

SACADA Database Code: 77

Topology: Ita

of independent nodes (IN): 1
Transitivity: [1343]
Space Group: Pm-3m
Pearson: cP24
Coordination Number (CN): 4

Year: 2004

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
Simple cubicta (SACADA #77)		2.335		0.761	260.9	209.6	29.7	SACADA ¹
SCF-C24								doi: 10.1134/1.1649442
SCF-C24		2.808	1.9		308.4			doi: 10.1081/FST-200039418
fullerite C24			1.6		205.5			doi: 10.1134/s1063783406070298
Cubic C24								doi: 10.3103/s1063457610020012
CA4								doi: 10.1134/s1063776111060173
Cubic C3		2.31	3.04					doi: 10.1103/PhysRevB.85.214104

Elasticity tensor (kBar)¹

5197.9814	1313.9247	1313.9247	0.0000	-0.0000	0.0000
1313.9247	5197.9814	1313.9247	-0.0000	-0.0000	-0.0000
1313.9247	1313.9247	5197.9814	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	2204.9671	-0.0000	0.0000
-0.0000	-0.0000	0.0000	-0.0000	2204.9671	0.0000
0.0000	-0.0000	0.0000	0.0000	0.0000	2204.9671

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 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].