SACADA Database Code: 270

Topology: $3^2,4^4$T9

# of independent nodes (IN): 6
Transitivity: [6(17)(20)(10)]
Space Group: Pccm
Pearson: oP48
Coordination Number (CN): 3, 4 (1:2)

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^2,4^4$T9 (SACADA #270)		2.827		0.909	292.2	261.6	43.0	SACADA[1]
3D (6,0)-IV	3		0.23		212.63	257.22	80.1	doi: 10.1038/srep01331

Elasticity tensor (kBar)[1]

7366.9270	2514.8125	625.2809	0.0000	-0.0000	0.0000
2514.8125	3386.6090	349.1614	-0.0000	-0.0000	-0.0000
625.2809	349.1614	11048.1266	-0.0000	-0.0000	0.0000
0.0000	-0.0000	-0.0000	2276.4517	0.0000	0.0000
-0.0000	-0.0000	-0.0000	0.0000	2478.1199	-0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	3870.1570

[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].