

## SACADA Database Code: 663

Topology: 4<sup>4</sup>T29-CA

# of independent nodes (IN): 4

Transitivity: [4961]

Space Group: Pmn21

Pearson: oP16

Coordination Number (CN): 4

Year: 2023

### 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>4</sup> T29-CA (SACADA #663)		3.095		0.425	369.4	317.9	49.8	SACADA <sup>1</sup>
4 <sup>4</sup> T29-CA								doi: <a href="https://doi.org/10.1107/S205252062300255X">10.1107/S205252062300255X</a>

<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].