SACADA Database Code: 3

Topology: dia (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1111]
Space Group: Fd-3m
Pearson: cF40
Coordination Number (CN): 2, 4 (4:1)

Year: 1992

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
dia (SACADA #3)		.899		1.778	83.7	4.7	0.8	SACADA[1]
								doi: 10.1002/anie.199211013
superdiamond								doi: 10.4028/www.scientific.net/MSF.191.1
								doi: 10.1039/B702109G
sp-sp3-yne-diamond								doi: 10.1038/nmat2885
								doi: 10.1103/PhysRevB.86.075151
Y-carbon		0.894	4.662		82.9			doi: 10.1103/PhysRevB.86.075151
yne-diamond			4.850		86.9	14.8	3.29	doi: 10.1209/0295-5075/100/56003
D-carbon			4.8		91.7	18.59		doi: 10.1039/C3TA10292K
Y-carbon		0.891			83.5	10.9	1.1	doi: 10.1073/pnas.1311028110
Y-carbon					84.6			doi: 10.1016/j.diamond.2014.04.005
Y-carbon		0.89			84.4	13.7		doi: 10.1039/C4RA01962H

Elasticity tensor (kBar)[1]

908.6885	800.8440	800.8440	-0.0000	0.0000	0.0000
800.8440	908.6885	800.8440	-0.0000	-0.0000	0.0000
800.8440	800.8440	908.6885	-0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	43.3260	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	43.3260	-0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	43.3260

[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].