SACADA Database Code: 252

Topology: $3^2,4^4T33$

# of independent nodes (IN): 6
Transitivity: [6764]
Space Group: Pmma
Pearson: oP12
Coordination Number (CN): 3, 4 (1:2)

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^2,4^4T33$ (SACADA #252)		3.251		0.809	381.6	290.0	37.6	SACADA[1]
oP12-carbon		3.3	Metal		389.9	314.2	42.2	doi: 10.3103/s1063457614040042

Elasticity tensor (kBar)[1]

6732.5970	248.0738	1126.1914	0.0000	0.0000	0.0000
248.0738	11898.1953	1594.3238	0.0000	-0.0000	-0.0000
1126.1914	1594.3238	11158.9216	0.0000	0.0000	-0.0000
0.0000	0.0000	0.0000	2168.3939	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	5292.8668	-0.0000
0.0000	-0.0000	-0.0000	0.0000	-0.0000	976.7854

[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].