

SACADA Database Code: 180

Topology: 3²,4T192

of independent nodes (IN): 3

Transitivity: [3653]

Space Group: Fm-3

Pearson: cF240

Coordination Number (CN): 3, 4 (3:2)

Year: 2008

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3 ² ,4T192 (SACADA #180)		1.641		0.929	9.4	3.5	0.5	SACADA ¹
C60 Polymers Model X	13							doi: 10.1021/ja076761k 

Elasticity tensor (kBar)¹

106.5203	86.5919	86.5919	0.0000	0.0000	-0.0000
86.5919	106.5203	86.5919	-0.0000	-0.0000	0.0000
86.5919	86.5919	106.5203	-0.0000	0.0000	-0.0000
0.0000	0.0000	-0.0000	76.0340	0.0000	-0.0000
0.0000	-0.0000	0.0000	0.0000	76.0340	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	-0.0000	76.0340

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 $2\pi \times 0.025 \text{ \AA}^{-1}$ 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 $\text{\AA}^{-1}$ 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].