

## SACADA Database Code: 390

Topology: 4<sup>8</sup>T24

# of independent nodes (IN): 8

Transitivity: [8(17)(17)8]

Space Group: C2

Pearson: mS32

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>8</sup> T24 (SACADA #390)		3.528		0.753	420.5	493.0	93.2	SACADA <sup>1</sup>
G79								doi: <a href="https://doi.org/10.1002/cphc.201700151">10.1002/cphc.201700151</a> ✉

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

11115.2963	567.5083	655.8788	-0.0000	-0.0000	-106.6843
567.5083	11747.9428	804.0227	-0.0000	0.0000	-249.0551
655.8788	804.0227	10946.7827	0.0000	0.0000	334.5270
-0.0000	-0.0000	0.0000	4739.7972	-354.8912	0.0000
-0.0000	-0.0000	0.0000	-354.8912	5111.9078	-0.0000
-106.6843	-249.0551	334.5270	0.0000	-0.0000	4290.3191

<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].