SACADA Database Code: 307

Topology: $3^6,4^3T5$

# of independent nodes (IN): 9
Transitivity: [9(17)(15)7]
Space Group: Immm
Pearson: oI120
Coordination Number (CN): 3, 4 (3:2)

Year: 2006

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^6,4^3T5$ (SACADA #307)		2.527		1.076	191.5	142.5	17.9	SACADA[1]
3D C60	15	2.55	0.2					doi: 10.1103/PhysRevLett.96.076602
cuboids								doi: 10.3103/s1063457610020012

Elasticity tensor (kBar)[1]

2291.5408	1260.3025	812.7584	0.0000	0.0000	-0.0000
1260.3025	4861.6322	435.7091	-0.0000	-0.0000	0.0000
812.7584	435.7091	6123.8107	-0.0000	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	1309.5372	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	1949.9988	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	931.2012

[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].