SACADA Database Code: 318

Topology: $3,4^{9}T2$

# of independent nodes (IN): 10
Transitivity: [(10)(20)(13)2]
Space Group: P-1
Pearson: aP20
Coordination Number (CN): 3, 4 (1:9)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^{9}T2$ (SACADA #318)		2.855		1.422	243.3	216.0	35.2	SACADA[1]
phaseII	105	2.79	4.0		316			doi: 10.1016/j.carbon.2013.06.086

Elasticity tensor (kBar)[1]

7154.6327	1031.8073	339.3786	250.0897	98.0740	-158.2360
1031.8073	5519.1106	567.7311	-720.8054	427.0750	-146.1829
339.3786	567.7311	5820.7184	-84.4777	417.5373	44.9836
250.0897	-720.8054	-84.4777	2576.5101	-158.8241	142.8935
98.0740	427.0750	417.5373	-158.8241	1537.9278	-38.4431
-158.2360	-146.1829	44.9836	142.8935	-38.4431	1640.8986

[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 $2\pi \times 0.025$ 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_v has been estimated according to Oganov's model [9].