SACADA Database Code: 158

Topology: mtn

# of independent nodes (IN): 3
Transitivity: [3432]
Space Group: Fd-3m
Pearson: cF136
Coordination Number (CN): 4

Year: 1993

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
mtn (SACADA #158)		3.064		0.667	384.1	423.3	79.0	SACADA[1]
C-MTN								doi: 10.1002/anie.199307011
C34								doi: 10.1103/PhysRevB.49.8048
f.c.c.-C34					364			doi: 10.1016/0009-2614(95)00946-2
f.c.c.-C34						435.9		doi: 10.1007/BF02451606
f.c.c.-C34								nonelink
clathrate II								link
C34								doi: 10.1103/PhysRevB.67.035211
C34								doi: 10.1016/j.apsusc.2003.11.043
clathrate II								doi: 10.1080/08957950500319464
C34								doi: 10.1016/j.crci.2009.05.004
f.c.c.-C34		3.1	3.7		381	439		doi: 10.1103/PhysRevB.82.075209
fcc-C136								doi: 10.1063/1.3359682
clathrate II								doi: 10.1021/ic102178d
clathrate II		3.06			404			doi: 10.1021/jp205676p
fcc-C136			3.60		381.9		87.9	doi: 10.1021/ja304380p
f.c.c.-C34								doi: 10.1007/978-94-007-6371-5_4
clat34					372			doi: 10.1103/PhysRevB.91.214104

Elasticity tensor (kBar)[1]

9480.1937	1020.8539	1020.8539	-0.0000	0.0000	-0.0000

1020.8539	9480.1937	1020.8539	-0.0000	0.0000	0.0000
1020.8539	1020.8539	9480.1937	0.0000	-0.0000	0.0000
-0.0000	-0.0000	0.0000	4235.5776	-0.0000	0.0000
-0.0000	0.0000	0.0000	-0.0000	4235.5776	0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	4235.5776

[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].