SACADA Database Code: 33

Topology: dia-a

# of independent nodes (IN): 1
Transitivity: [1222]
Space Group: Fd-3m
Pearson: cF32
Coordination Number (CN): 4

Year: 1985

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
Tetrahedraldia-a (SACADA #33)		1.507		1.848	158.4	48.2	7.4	SACADA[1]
diamond								doi: 10.1021/ja00297a011
T-carbon								doi: 10.1134/S0012500810100010
T-carbon		1.50	2.25		169		61.1	doi: 10.1103/PhysRevLett.106.155703
T-carbon								doi: 10.1103/PhysRevB.84.121405
CA1								doi: 10.1134/s1063776111060173
T-carbon								link
T-carbon		1.501	2.253					doi: 10.1039/c2cp43221h
T-carbon								doi: 10.3103/s1063457613010012
T-carbon		1.503			159.8			doi: 10.1073/pnas.1311028110
T-carbon		1.50			162	52		doi: 10.1039/C4RA01962H

Elasticity tensor (kBar)[1]

1958.7510	1396.6477	1396.6477	-0.0000	-0.0000	-0.0000
1396.6477	1958.7510	1396.6477	-0.0000	0.0000	-0.0000
1396.6477	1396.6477	1958.7510	-0.0000	-0.0000	0.0000
-0.0000	0.0000	0.0000	690.7247	-0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	690.7247	0.0000
0.0000	-0.0000	0.0000	0.0000	-0.0000	690.7247

[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].