SACADA Database Code: 315

Topology: $3^6,4^4$T6

# of independent nodes (IN): 10
Transitivity: [(10)(17)(11)4]
Space Group: R-3
Pearson: hR180
Coordination Number (CN): 3, 4 (3:2)

Year: 2008

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^6,4^4$T6 (SACADA #315)		2.366		1.058	191.9	145.6	18.9	SACADA[1]
C60 Polymers R-3		2.61	0.5					doi: 10.1021/ja076761k
C60 Polymers R-3								doi: 10.1039/B918480E
3D fullerite with tetragonal unit cell								doi: 10.3103/s1063457610020012

Elasticity tensor (kBar)[1]

3777.0209	725.3545	1056.6888	-0.0000	-173.0917	-52.2057
725.3545	3777.0209	1056.6888	-0.0000	173.0917	52.2057
1056.6888	1056.6888	4091.7028	-0.0000	-0.0000	0.0000
-0.0000	-0.0000	-0.0000	1525.8332	52.2057	-173.0917
-173.0917	173.0917	-0.0000	52.2057	1434.5832	-0.0000
-52.2057	52.2057	0.0000	-173.0917	-0.0000	1434.5833

[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].