

## SACADA Database Code: 439

Topology: 4<sup>6</sup>T34

# of independent nodes (IN): 6

Transitivity: [6(13)(13)4]

Space Group: P-1

Pearson: aP12

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>6</sup> T34 (SACADA #439)		3.360		1.143	359.0	386.1	71.5	SACADA <sup>1</sup>
G142								doi: <a href="https://doi.org/10.1002/cphc.201700151">10.1002/cphc.201700151</a>

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

10689.6027	673.9238	931.3330	-750.9313	103.6396	109.8196
673.9238	8934.7323	1064.6977	-58.1832	4.7508	-36.9171
931.3330	1064.6977	7573.5199	152.5342	-234.7017	-384.1332
-750.9313	-58.1832	152.5342	4567.4348	-57.6447	86.4838
103.6396	4.7508	-234.7017	-57.6447	2703.4038	106.9869
109.8196	-36.9171	-384.1332	86.4838	106.9869	4308.7211

<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].