Density, g/cm <sup>3</sup> | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs  |
|------------------|---------------|----------------------------|---------|--------------------------|-----------|------------|--------------|---|
| bto (SACADA #22) |               | 3.149                      |         | 1.379                    | 382.3     | 209.8      | 25.7         | SACADA <sup>1</sup>   |
| H-6              |               | 3.4                        | Metal   |                          | 580       |            |              | doi: <a href="#">10.1557/JMR.1990.2273</a> <sup>↗</sup>         |
| H-6              |               | 3.17                       |         |                          | 372       |            |              | doi: <a href="#">10.1103/PhysRevB.43.6742</a> <sup>↗</sup>      |
| 6(3)6-09         |               | 3.19                       |         |                          |           |            |              | doi: <a href="#">10.1016/S0009-2614(01)00126-9</a> <sup>↗</sup> |
| H-6              |               | 3.16                       |         |                          | 370       |            |              | doi: <a href="#">10.1007/978-94-010-1013-9_1</a> <sup>↗</sup>   |
| H-6              |               |                            |         |                          | 384       |            |              | doi: <a href="#">10.1103/PhysRevB.78.125415</a> <sup>↗</sup>    |
| H-6              |               |                            |         |                          |           |            |              | <a href="#">link</a> <sup>↗</sup>                               |
| H-6              |               | 3.093                      | Metal   |                          |           |            |              | doi: <a href="#">10.1039/c2cp43221h</a> <sup>↗</sup>            |
| H-6              |               |                            |         |                          |           |            |              | doi: <a href="#">10.1038/srep04339</a> <sup>↗</sup>             |
| H-6              |               |                            | Metal   |                          | 273       |            |              | doi: <a href="#">10.1016/j.commat.2013.10.032</a> <sup>↗</sup>  |
| H-6              |               |                            |         |                          |           |            |              | doi: <a href="#">10.1039/c6ra10809a</a> <sup>↗</sup>            |

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

|           |           |            |           |           |           |
|-----------|-----------|------------|-----------|-----------|-----------|
| 6016.8621 | 3359.7431 | 922.7967   | 0.0000    | 0.0000    | 0.0000    |
| 3359.7431 | 6016.8621 | 922.7967   | 0.0000    | -0.0000   | -0.0000   |
| 922.7967  | 922.7967  | 12494.5814 | -0.0000   | 0.0000    | -0.0000   |
| 0.0000    | 0.0000    | -0.0000    | 1328.5595 | 0.0000    | 0.0000    |
| 0.0000    | -0.0000   | 0.0000     | 0.0000    | 1992.7088 | -0.0000   |
| 0.0000    | -0.0000   | -0.0000    | 0.0000    | -0.0000   | 1992.7070 |

<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].