SACADA Database Code: 60

Topology: crb

# of independent nodes (IN): 1
Transitivity: [1232]
Space Group: I4/mmm
Pearson: tI8
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
crb (SACADA #60)		3.360		0.210	418.4	423.5	76.5	SACADA[1]
8-tetra(2,2)-tubulane								doi: 10.1016/0009-2614(93)80059-X
(R2)								doi: 10.1016/S0379-6779(97)81165-4
bct-C4								doi: 10.1103/PhysRevB.59.733
Rectangulated carbon								doi: 10.1016/s0038-1098(02)00136-9
D					397			doi: 10.1103/PhysRevB.70.045101
3D (2,2)-II		3.331			373.2			doi: 10.1088/0953-8984/16/49/023
bct-carbon								doi: 10.1103/PhysRevB.82.134126
bct-C4					414	427		doi: 10.1103/PhysRevLett.104.125504
bct-C4								doi: 10.1002/pssr.201004187
crb								doi: 10.1039/c004039h
bct-C4								doi: 10.1088/0253-6102/55/3/26
3D-(2,2)		3.438			420.1	427.1	92.6	doi: 10.1021/nn202053t
LA3		3.438			420.1	427.1	92.6	doi: 10.1134/s1063776111060173
bct-C4								link
bct4-carbon								doi: 10.1103/PhysRevB.84.092103
bct-carbon								doi: 10.1103/PhysRevB.83.155452
bct-C4								doi: 10.7498/aps.61.093104
bct-C4								doi: 10.1021/ja304380p
bct-C4								doi: 10.1134/S0012501612010010

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
bct-C4								doi: 10.1103/PhysRevB.85.144115
bct-C4								doi: 10.1038/srep00471
bct-C4								doi: 10.1103/PhysRevB.85.155428
								link
bct-C4								doi: 10.3103/s1063457613010012
3D (2,2)-II								doi: 10.1038/srep01331
C4					415.6	434.2	93.6	doi: 10.1016/j.ssc.2013.07.001
crb								doi: 10.1524/zkri.2013.1620
bct-C4								doi: 10.1016/j.carbon.2014.06.050
bct-C4		3.42	3.71		432			doi: 10.1039/c3tc32083a
bct-C4								doi: 10.1142/s0217984915300112

Elasticity tensor (kBar)[1]

9530.5048	1854.7828	688.5936	0.0000	0.0000	0.0000
1854.7828	9530.5048	688.5936	-0.0000	-0.0000	-0.0000
688.5936	688.5936	12193.6108	0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	3129.8642	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	4544.1351	0.0000
0.0000	-0.0000	0.0000	-0.0000	0.0000	4544.1403

[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].