SACADA Database Code: 159

Topology: mep

# of independent nodes (IN): 3
Transitivity: [3432]
Space Group: Pm-3n
Pearson: cP46
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
mep (SACADA #159)		3.092		0.700	380.9	429.9	80.7	SACADA[1]
C-MEP								doi: 10.1002/anie.199307011
C-46								doi: 10.1103/PhysRevB.49.8048
C-46					364			doi: 10.1016/0009-2614(95)00946-2
sc-C46								doi: 10.1007/BF02451606
sc-C46								nonelink
clathrate I								link
C-46								doi: 10.1088/0953-8984/13/26/313
C-46								doi: 10.1103/PhysRevB.67.035211
C-46								doi: 10.1016/j.apsusc.2003.11.043
C-46								doi: 10.1103/PhysRevLett.92.215505
clathrate I								doi: 10.1080/08957950500319464
C-46								doi: 10.1016/j.crci.2009.05.004
C-46		3.13	3.7		396	403		doi: 10.1103/PhysRevB.82.075209
sc-C46								doi: 10.1063/1.3359682
clathrate I								doi: 10.1021/ic102178d
clathrate I		3.08			402			doi: 10.1021/jp205676p
KII		3.06	4.11		368.7		83.0	doi: 10.1063/1.4802002
sc-C46								doi: 10.1007/978-94-007-6371-5_4
clat46					368			doi: 10.1103/PhysRevB.91.214104

Elasticity tensor (kBar)[1]

9260.1932	1083.2327	1083.2327	0.0000	-0.0000	0.0000
1083.2327	9260.1932	1083.2327	-0.0000	-0.0000	-0.0000
1083.2327	1083.2327	9260.1932	0.0000	0.0000	0.0000
0.0000	-0.0000	0.0000	4445.1436	0.0000	-0.0000
-0.0000	-0.0000	0.0000	0.0000	4445.1436	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	4445.1436

[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].