

SACADA Database Code: 504

Topology: 4³T187

of independent nodes (IN): 3

Transitivity: [3883]

Space Group: C2/c

Pearson: mS24

Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ³ T187 (SACADA #504)		3.320		0.978	382.1	400.5	73.5	SACADA ¹
G217								doi: 10.1002/cphc.201700151 cf

Elasticity tensor (kBar)¹

9554.9218	860.4384	857.0890	0.0000	-0.0000	620.3190
860.4384	8433.4334	757.2411	-0.0000	0.0000	-253.3970
857.0890	757.2411	11751.1022	-0.0000	0.0000	-366.9321
0.0000	-0.0000	-0.0000	3008.3198	-70.1114	0.0000
-0.0000	0.0000	0.0000	-70.1114	3610.0035	0.0000
620.3190	-253.3970	-366.9321	0.0000	0.0000	4685.2406

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].