SACADA Database Code: 173

Topology: mct

# of independent nodes (IN): 3
Transitivity: [3552]
Space Group: Im-3m
Pearson: cI192
Coordination Number (CN): 3

Year: 1991

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
mct (SACADA #173)		1.164		0.737	117.7	51.3	7.1	SACADA[1]
P8								doi: 10.1038/352762a0
P8		1.16			103			doi: 10.1016/0008-6223(92)90066-6
P192								doi: 10.1103/PhysRevLett.69.921
P192								doi: 10.1103/PhysRevB.46.1941
P8								doi: 10.1098/rsta.1993.0045
P8								doi: 10.1016/0009-2614(93)85009-d
P8								link
P8		1.14			114			doi: 10.1016/0956-7151(94)90210-0
P8								link
P192								doi: 10.1021/jp9613201
P8								doi: 10.1016/s0960-8974(97)00003-x
P8								doi: 10.1088/1367-2630/5/1/126
P8			1.4		149	54.3		doi: 10.1088/1367-2630/5/1/123

Elasticity tensor (kBar)[1]

1583.3882	974.2138	974.2138	0.0000	0.0000	-0.0000
974.2138	1583.3882	974.2138	0.0000	0.0000	0.0000
974.2138	974.2138	1583.3882	-0.0000	-0.0000	-0.0000
0.0000	0.0000	-0.0000	729.4125	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	729.4125	0.0000
-0.0000	0.0000	0.0000	0.0000	0.0000	729.4125

[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].