

## SACADA Database Code: 90

Topology: [twf](#) 

# of independent nodes (IN): 1

Transitivity: -


Space Group: P6222

Pearson: hP6

Coordination Number (CN): 3

Year: 2001

## Data

Name	Pressure, GPa	Density, g/cm <sup>3</sup>	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
twf (SACADA #90)		3.395		1.384	-	-	-	SACADA <sup>1</sup>
6(3)1-06		3.41						doi: <a href="https://doi.org/10.1016/S0009-2614(01)00126-9">10.1016/S0009-2614(01)00126-9</a> 

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

10085.0979	1497.6720	1980.2165	0.0000	-0.0000	-0.0000
1497.6720	10085.0979	1980.2165	0.0000	0.0000	-0.0000
1980.2165	1980.2165	5314.2930	0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	4293.7130	0.0000	0.0000
0.0000	0.0000	-0.0000	0.0000	-2487.5063	-0.0000
-0.0000	-0.0000	0.0000	0.0000	-0.0000	-2487.5067

<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].