

SACADA Database Code: 566

Topology: 4³T63-CA

of independent nodes (IN): 3
Transitivity: [3873]
Space Group: P2/n
Pearson: mP12
Coordination Number (CN): 4

Year: 2021

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ³ T63-CA (SACADA #566)		3.478		0.899	376.1	403.8	74.7	SACADA ¹
4 ³ T63-CA								doi: 10.1038/s41524-021-00491-y ✉

Elasticity tensor (kBar)¹

9455.2920	28.1089	1045.1990	0.0000	-0.0000	296.5338
28.1089	10681.4968	473.5838	0.0000	0.0000	-588.2510
1045.1990	473.5838	10699.9963	-0.0000	-0.0000	519.6490
0.0000	0.0000	-0.0000	2756.6197	241.5712	0.0000
-0.0000	0.0000	-0.0000	241.5712	3956.7386	0.0000
296.5338	-588.2510	519.6490	0.0000	0.0000	4180.0990

¹ 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 Γ -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 ν — 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].