

## SACADA Database Code: 361

Topology: 4<sup>7</sup>T22

# of independent nodes (IN): 7

Transitivity: [7(12)(10)6]

Space Group: P21/m

Pearson: mP14

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
4 <sup>7</sup> T22 (SACADA #361)		3.419		0.674	409.2	466.1	87.7	SACADA <sup>1</sup>
G12								doi: <a href="https://doi.org/10.1002/cphc.201700151">10.1002/cphc.201700151</a> ✉

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

10238.2592	896.3909	855.9844	0.0000	0.0000	-214.1573
896.3909	10987.8706	487.5045	0.0000	0.0000	318.6949
855.9844	487.5045	11131.1236	-0.0000	-0.0000	-182.6344
0.0000	0.0000	-0.0000	4853.5595	408.1483	0.0000
0.0000	0.0000	-0.0000	408.1483	4540.8090	-0.0000
-214.1573	318.6949	-182.6344	0.0000	-0.0000	3978.3081

<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].