SACADA Database Code: 297

Topology: 48T6

of independent nodes (IN): 8

Transitivity: [8(16)(13)5] Space Group: P-3m1

Pearson: hP58

Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ⁸ T6 (SACADA #297)		2.974		0.858	351.1	373.6	69.0	SACADA ¹
KVIII		2.94	3.13		338.8		79.3	doi: 10.1063/1.4802002

Elasticity tensor (kBar)¹

8585.7671	1097.1046	1032.0298	0.0000	99.0566	0.0000
1097.1046	8585.7671	1032.0298	0.0000	-99.0566	-0.0000
1032.0298	1032.0298	8120.9817	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	3744.3312	-0.0000	99.0566
99.0566	-99.0566	0.0000	-0.0000	3784.9883	0.0000
0.0000	-0.0000	0.0000	99.0566	0.0000	3784.9883

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 $2\pi \times 0.025~\text{Å}^{-1}$ 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 Å^{-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_{ν} has been estimated according to Oganov's model [9].