SACADA Database Code: 273

Topology: mtt

# of independent nodes (IN): 7
Transitivity: [7(10)85]
Space Group: Pmmn
Pearson: oP24
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
mtt (SACADA #273)		3.086		0.879	360.9	371.7	67.7	SACADA[1]
C-MTT			3.68					doi: 10.1002/anie.199307011

Elasticity tensor (kBar)[1]

8589.9903	586.4027	1394.8868	0.0000	0.0000	0.0000
586.4027	9993.8965	705.5481	-0.0000	-0.0000	-0.0000
1394.8868	705.5481	8538.8917	-0.0000	0.0000	0.0000
0.0000	-0.0000	-0.0000	3916.6349	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	3988.0107	-0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	2786.6702

[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].