SACADA Database Code: 25

Topology: lig

# of independent nodes (IN): 1
Transitivity: [1221]
Space Group: I41/amd
Pearson: tI16
Coordination Number (CN): 3

Year: 1981

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
lig (SACADA #25)		2.382		1.033	253.6	112.2	15.5	SACADA[1]
								link
Structure III								doi: 10.1007/bf00750899
C2(4)			2.44		275			doi: 10.1007/BF00746187
C2(4)								doi: 10.1007/bf00747369
C2(4)								doi: 10.1070/RC1984v053n07ABEH003084
C2(4)								doi: 10.1007/bf00749588
BCT8		2.35	2.72		333			doi: 10.1103/PhysRevB.57.R661
cT8								doi: 10.1038/srep03077
cT8								doi: 10.1038/srep04339
cT8			2.41		283			doi: 10.1103/PhysRevLett.116.195501
cT8		2.44			253.6	111.7		doi: 10.1016/j.diamond.2016.12.005

Elasticity tensor (kBar)[1]

5311.4713	1531.8572	2198.4553	0.0000	-0.0000	0.0000
1531.8572	5311.4713	2198.4553	-0.0000	0.0000	0.0000
2198.4553	2198.4553	2328.3612	0.0000	0.0000	-0.0000
0.0000	-0.0000	0.0000	852.7995	-0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	1735.0783	0.0000
0.0000	0.0000	-0.0000	0.0000	0.0000	1735.0780

[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].