SACADA Database Code: 5

Topology: srs

# of independent nodes (IN): 1
Transitivity: [1111]
Space Group: I4132
Pearson: cI8
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
srs (SACADA #5)		2.305		1.262	-	-	-	SACADA[1]
								link
Structure I								doi: 10.1007/bf00750899
C1(41)								doi: 10.1007/BF00746150
C1(41)								doi: 10.1070/RC1984v053n07ABEH003084
C1(41)								doi: 10.1007/bf00749588
C1(41)								doi: 10.1007/bf00752165
10[3]		2.269	Metal					doi: 10.1103/PhysRevLett.68.2325
4(3)1		2.33						doi: 10.1016/S0009-2614(01)00126-9
K4			Metal		273			doi: 10.1103/PhysRevB.78.125415
K4								doi: 10.1209/0295-5075/87/56003
K4								doi: 10.1103/PhysRevLett.102.055703
K4								doi: 10.1103/PhysRevLett.102.229601
K4								link
K4								link
K4			Metal		270.2			doi: 10.1063/1.4773584
K4		2.269	Metal					doi: 10.1039/c2cp43221h
K4								doi: 10.1038/srep04339
K4								doi: 10.1142/s0217984915300112
srs								doi: 10.1007/s11224-016-0782-1

Elasticity tensor (kBar)[1]

1902.3222	2988.8823	2988.8823	0.0000	0.0000	-0.0000
2988.8823	1902.3222	2988.8823	0.0000	-0.0000	0.0000
2988.8823	2988.8823	1902.3222	-0.0000	0.0000	0.0000
-0.0000	0.0000	-0.0000	-2036.3452	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	-2036.3452	0.0000
-0.0000	-0.0000	0.0000	0.0000	0.0000	-2036.3452

[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].